

Learning Theory from First Principles

DRAFT

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Preface

This draft textbook is extracted from lecture notes from a class that I have taught (unfortunately online, but this gave me an opportunity to write more detailed notes) during the Fall 2020 semester, with an extra pass during the class I taught in the Spring 2021, Fall 2021, and Fall 2022 semesters. A final pass will be made during the Fall 2023 semester.

The goal of the class (and thus of this textbook) is to present old and recent results in learning theory for the most widely-used learning architectures. This class is geared towards theory-oriented students as well as students who want to acquire a basic mathematical understanding of algorithms used throughout machine learning and associated fields that are significant users of learning methods such as computer vision or natural language processing. Moreover, it is well suited to students and researchers coming from other areas of applied mathematics and that want to learn about the theory behind machine learning.

A particular effort will be made to prove **many results from first principles** while keeping the exposition as simple as possible. This will naturally lead to a choice of key results showcasing the essential concepts in learning theory in simple but relevant instances. Some general results will also be presented without proof. Of course, the concept of first principles is subjective, and I will assume a good knowledge of linear algebra, probability theory, and differential calculus.

Moreover, I will focus on the part of learning theory that does not exist outside of algorithms that can be run in practice, and thus all algorithmic frameworks described in this book are routinely used. For most learning methods, some simple **illustrative experiments** are presented, with accompanying code (Matlab for the moment, Python underway, Julia in the future) so that students can see for themselves that the algorithms are simple and effective in synthetic experiments.

Note that this is *not* an introductory textbook on machine learning. There are already several good ones in several languages (see, e.g., [Alpaydin, 2020](#); [Azencott, 2019](#)).

Book organization. The book comprises three main parts: introduction, core part, and special topics. Readers are encouraged to read the first two parts to understand the main

concepts fully and can pick from the special topic chapters in a second reading, or if used in a two-semester class.

All chapters start with a summary of the main concepts and results that will be covered. All simulations experiments are available at <https://www.di.ens.fr/~fbach/ltpf/> as Matlab code. Python code is currently being finalized.

Sections or exercises which are more advanced are denoted by ♦, ♦♦, or ♦♦♦. Comments or suggestions are most welcome and should be sent to francis.bach@inria.fr.

Many topics are not covered, and many more are not covered in depth. There are many good textbooks on learning theory that go deeper or wider ([Christmann and Steinwart, 2008](#); [Mohri et al., 2018](#); [Shalev-Shwartz and Ben-David, 2014](#)). See also the nice notes from Alexander Rakhlin and Karthik Sridharan,¹ as well as from Michael Wolf.²

In particular, the book focuses primarily on real-valued prediction functions, as it is the de-facto standard for modern machine learning techniques, even when predicting discrete-valued outputs. Thus, although its historical importance and influence are crucial, I choose not to present the Vapnik-Chervonenkis dimension (see [Vapnik and Chervonenkis, 2015](#)), and instead based our generic bounds on Rademacher complexities. This focus on real-valued prediction functions makes least-squares regression a central part of the theory, which seems to be well appreciated by students. Moreover, this allows drawing links with the related statistical literature.

Some areas, such as online learning or probabilistic methods, are described in a single chapter to draw links with the classical theory and encourage readers to learn more about them through dedicated books. I have also included a chapter on over-parameterized models which presents modern topics in machine learning.

This is still a work in progress. In particular, there are still a lot of typos, probably some mistakes, and almost surely places where more details are needed; readers are most welcome to report them to me (and then get credit for it). I am convinced that more straightforward mathematical arguments are possible in many places in the book. Please let me know if you are aware of elegant and simple ideas I have overlooked.

Mathematical notations. Throughout the textbook, I will try to provide unified notations:

- Random variables: given a set \mathcal{X} , we will use the lower-case notation for a random variable with values in \mathcal{X} , as well as for its observations. Probability distributions will be denoted μ or p and expectations as $\mathbb{E}[f(x)] = \int_{\mathcal{X}} f(x) d\mu(x)$. This is slightly ambiguous but will not cause major problems (and is standard in research papers).

¹http://www.mit.edu/~rakhlin/courses/stat928/stat928_notes.pdf

²https://www-m5.ma.tum.de/foswiki/pub/M5/Allgemeines/MA4801_2021S/ML.pdf

- Norms on \mathbb{R}^d : we will consider the usual ℓ_p -norms on \mathbb{R}^d , defined through $\|x\|_p^p = \sum_{i=1}^d |x_i|^p$ for $p \in [1, \infty)$, with $\|x\|_\infty = \max_{i \in \{1, \dots, d\}} |x_i|$.
- For a symmetric matrix $A \in \mathbb{R}^{n \times n}$, $A \succcurlyeq 0$ means that A is positive semi-definite (that is, all of its eigenvalues are non-negative), and for two symmetric matrices A and B , $A \succcurlyeq B$ means that $A - B \succcurlyeq 0$.
- For a differentiable function $f : \mathbb{R}^d \rightarrow \mathbb{R}$, its gradient at x is denoted $f'(x) \in \mathbb{R}^d$, and if it is twice differentiable, its Hessian is denoted $f''(x) \in \mathbb{R}^{d \times d}$.

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Part I

Preliminaries

Chapter 1

Mathematical preliminaries

Chapter summary

- Linear algebra: a bag of tricks to avoid lengthy and faulty computations.
- Concentration inequalities: for n independent random variables, the deviation between the empirical average and the expectation is of order $O(1/\sqrt{n})$. What is in the big O , and how does it depend explicitly on problem parameters?

The mathematical analysis and design of machine learning algorithms require specialized tools beyond classic linear algebra, differential calculus, and probability. In this chapter, I will review these non-elementary mathematical tools used throughout the book: first linear algebra tricks, then concentration inequalities. The chapter can be safely skipped since relevant results will be referenced when needed.

1.1 Linear algebra and differentiable calculus

This section reviews basic linear algebra and differential calculus results that will be used throughout the book. Using these may usually greatly simplify computations. As much as possible, matrix notations will be used.

1.1.1 Minimization of quadratic forms

Given a positive definite (and hence invertible) symmetric matrix $A \in \mathbb{R}^{n \times n}$ and a vector $b \in \mathbb{R}^n$, the minimization of quadratic forms with linear terms can be done in closed form

as:

$$\inf_{x \in \mathbb{R}^n} \frac{1}{2} x^\top A x - b^\top x = -\frac{1}{2} b^\top A^{-1} b,$$

with minimizer $x_* = A^{-1}b$ obtained by zeroing the gradient $f'(x) = Ax - b$ of $f(x) = \frac{1}{2}x^\top Ax - b^\top x$. Moreover, we have:

$$\frac{1}{2}x^\top Ax - b^\top x = \frac{1}{2}(x - x_*)^\top A(x - x_*) - \frac{1}{2}b^\top A^{-1}b.$$

If A was not invertible (simply positive semi-definite) and b was not in the column space of A , then the infimum would be $-\infty$.

Note that this result is often used in various forms, such as

$$b^\top x \leq \frac{1}{2}b^\top A^{-1}b + \frac{1}{2}x^\top Ax \text{ with equality if and only if } b = Ax.$$

This form is exactly the Fenchel-Young inequality¹ for quadratic forms (see Chapter 5), and is often used in one dimension in the form $ab \leq \frac{a^2}{2\eta} + \frac{\eta b^2}{2}$, for any $\eta \geq 0$ (and equality if and only if $\eta = a/b$).

1.1.2 Inverting a 2×2 matrix

Solving small systems happens frequently, as well as inverting small matrices. This can be easily done in two dimensions. Let $M = \begin{pmatrix} a & b \\ c & d \end{pmatrix}$ be a 2×2 matrix. If $ad - bc \neq 0$, then we may invert it as follows

$$M^{-1} = \frac{1}{ad - bc} \begin{pmatrix} d & -b \\ -c & a \end{pmatrix}.$$

This can be checked by multiplying the two matrices or using Cramer's rule,² and can be generalized to matrices defined by blocks, as we present next.

1.1.3 Inverting matrices defined by blocks, matrix inversion lemma

The example above may be generalized to matrices of the form $M = \begin{pmatrix} A & B \\ C & D \end{pmatrix}$, with blocks of consistent sizes (note that A and D have to be square matrices). The inverse of M may be obtained by applying directly Gaussian elimination³ done in block form. Given the two

¹See https://en.wikipedia.org/wiki/Convex_conjugate.

²See https://en.wikipedia.org/wiki/Cramer%27s_rule.

³See https://en.wikipedia.org/wiki/Gaussian_elimination.

matrices $M = \begin{pmatrix} A & B \\ C & D \end{pmatrix}$ and $N = \begin{pmatrix} I & 0 \\ 0 & I \end{pmatrix}$, we may linearly combine lines (with the same coefficients for the two matrices). Once M has been transformed into the identity matrix, N has been transformed to the inverse of M .

We make the simplifying assumption that A is invertible, we use the notation $(M/A) = D - CA^{-1}B$ for the Schur complement of the block A , and also assume that (M/A) is invertible. We thus get by Gaussian elimination, referring to L_i , $i = 1, 2$, as the two lines of blocks, so that for the first matrix $M = \begin{pmatrix} L_1 \\ L_2 \end{pmatrix}$:

$$\begin{aligned} \text{Original matrices: } & \begin{pmatrix} A & B \\ C & D \end{pmatrix} \quad \begin{pmatrix} I & 0 \\ 0 & I \end{pmatrix} \\ L_2 \leftarrow L_2 - CA^{-1}L_1 : & \begin{pmatrix} A & B \\ 0 & (M/A) \end{pmatrix} \quad \begin{pmatrix} I & 0 \\ -CA^{-1} & I \end{pmatrix} \\ L_2 \leftarrow (M/A)^{-1}L_2 : & \begin{pmatrix} A & B \\ 0 & I \end{pmatrix} \quad \begin{pmatrix} I & 0 \\ -(M/A)^{-1}CA^{-1} & (M/A)^{-1} \end{pmatrix} \\ L_1 \leftarrow L_1 - BL_2 : & \begin{pmatrix} A & 0 \\ 0 & I \end{pmatrix} \quad \begin{pmatrix} I + B(M/A)^{-1}CA^{-1} & -B(M/A)^{-1} \\ -(M/A)^{-1}CA^{-1} & (M/A)^{-1} \end{pmatrix} \\ L_1 \leftarrow A^{-1}L_1 : & \begin{pmatrix} I & 0 \\ 0 & I \end{pmatrix} \quad \begin{pmatrix} A^{-1} + A^{-1}B(M/A)^{-1}CA^{-1} & -A^{-1}B(M/A)^{-1} \\ -(M/A)^{-1}CA^{-1} & (M/A)^{-1} \end{pmatrix}. \end{aligned}$$

This shows that

$$M^{-1} = \begin{pmatrix} A & B \\ C & D \end{pmatrix}^{-1} = \begin{pmatrix} A^{-1} + A^{-1}B(M/A)^{-1}CA^{-1} & -A^{-1}B(M/A)^{-1} \\ -(M/A)^{-1}CA^{-1} & (M/A)^{-1} \end{pmatrix}. \quad (1.1)$$

Moreover, by doing the same operations but by putting to zero first the upper-right block, and assuming D and $(M/D) = A - BD^{-1}C$ are invertible, we obtain:

$$M^{-1} = \begin{pmatrix} A & B \\ C & D \end{pmatrix}^{-1} = \begin{pmatrix} (M/D)^{-1} & -(M/D)^{-1}BD^{-1} \\ -D^{-1}C(M/D)^{-1} & D^{-1} + D^{-1}C(M/D)^{-1}BD^{-1} \end{pmatrix}. \quad (1.2)$$

By identifying the upper-left and lower-right blocks in Eq. (1.1) and Eq. (1.2), we obtain the identities (sometimes referred to as Woodbury matrix identities, or the *matrix inversion lemma*):

$$\begin{aligned} (A - BD^{-1}C)^{-1} &= A^{-1} + A^{-1}B(D - CA^{-1}B)^{-1}CA^{-1} \\ (D - CA^{-1}B)^{-1} &= D^{-1} + D^{-1}C(A - BD^{-1}C)^{-1}BD^{-1}. \end{aligned}$$

Another classical formulation is:

$$(A - BD^{-1}C)^{-1}B = A^{-1}B(D - CA^{-1}B)^{-1}D.$$

These are particularly interesting when the blocks A and D have very different sizes, as the inverse of a large matrix may be obtained from the inverse of a small matrix.

The lemma is often applied when $C = B^\top$, $A = I$ and $D = -I$, which leads to

$$(I + BB^\top)^{-1} = I - B(I + B^\top B)^{-1}B^\top,$$

and, once right-multiplied by B , this leads to the compact formula (which is easier to rederive and remember):

$$(I + BB^\top)^{-1}B = B(I + B^\top B)^{-1}.$$

These equalities are commonly used both for theoretical and algorithmic purposes.

Exercise 1.1 (♦) *Show that we can “diagonalize” by blocks the matrices M and M^{-1} as:*

$$\begin{aligned} M &= \begin{pmatrix} A & B \\ C & D \end{pmatrix} = \begin{pmatrix} I & 0 \\ CA^{-1} & I \end{pmatrix} \begin{pmatrix} A & 0 \\ 0 & (M/A) \end{pmatrix} \begin{pmatrix} I & A^{-1}B \\ 0 & I \end{pmatrix} \\ M^{-1} &= \begin{pmatrix} A & B \\ C & D \end{pmatrix}^{-1} = \begin{pmatrix} I & -A^{-1}B \\ 0 & I \end{pmatrix} \begin{pmatrix} A^{-1} & 0 \\ 0 & (M/A)^{-1} \end{pmatrix} \begin{pmatrix} I & 0 \\ -CA^{-1} & I \end{pmatrix}. \end{aligned}$$

Conditional covariance matrices for Gaussian vectors (♦). The identities above can be used to compute conditional mean vectors and covariance matrices for Gaussian vectors (in this book, we will use the denominations “normal” and “Gaussian” interchangeably). If we have a Gaussian vector $\begin{pmatrix} x \\ y \end{pmatrix}$ with $x \in \mathbb{R}^m$ and $y \in \mathbb{R}^n$, with mean vector defined by

block as $\mu = \begin{pmatrix} \mu_x \\ \mu_y \end{pmatrix}$, and covariance matrix $\Sigma = \begin{pmatrix} \Sigma_{xx} & \Sigma_{xy} \\ \Sigma_{yx} & \Sigma_{yy} \end{pmatrix} \succcurlyeq 0$ (defined with blocks of appropriate sizes), then the joint density $p(x, y)$ of (x, y) is proportional to

$$\exp \left(-\frac{1}{2} \begin{pmatrix} x - \mu_x \\ y - \mu_y \end{pmatrix}^\top \begin{pmatrix} \Sigma_{xx} & \Sigma_{xy} \\ \Sigma_{yx} & \Sigma_{yy} \end{pmatrix}^{-1} \begin{pmatrix} x - \mu_x \\ y - \mu_y \end{pmatrix} \right).$$

By writing it as the product of a function of x and of a function of (x, y) , we can get that x is Gaussian with mean μ_x and covariance matrix Σ_x , and that given x , y is Gaussian with mean $\mu_{y|x} = \mu_y + \Sigma_{yx}\Sigma_{xx}^{-1}(x - \mu_x)$ and covariance matrix $\Sigma_{y|x} = \Sigma_{yy} - \Sigma_{yx}\Sigma_{xx}^{-1}\Sigma_{xy}$.

Exercise 1.2 (♦) *Prove the identities $\mu_{y|x} = \mu_y + \Sigma_{yx}\Sigma_{xx}^{-1}(x - \mu_x)$ and covariance matrix $\Sigma_{y|x} = \Sigma_{yy} - \Sigma_{yx}\Sigma_{xx}^{-1}\Sigma_{xy}$.*

1.1.4 Eigenvalue and singular value decomposition

In this book, we will often use eigenvalue decompositions of symmetric matrices. If $A \in \mathbb{R}^{n \times n}$ is a symmetric matrix, there exists an orthogonal matrix $U \in \mathbb{R}^{n \times n}$ (that is, such that

$U^\top U = UU^\top = I$), and a vector $\lambda \in \mathbb{R}^n$ of eigenvalues, such that $A = U \text{Diag}(\lambda)U^\top$. If $u_i \in \mathbb{R}^n$ denotes the i -th column of U , then we have $A = \sum_{i=1}^n \lambda_i u_i u_i^\top$, and $Au_i = \lambda_i u_i$. A symmetric matrix is said to be positive semi-definite if and only if all its eigenvalues are non-negative.

Given a rectangular matrix $X \in \mathbb{R}^{n \times d}$, such that $n \geq d$, there exists an orthogonal matrix $V \in \mathbb{R}^{d \times d}$ (that is, such that $V^\top V = VV^\top = I$), a matrix $U \in \mathbb{R}^{n \times d}$ with orthonormal columns (that is, such that $U^\top U = I$), a vector $s \in \mathbb{R}_+^d$ of singular values, such that $X = U \text{Diag}(s)V^\top$; this is often called the “economy-size” singular value decomposition (SVD) of the matrix X . If $u_i \in \mathbb{R}^n$ and $v_i \in \mathbb{R}^d$ denote the i -th columns of U and V , then we have $X = \sum_{i=1}^d s_i u_i v_i^\top$, and $Xv_i = s_i u_i$, $X^\top u_i = s_i v_i$.

There are several ways of relating eigenvalues and singular values. For example, if s_i is a singular value of X , then s_i^2 is an eigenvalue of XX^\top and $X^\top X$. Moreover, the eigenvalues of the matrix $\begin{pmatrix} 0 & X \\ X^\top & 0 \end{pmatrix}$ are zero, the singular values of X , and their opposites. For further properties of eigenvalues and singular values, see [Golub and Loan \(1996\)](#), [Stewart and Sun \(1990\)](#) and [Bhatia \(2013\)](#).

Exercise 1.3 Express the eigenvectors of XX^\top and $X^\top X$ using the singular vectors of X .

Exercise 1.4 Express the eigenvectors of $\begin{pmatrix} 0 & X \\ X^\top & 0 \end{pmatrix}$ using the singular vectors of X .

1.1.5 Differential calculus

Throughout the book, we will compute gradients and Hessians of functions in almost all cases in matrix notations. Here are some classic examples:

- Quadratic forms: assuming $A = A^\top$, with $f(x) = \frac{1}{2}x^\top Ax - b^\top x$, $f'(x) = Ax - b$, $f''(x) = A$. If A is not symmetric, then $f'(x) = \frac{1}{2}(A + A^\top)x$ and $f''(x) = \frac{1}{2}(A + A^\top)$.
- Least-squares with $X \in \mathbb{R}^{n \times d}$ and $y \in \mathbb{R}^n$: $f(w) = \frac{1}{2n}\|y - Xw\|_2^2$. Then $f'(w) = \frac{1}{n}X^\top(Xw - y)$, $f''(w) = \frac{1}{n}X^\top X$.

Exercise 1.5 Show that for the logistic regression objective function $f(w) = \frac{1}{n} \sum_{i=1}^n \log(1 + \exp(-y_i(Xw)_i))$ with $X \in \mathbb{R}^{n \times d}$ and $y \in \{-1, 1\}^n$, then $f'(w) = \frac{1}{n}X^\top g$, where $g \in \mathbb{R}^n$ is defined as $g_i = -y_i \sigma(-y_i(Xw)_i)$, with $\sigma(u) = (1 + e^{-u})^{-1}$ is the sigmoid function. Show that the Hessian is $\frac{1}{n}X^\top \text{Diag}(h)X$, with $h \in \mathbb{R}^n$ defined as $h_i = \sigma(y_i(Xw)_i)\sigma(-y_i(Xw)_i)$.

1.2 Concentration inequalities

All results presented in this textbook rely on the simple probabilistic assumption that data are independently and identically distributed (i.i.d.). The primary tool is then to relate empirical averages to expectations.

The key (very classical) insight behind probabilistic inequalities used in machine learning is that when you have n *independent zero-mean* random variables, the natural “magnitude” of their average is $1/\sqrt{n}$ times smaller than their average magnitude. The simplest instance of this phenomenon is that if $Z_1, \dots, Z_n \in \mathbb{R}$ are independent and identically distributed with variance $\sigma^2 = \mathbb{E}(Z - \mathbb{E}[Z])^2$, then the variance of the sum is the sum of variances, and

$$\text{var}\left(\frac{1}{n} \sum_{i=1}^n Z_i\right) = \frac{1}{n^2} \sum_{i=1}^n \text{var}(Z_i) = \frac{\sigma^2}{n}.$$



Be careful with error measures or magnitudes: some are squared, some are not. Therefore, the $1/\sqrt{n}$ becomes $1/n$ after taking the square (this is trivial but typically leads to confusion).

The equality above can be interpreted as

$$\mathbb{E}\left[\left(\frac{1}{n} \sum_{i=1}^n Z_i - \mathbb{E}[Z]\right)^2\right] = \frac{\sigma^2}{n},$$

which provides the simplest proof of the law of large numbers when variances exist and also highlights the convergence in squared mean of the random variable $\frac{1}{n} \sum_{i=1}^n Z_i$ to the constant $\mathbb{E}[Z]$. This also implies convergence in probability using Markov’s inequality:

$$\mathbb{P}\left(\left|\frac{1}{n} \sum_{i=1}^n Z_i - \mathbb{E}[Z]\right| \geq \varepsilon\right) \leq \frac{1}{\varepsilon^2} \mathbb{E}\left[\left(\frac{1}{n} \sum_{i=1}^n Z_i - \mathbb{E}[Z]\right)^2\right] = \frac{\sigma^2}{n\varepsilon^2}.$$

To characterize the deviations more finely, there are two classical tools: the *central limit theorem*, which states that $\frac{1}{n} \sum_{i=1}^n Z_i$ is approximately Gaussian with mean $\mathbb{E}[Z]$ and variance σ^2/n . This is an asymptotic statement (formally $\sqrt{n}\left(\frac{1}{n} \sum_{i=1}^n Z_i - \mathbb{E}[Z]\right)$ converges in distribution to a Gaussian distribution with mean zero and variance σ^2). Although it gives the correct scaling in n , in this textbook, we will look primarily at non-asymptotic results that quantify the deviation for any n .



In what follows, we will always provide versions of inequalities for *averages* of random variables (some authors equivalently consider sums).

Before describing various concentration inequalities, let us recall the classical *union bound*: given events indexed by $f \in \mathcal{F}$ (which can have a countably infinite number of

elements), we have:

$$\mathbb{P}\left(\bigcup_{f \in \mathcal{F}} A_f\right) \leq \sum_{f \in \mathcal{F}} \mathbb{P}(A_f).$$

It has (among many other uses in machine learning) a direct application in upper-bounding the tail probability of the supremum of random variables:

$$\mathbb{P}\left(\sup_{f \in \mathcal{F}} Z_f > t\right) = \mathbb{P}\left(\bigcup_{f \in \mathcal{F}} \{Z_f > t\}\right) \leq \sum_{f \in \mathcal{F}} \mathbb{P}(Z_f > t).$$

We will only cover the most valuable inequalities for machine learning. For more advanced inequalities, see, e.g., [Boucheron et al. \(2013\)](#); [Vershynin \(2018\)](#).

Homogeneity. ! Random variables or vectors typically have a unit, and it is always helpful to perform some basic dimensional analysis⁴ to spot mistakes. For example, when performing linear predictions of the form $y = x^\top \theta$, the unit of y is the one of x times the one of θ . Typically, these units are encapsulated in the constants describing the problem (such as the noise standard deviation for y or bounds for x and θ).

1.2.1 Hoeffding's inequality

The simplest concentration inequality considers bounded real-valued random variables.

Proposition 1.1 (Hoeffding's inequality) *If Z_1, \dots, Z_n are independent random variables such that $Z_i \in [0, 1]$ almost surely, then, for any $t \geq 0$,*

$$\mathbb{P}\left(\frac{1}{n} \sum_{i=1}^n Z_i - \frac{1}{n} \sum_{i=1}^n \mathbb{E}[Z_i] \geq t\right) \leq \exp(-2nt^2). \quad (1.3)$$

Proof The usual proof uses standard convexity arguments and is divided into two parts.

- (1) Lemma: If $Z \in [0, 1]$ almost surely, then $\mathbb{E}[\exp(s(Z - \mathbb{E}[Z]))] \leq \exp(s^2/8)$ for any $s \geq 0$.

Proof: we can compute the first two derivatives of $\varphi : s \mapsto \log(\mathbb{E}[\exp(s(Z - \mathbb{E}[Z]))])$, which is a “log-sum-exp” function, often referred to as the “cumulant generating function”, so that the second derivative is related to a certain variance. We can compute

⁴https://en.wikipedia.org/wiki/Dimensional_analysis

the derivatives of φ as:

$$\begin{aligned}\varphi'(s) &= \frac{\mathbb{E}[(Z - \mathbb{E}[Z])e^{s(Z-\mathbb{E}[Z])}]}{\mathbb{E}[e^{s(Z-\mathbb{E}[Z])}]}, \\ \varphi''(s) &= \frac{\mathbb{E}[(Z - \mathbb{E}[Z])^2 e^{s(Z-\mathbb{E}[Z])}]}{\mathbb{E}[e^{s(Z-\mathbb{E}[Z])}]} - \left[\frac{\mathbb{E}[(Z - \mathbb{E}[Z])e^{s(Z-\mathbb{E}[Z])}]}{\mathbb{E}[e^{s(Z-\mathbb{E}[Z])}]} \right]^2.\end{aligned}$$

We thus get $\varphi(0) = \varphi'(0) = 0$, and $\varphi''(s)$ is the variance of some random variable $\tilde{Z} \in [0, 1]$, with distribution with density $z \mapsto e^{s(z-\mathbb{E}[Z])}$ with respect to μ , where μ is the distribution of Z . We recall that the variance of \tilde{Z} is the minimum squared deviation to a constant and can thus bound this variance as

$$\text{var}(\tilde{Z}) = \inf_{\nu \in [0,1]} \mathbb{E}[(\tilde{Z} - \nu)^2] \leq \mathbb{E}[(\tilde{Z} - 1/2)^2] = \frac{1}{4} \mathbb{E}[(2\tilde{Z} - 1)^2] \leq \frac{1}{4},$$

since $2\tilde{Z} - 1 \in [-1, 1]$ almost surely. Thus, for all $s \geq 0$, $\varphi''(s) \leq 1/4$, and by Taylor's formula, $\varphi(s) \leq \frac{s^2}{8}$.

- (2) We recall Markov's inequality for any non-negative random variable X and $a > 0$, which states $\mathbb{P}(X \geq a) \leq \frac{1}{a} \mathbb{E}[X]$. For any $t \geq 0$, and denoting $\bar{Z} = \frac{1}{n} \sum_{i=1}^n Z_i$:

$$\begin{aligned}&\mathbb{P}(\bar{Z} - \mathbb{E}[\bar{Z}] \geq t) \\ &= \mathbb{P}(\exp(s(\bar{Z} - \mathbb{E}[\bar{Z}])) \geq \exp(st)) \text{ by monotonicity of the exponential,} \\ &\leq \exp(-st) \mathbb{E}[\exp(s(\bar{Z} - \mathbb{E}[\bar{Z}]))] \text{ using Markov's inequality,} \\ &\leq \exp(-st) \prod_{i=1}^n \mathbb{E}\left[\exp\left(\frac{s}{n}(Z_i - \mathbb{E}[Z_i])\right)\right] \text{ by independence,} \\ &\leq \exp(-st) \prod_{i=1}^n \exp\left(\frac{s^2}{8n^2}\right) = \exp\left(-st + \frac{s^2}{8n}\right), \text{ using the lemma above,}\end{aligned}$$

which is minimized for $s = 4nt$. We then get the result.

■

Note the difference with the central limit theorem, which states that when n goes to infinity, the probability in Eq. (1.3) is asymptotically equivalent to

$$\frac{1}{\sqrt{2\pi\sigma^2/n}} \int_t^\infty \exp\left(-\frac{nz^2}{2\sigma^2}\right) dz \text{ which can be shown to be less than } \exp\left(-\frac{nt^2}{2\sigma^2}\right),$$

where $\sigma^2 = \lim_{n \rightarrow +\infty} \frac{1}{n} \sum_{i=1}^n \text{var}(Z_i)$. The central limit theorem is more precise (as it involves the variance of Z_i 's and not an almost sure bound) but is asymptotic. Bernstein inequalities (see Section 1.2.3) will be in between as they use both the variance and an almost sure bound.

Extensions. We get the following corollary by just applying the inequality to Z_i 's and $1 - Z_i$'s and using the union bound.

Corollary 1.1 (Two-sided Hoeffding's inequality) *If Z_1, \dots, Z_n are independent random variables such that $Z_i \in [0, 1]$ almost surely, then, for any $t \geq 0$,*

$$P\left(\left|\frac{1}{n} \sum_{i=1}^n Z_i - \frac{1}{n} \sum_{i=1}^n \mathbb{E}[Z_i]\right| \geq t\right) \leq 2 \exp(-2nt^2).$$

We can make the following observations:

- Hoeffding's inequality can be extended to the assumption that $Z_i \in [a, b]$ almost surely, leading to

$$\mathbb{P}\left(\left|\frac{1}{n} \sum_{i=1}^n Z_i - \frac{1}{n} \sum_{i=1}^n \mathbb{E}[Z_i]\right| \geq t\right) \leq 2 \exp(-2nt^2/(b-a)^2).$$

- Such an inequality is often used “in the other direction”, starting from the probability and deriving t from it as follows. For any $\delta \in (0, 1)$, with probability greater than $1 - \delta$, we have:

$$\left|\frac{1}{n} \sum_{i=1}^n Z_i - \frac{1}{n} \sum_{i=1}^n \mathbb{E}[Z_i]\right| < \frac{|a-b|}{\sqrt{2n}} \sqrt{\log\left(\frac{2}{\delta}\right)}.$$

Note the dependence in n as $1/\sqrt{n}$ and the logarithmic dependence in δ (which corresponds to the exponential tail bound in t).

Exercise 1.6 Show that the one-sided inequality: with probability greater than $1 - \delta$,

$$\frac{1}{n} \sum_{i=1}^n Z_i - \frac{1}{n} \sum_{i=1}^n \mathbb{E}[Z_i] < \frac{|a-b|}{\sqrt{2n}} \sqrt{\log\left(\frac{1}{\delta}\right)}.$$

- When $Z_i \in [a_i, b_i]$ almost surely, with potentially different a_i 's and b_i 's, the probability upper-bound can be replaced by $2 \exp(-2nt^2/c^2)$, where $c^2 = \frac{1}{n} \sum_{i=1}^n (b_i - a_i)^2$.
- The result extends to martingales with essentially the same proof, leading to Azuma's inequality.⁵
- Hoeffding's inequality is often applied to so-called “sub-Gaussian” random variables, that is, random variables X for which there exists $\tau \in \mathbb{R}_+$ such that the following bound on the Laplace transform of X holds:

$$\forall s \in \mathbb{R}, \mathbb{E}\left[\exp(s[X - \mathbb{E}[X]])\right] \leq \exp\left(\frac{\tau^2 s^2}{2}\right),$$

⁵See https://en.wikipedia.org/wiki/Azuma%27s_inequality.

which is exactly what we used in the proof. In other words, a random variable with values in $[a, b]$ is sub-Gaussian with constant $\tau^2 = (b - a)^2/4$. For these sub-Gaussian variables, we have similar concentration inequalities (see next exercise). Moreover, for such sub-Gaussian random variables, we have the usual two versions of the tail bound:

$$\forall t \geq 0, \mathbb{P}(|Z - \mathbb{E}[Z]| \geq t) \leq 2 \exp\left(-\frac{t^2}{2\tau^2}\right) \quad (1.4)$$

$$\Leftrightarrow \forall \delta \in (0, 1], |Z - \mathbb{E}[Z]| \leq \tau \sqrt{2 \log\left(\frac{2}{\delta}\right)} \text{ with probability } 1 - \delta. \quad (1.5)$$

Exercise 1.7 Show that a Gaussian random variable with variance σ^2 is sub-Gaussian with constant σ^2 .

Exercise 1.8 If Z_1, \dots, Z_n are independent random variables which are sub-Gaussian with constant τ^2 , then, for any $t \geq 0$, $P\left(\left|\frac{1}{n} \sum_{i=1}^n Z_i - \frac{1}{n} \sum_{i=1}^n \mathbb{E}[Z_i]\right| \geq t\right) \leq 2 \exp\left(-\frac{nt^2}{2\tau^2}\right)$.

- Sub-Gaussian random variables can be defined in several other ways, equivalent to constants with the bound on the Laplace transform. See the exercises below.

Exercise 1.9 (♦) Let Z be a random variable which is sub-Gaussian with constant τ^2 . Then, by using the tail bound $\mathbb{P}(|Z - \mathbb{E}[Z]| \geq t) \leq 2 \exp\left(-\frac{t^2}{2\tau^2}\right)$ in Eq. (1.4), show that for any positive integer q , $\mathbb{E}[(Z - \mathbb{E}[Z])^{2q}] \leq (2q)q!(2\tau^2)^q$.

Exercise 1.10 (♦♦) Let Z be a random variable such that for any positive integer q , $\mathbb{E}[(Z - \mathbb{E}[Z])^{2q}] \leq (2q)q!(2\tau^2)^q$. Then show that Z is sub-Gaussian with parameter $24\tau^2$.

1.2.2 McDiarmid's inequality

Given n independent random variables, it may be useful to concentrate other quantities than their average. What is needed is that the function of these random variables has “bounded variation”.

Proposition 1.2 (McDiarmid's inequality) Let Z_1, \dots, Z_n be independent random variables (in any measurable space \mathcal{Z}), and $f : \mathcal{Z}^n \rightarrow \mathbb{R}$ a function of “bounded variation”, that is, such that for all i , and all $z_1, \dots, z_n, z'_i \in \mathcal{Z}$, we have

$$|f(z_1, \dots, z_{i-1}, z_i, z_{i+1}, \dots, z_n) - f(z_1, \dots, z_{i-1}, z'_i, z_{i+1}, \dots, z_n)| \leq c.$$

Then

$$\mathbb{P}(|f(Z_1, \dots, Z_n) - \mathbb{E}[f(Z_1, \dots, Z_n)]| \geq t) \leq 2 \exp(-2t^2/(nc^2)).$$

Proof (♦) The proof generalizes Hoeffding's inequality, which corresponds to $f(z) = \frac{1}{n} \sum_{i=1}^n z_i$ and $c = 1$. We will only consider the one-sided inequality

$$\mathbb{P}(f(Z_1, \dots, Z_n) - \mathbb{E}[f(Z_1, \dots, Z_n)] \geq t) \leq \exp(-2t^2/(nc^2)),$$

which is sufficient to get the two-sided bound.

We simply introduce the random variables, for $i \in \{1, \dots, n\}$:

$$V_i = \mathbb{E}[f(Z_1, \dots, Z_n)|Z_1, \dots, Z_i] - \mathbb{E}[f(Z_1, \dots, Z_n)|Z_1, \dots, Z_{i-1}].$$

We have $\mathbb{E}[V_i|Z_1, \dots, Z_{i-1}] = 0$, and from the bounded variation assumption $|V_i| \leq c$ almost surely. Moreover, $f(Z_1, \dots, Z_n) - \mathbb{E}[f(Z_1, \dots, Z_n)] = \sum_{i=1}^n V_i$. Using the same argument as in part (1) of the proof of Hoeffding's inequality, we get for any $s > 0$, $\mathbb{E}(e^{sV_i}|Z_1, \dots, Z_{i-1}) \leq e^{s^2 c^2/8}$, and we can obtain a proof with the same steps as part (2) of Hoeffding's inequality by being careful with conditioning. See [Boucheron et al. \(2013\)](#) for details. ■

This inequality will be used to provide high-probability bounds on the estimation error in empirical risk minimization in Section [4.4.1](#).

Exercise 1.11 (♦) Use McDiarmid's inequality to prove a Hoeffding-type bound for vectors, that is, if $Z_1, \dots, Z_n \in \mathbb{R}^d$ are independent centered vectors such that $\|Z_i\|_2 \leq c$ almost surely, then with probability greater than $1 - \delta$, we have

$$\left\| \frac{1}{n} \sum_{i=1}^n Z_i \right\|_2 \leq \frac{c}{\sqrt{n}} \left(1 + \sqrt{2 \log \frac{1}{\delta}} \right).$$

1.2.3 Bernstein's inequality (♦)

As mentioned earlier, Hoeffding's inequality only uses an almost sure bound, but not explicitly the variance, as the central limit theorem is using (but only with an asymptotic result). Bernstein's inequality allows using the variance to get a finer non-asymptotic result.

Proposition 1.3 (Bernstein's inequality) Let Z_1, \dots, Z_n be n independent random variables such that $|Z_i| \leq c$ almost surely and $\mathbb{E}[Z_i] = 0$. Then

$$\mathbb{P}\left(\left|\frac{1}{n} \sum_{i=1}^n Z_i\right| \geq t\right) \leq 2 \exp\left(-\frac{nt^2}{2\sigma^2 + 2ct/3}\right), \quad (1.6)$$

where $\sigma^2 = \frac{1}{n} \sum_{i=1}^n \text{var}(Z_i)$. Moreover, with probability greater than $1 - \delta$, we have:

$$\left|\frac{1}{n} \sum_{i=1}^n Z_i\right| \leq \sqrt{\frac{2\sigma^2 \log(2/\delta)}{n}} + \frac{c \log(2/\delta)}{3n}.$$

Proof The proof is also divided into two parts, with first a lemma on the Laplace transform.

- (a) Lemma: if $|Z| \leq c$ almost surely, $\mathbb{E}[Z] = 0$, and $\mathbb{E}[Z^2] = \sigma^2$, then for any $s > 0$, we have $\mathbb{E}[e^{sZ}] \leq \exp\left(\frac{\sigma^2}{c^2}(e^{sc} - 1 - sc)\right)$.

Proof: using the power series expansion of the exponential, we get:

$$\begin{aligned}\mathbb{E}[e^{sZ}] &= 1 + \mathbb{E}[sZ] + \sum_{k=2}^{\infty} \frac{s^k}{k!} \mathbb{E}[Z^k] = 1 + \sum_{k=2}^{\infty} \frac{s^k}{k!} \mathbb{E}[Z^k] \text{ because } Z \text{ has zero mean,} \\ &\leq 1 + \sum_{k=2}^{\infty} \frac{s^k}{k!} \mathbb{E}[|Z|^{k-2}|Z|^2] \leq 1 + \sum_{k=2}^{\infty} \frac{s^k}{k!} c^{k-2} \sigma^2 = 1 + \frac{\sigma^2}{c^2}(e^{sc} - 1 - sc).\end{aligned}$$

Using the bound $1 + \alpha \leq e^\alpha$ valid for all $\alpha \in \mathbb{R}$ leads to the desired result.

- (b) With $\sigma_i^2 = \text{var}(Z_i)$, we have the one-sided inequality:

$$\begin{aligned}\mathbb{P}\left(\frac{1}{n} \sum_{i=1}^n Z_i \geq t\right) &= \mathbb{P}\left(\exp\left(s \sum_{i=1}^n Z_i\right) \geq \exp(nst)\right) \\ &\quad \text{by monotonicity of the exponential,} \\ &\leq \mathbb{E}\left[\exp\left(s \sum_{i=1}^n Z_i\right)\right] e^{-nst} \text{ using Markov's inequality,} \\ &\leq e^{-nst} \prod_{i=1}^n \exp\left(\frac{\sigma_i^2}{c^2}(e^{sc} - 1 - sc)\right) = e^{-nst} \exp\left(\frac{n\sigma^2}{c^2}(e^{sc} - 1 - sc)\right),\end{aligned}$$

using the lemma above. Thus, by choosing $s = \frac{1}{c} \log(1 + \frac{tc}{\sigma^2})$, we get a bound equal to

$$\exp\left(-\frac{nt}{c} \log(1 + \frac{tc}{\sigma^2}) + \frac{n\sigma^2}{c^2}\left(1 + \frac{tc}{\sigma^2} - 1 - \log(1 + \frac{tc}{\sigma^2})\right)\right) = \exp\left(-\frac{n\sigma^2}{c^2} h(ct/\sigma^2)\right),$$

with $h(\alpha) = (1 + \alpha) \log(1 + \alpha) - \alpha$. It turns out that $h(\alpha) \geq \frac{\alpha^2}{2+2\alpha/3}$, which leads to the first inequality. The second inequality can be obtained by standard algebra. See [Boucheron et al. \(2013\)](#) for details. ■

Note here that we get the same dependence as for the central limit theorem for small deviations t (and a strict improvement on Hoeffding because the variance is essentially bounded by the squared diameter of the support), while for large t , the dependence in t is worse than Hoeffding's inequality.

Beyond zero mean random variables. Bernstein's inequality can also be applied when the random variables Z_i do not have zero means. Then Eq. (1.6) is replaced by

$$\mathbb{P}\left(\left|\frac{1}{n} \sum_{i=1}^n Z_i - \frac{1}{n} \sum_{i=1}^n \mathbb{E}[Z_i]\right| \geq t\right) \leq 2 \exp\left(-\frac{nt^2}{2\sigma^2 + 2ct/3}\right).$$

Exercise 1.12 (♦) Prove the inequality above.

1.2.4 Expectation of the maximum

Concentration inequalities bound the deviation from the expectation. Often, computing the expectation is the tricky part, in particular for maxima of random variables. In a nutshell, taking the maximum of n bounded random variables leads to an extra factor of $\sqrt{\log n}$. Note here that we do not impose independence. We will consider other tools such as Rademacher complexities in Section 4.5. See Figure 1.1 for an illustration.

⚠ This logarithmic factor appears many times in this textbook and can often be traced back to the expectation of a maximum and to the Gaussian decay of tail bounds.

⚠ The variables do not need to be independent.

Proposition 1.4 (Expectation of the maximum) *If Z_1, \dots, Z_n are (potentially dependent) zero-mean real random variables which are sub-Gaussian with constant τ^2 , then*

$$\mathbb{E}[\max\{Z_1, \dots, Z_n\}] \leq \sqrt{2\tau^2 \log n}.$$

Proof We have:

$$\begin{aligned} \mathbb{E}[\max\{Z_1, \dots, Z_n\}] &\leq \frac{1}{t} \log \mathbb{E}[e^{t \max\{Z_1, \dots, Z_n\}}] \text{ by Jensen's inequality,} \\ &= \frac{1}{t} \log \mathbb{E}[\max\{e^{tZ_1}, \dots, e^{tZ_n}\}] \\ &\leq \frac{1}{t} \log \mathbb{E}[e^{tZ_1} + \dots + e^{tZ_n}] \text{ bounding the max by the sum,} \\ &\leq \frac{1}{t} \log(ne^{\tau^2 t^2/2}) = \frac{\log n}{t} + \tau^2 \frac{t}{2} = \sqrt{2\tau^2 \log n} \text{ with } t = \tau^{-1} \sqrt{2 \log n}, \end{aligned}$$

using the definition of sub-Gaussianity in Section 1.2.1 (and the fact that the variables have zero means). ■

While we consider a direct proof using Laplace transforms above, we can prove a similar result using Gaussian tail bounds together with the union bound

$$\mathbb{P}(\max\{U_1, \dots, U_n\} \geq t) \leq \mathbb{P}(U_1 \geq t) + \dots + \mathbb{P}(U_n \geq t),$$

for well-chosen random variables U_1, \dots, U_n . In other words, the dependence in the probability δ as $\sqrt{\log(\frac{2}{\delta})}$ in Eq. (1.5) is directly related to the term $\sqrt{\log n}$ above (see exercise below). We will see a different dependence in n in Section 8.1.2 for the maximum of squared norms of Gaussians.

Exercise 1.13 Assume Z_1, \dots, Z_n are random variables that are sub-Gaussian with constant τ^2 and have zero means. Show that $\mathbb{E}[\max\{|Z_1|, \dots, |Z_n|\}] \leq \sqrt{2\tau^2 \log(2n)}$. Prove the same result up to a universal constant using the tail bounds $\mathbb{P}(|Z_i| \geq t) \leq 2 \exp(-\frac{t^2}{2\tau^2})$ together with the union bound, and the property $\mathbb{E}[|Y|] = \int_0^{+\infty} \mathbb{P}(|Y| \geq t) dt$ for any random variable Y such that $\mathbb{E}[|Y|]$ exists.

Exercise 1.14 (♦♦) Assume Z_1, \dots, Z_n are independent Gaussian random variables with mean zero and variance σ^2 . Provide a lower bound for $\mathbb{E}[\max\{Z_1, \dots, Z_n\}]$ of the form $c\sqrt{\log n}$ for $c > 0$.

Exercise 1.15 (♦♦) We consider a convex function $f : \mathbb{R}^d \rightarrow \mathbb{R}$ such that $f(0) = 0$ and f is L -smooth with respect to the norm Ω , that is, f is continuously differentiable and for all $\theta, \eta \in \mathbb{R}^d$, $f(\theta) \leq f(\eta) + f'(\eta)^\top(\theta - \eta) + \frac{L}{2}\Omega(\theta - \eta)^2$. Let $Z_i \in \mathbb{R}^d$ be independent zero-mean random vectors with $\mathbb{E}[\Omega(Z_i)^2] \leq \sigma^2$, for $i = 1, \dots, n$. Show by induction in n that $\mathbb{E}[f(Z_1 + \dots + Z_n)] \leq nL\frac{\sigma^2}{2}$.

1.2.5 Estimation of expectations through quadrature (♦)

In machine learning, the generalization error is an expectation of a function (the loss associated with a specific prediction function) of a random variable (the pair input/output). This generalization error is naturally approximated by an empirical average given some independent and identically distributed (i.i.d.) samples, with a convergence rate of $O(1/\sqrt{n})$ from n samples (as shown, for example, from Hoeffding's inequality).

In this section, we briefly present *quadrature* methods whose aim is to estimate the same expectation but with observations that are potentially non-random. For simplicity, we consider a random variable X uniformly distributed in $[0, 1]$, and the task of computing the expectation of a function $f : [0, 1] \rightarrow \mathbb{R}$, that is, $I = \mathbb{E}[f(X)] = \int_0^1 f(x) dx$, noting that there are many variants of such methods (see, e.g., [Davis and Rabinowitz, 1984](#); [Brass and Petras](#),

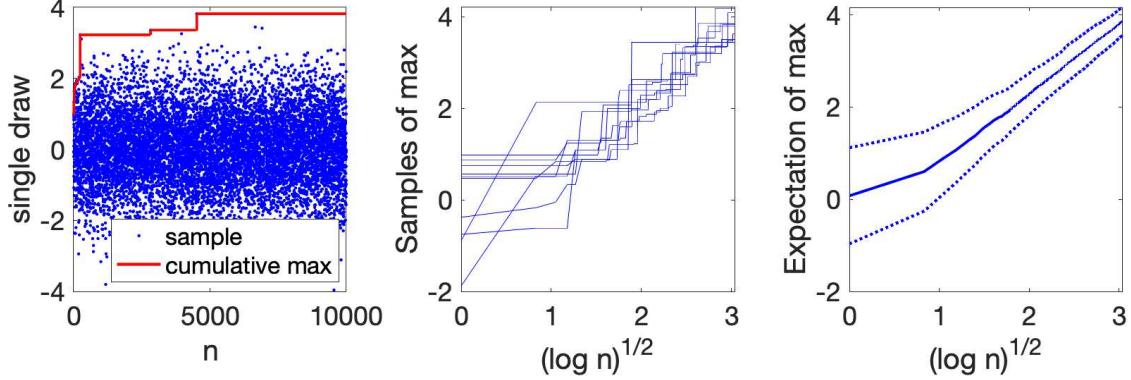


Figure 1.1: Expectation of the maximum of n independent standard Gaussian random variables. Left: illustration of the cumulative maximum $\max\{Z_1, \dots, Z_n\}$. Middle: 10 samples of the cumulative maximum as a function of $\sqrt{\log n}$. Right: mean and standard deviations from 1000 replications. Notice the linear growth in $\sqrt{\log n}$ compatible with our bounds.

2011), and that these techniques extend to higher dimensions (Holtz, 2010). Moreover, while we focus on equally spaced data in the interval, “quasi-random” methods lead to better convergence rates (Niederreiter, 1992).

We consider uniformly spaced grid points on $[0, 1]$, as it can serve as an idealization of random sampling when studying regression models, in particular in Chapter 6 and Chapter 7. That is, we consider $x_i = \frac{i}{n}$ for $i \in \{0, \dots, n\}$ (with $n + 1$ points). The classical trapezoidal rule considers the approximation

$$\hat{I} = \frac{1}{n} \left[\frac{1}{2} f(x_0) + \sum_{i=1}^{n-1} f(x_i) + \frac{1}{2} f(x_n) \right].$$

The error $|I - \hat{I}|$ then depends on the regularity of f . We have a decomposition of the error as the integral between f and its piecewise affine interpolant:

$$\begin{aligned} I - \hat{I} &= \sum_{i=1}^n \left(\int_{x_{i-1}}^{x_i} f(x) dx - \frac{x_i - x_{i-1}}{2} [f(x_i) + f(x_{i-1})] \right) \\ &= \sum_{i=1}^n \left(\int_{x_{i-1}}^{x_i} f(x) dx - \int_{x_{i-1}}^{x_i} \left\{ \frac{x_i - x}{x_i - x_{i-1}} f(x_{i-1}) + \frac{x - x_{i-1}}{x_i - x_{i-1}} f(x_i) \right\} dx \right). \end{aligned}$$

If f is twice differentiable and has a second-derivative bounded by L uniformly in absolute value, then we have the bound (which can be obtained by Taylor’s formula):

$$|I - \hat{I}| \leq \sum_{i=1}^n \frac{L}{2} \int_{x_{i-1}}^{x_i} (x_i - x)(x - x_{i-1}) dx = \sum_{i=1}^n \frac{L}{12} (x_i - x_{i-1})^3 dx = \frac{L}{12n^2}.$$

We thus have an error bound in $O(1/n^2)$ if we assume two bounded derivatives. We typically get an error of $O(1/n^s)$ for such numerical integration methods if we assume s bounded derivatives (with the appropriate rule, such as Simpson's rule, which makes a piecewise quadratic interpolation). See the exercises below.

Exercise 1.16 *Show that the trapezoidal rule leads to an error in $O(1/n)$ if we only assume one bounded derivative.*

Exercise 1.17 (♦) *Show that for 1-periodic functions, the trapezoidal rule leads to an error in $O(1/n^s)$ if we assume s bounded derivatives.*

1.2.6 Concentration inequalities for matrices (♦♦)

It turns out the concentration inequalities that have been presented in this chapter apply equally well to matrices with the positive semi-definite order. The following bounds are adapted from [Tropp \(2012\)](#) and presented without proofs, with the following notations: $\lambda_{\max}(M)$ denote the largest eigenvalue of the symmetric matrix M , while $\|M\|_{\text{op}}$ denotes the largest singular value of a potentially rectangular matrix M , and $A \preceq B$ if and only if $B - A$ is positive semi-definite.

Proposition 1.5 (Matrix Hoeffding bound) (Tropp, 2012, Theorem 1.3) *Given n independent symmetric matrices $M_i \in \mathbb{R}^{d \times d}$, such that for all $i \in \{1, \dots, n\}$, $\mathbb{E}[M_i] = 0$, $M_i^2 \preceq C_i^2$ almost surely. Then for all $t \geq 0$,*

$$\mathbb{P}\left(\lambda_{\max}\left(\frac{1}{n} \sum_{i=1}^n M_i\right) \geq t\right) \leq d \cdot \exp\left(-\frac{nt^2}{8\sigma^2}\right),$$

for $\sigma^2 = \lambda_{\max}\left(\frac{1}{n} \sum_{i=1}^n C_i^2\right)$.

Proposition 1.6 (Matrix Bernstein bound) (Tropp, 2012, Theorem 1.4) *Given n independent symmetric matrices $M_i \in \mathbb{R}^{d \times d}$, such that for all $i \in \{1, \dots, n\}$, $\mathbb{E}[M_i] = 0$, $\lambda_{\max}(M_i) \leq c$ almost surely. Then for all $t \geq 0$,*

$$\mathbb{P}\left(\lambda_{\max}\left(\frac{1}{n} \sum_{i=1}^n M_i\right) \geq t\right) \leq d \cdot \exp\left(-\frac{nt^2/2}{\sigma^2 + ct/3}\right),$$

for $\sigma^2 = \lambda_{\max}\left(\frac{1}{n} \sum_{i=1}^n \mathbb{E}[M_i^2]\right)$.

We can make the following observations:

- Note the similarity with the corresponding bounds for scalar random variables when $d = 1$. McDiarmid's inequality can also be extended ([Tropp, 2012](#), Corollary 7.5).
- These bounds apply as well to rectangular matrices $M_i \in \mathbb{R}^{d_1 \times d_2}$ by considering the symmetric matrices $\widetilde{M}_i = \begin{pmatrix} 0 & M_i \\ M_i^\top & 0 \end{pmatrix} \in \mathbb{R}^{(d_1+d_2) \times (d_1+d_2)}$, whose eigenvalues are plus and minus the singular values of M_i ; see Section 1.1.4 and [Stewart and Sun \(1990, Theorem 4.2\)](#).

Exercise 1.18 Assume the matrices $M_i \in \mathbb{R}^{d_1 \times d_2}$ are independent, have zero mean, and such that $\|M_i\|_{\text{op}} \leq c$ almost surely for all $i \in \{1, \dots, n\}$. Show that

$$\mathbb{P}\left(\left\|\frac{1}{n} \sum_{i=1}^n M_i\right\|_{\text{op}} \geq t\right) \leq (d_1 + d_2) \cdot \exp\left(-\frac{nt^2}{8c^2}\right).$$

Moreover, with $\sigma^2 = \max\left\{\lambda_{\max}\left(\frac{1}{n} \sum_{i=1}^n M_i^\top M_i\right), \lambda_{\max}\left(\frac{1}{n} \sum_{i=1}^n M_i M_i^\top\right)\right\}$, show that

$$\mathbb{P}\left(\left\|\frac{1}{n} \sum_{i=1}^n M_i\right\|_{\text{op}} \geq t\right) \leq (d_1 + d_2) \cdot \exp\left(-\frac{nt^2/2}{\sigma^2 + ct/3}\right).$$

Infinite-dimensional covariance operators (♦♦). As used within Chapter 7, we will need to extend the results above, which depend on the underlying dimension, to the notion of “intrinsic dimension”, which can still be finite if the underlying dimension is infinite. That is, we have:

Proposition 1.7 (Matrix Bernstein bound - intrinsic dimension) ([Minsker, 2017, Eq. \(3.9\)](#)) Given n independent random bounded self-adjoint operators M_i on a Hilbert spaces, such that for all $i \in \{1, \dots, n\}$, $\mathbb{E}[M_i] = 0$, $\lambda_{\max}(M_i) \leq c$ almost surely, and $\frac{1}{n} \sum_{i=1}^n \mathbb{E}[M_i^2] \leq V$. Then for all $t \geq 0$,

$$\mathbb{P}\left(\lambda_{\max}\left(\frac{1}{n} \sum_{i=1}^n M_i\right) \geq t\right) \leq d \cdot \left(1 + \frac{6}{n^2 t^4} (\sigma^2 + ct/3)^2\right) \exp\left(-\frac{nt^2/2}{\sigma^2 + ct/3}\right),$$

for $\sigma^2 \geq \lambda_{\max}(V)$ and $d = \frac{\text{tr}(V)}{\sigma^2}$. When $t \geq \frac{c}{3n} + \frac{\sigma}{\sqrt{n}}$, then we get the bound $7d \exp\left(-\frac{nt^2/2}{\sigma^2 + ct/3}\right)$.

Chapter 2

Introduction to supervised learning

Chapter summary

- Decision theory (loss, risk, optimal predictors): what is the optimal prediction and performance given infinite data and infinite computational resources?
- Statistical learning theory: when is an algorithm “consistent”?
- No free lunch theorems: learning is impossible without making assumptions.

| | |
|---|--|
| \mathcal{X} | input space |
| \mathcal{Y} | output space |
| p | joint distribution on $\mathcal{X} \times \mathcal{Y}$ |
| $(x_1, y_1, \dots, x_n, y_n)$ | training data |
| $f : \mathcal{X} \rightarrow \mathcal{Y}$ | prediction function |
| $\ell(y, z)$ | loss function between output y and prediction z |
| $\mathcal{R}(f) = \mathbb{E}[\ell(y, f(x))]$ | expected risk of prediction function f |
| $\widehat{\mathcal{R}}(f) = \frac{1}{n} \sum_{i=1}^n \ell(y_i, f(x_i))$ | empirical risk of prediction function f |
| $f^*(x') = \arg \min_{z \in \mathcal{Y}} \mathbb{E}[\ell(y, z) x = x']$ | Bayes prediction at x' |
| $\mathcal{R}^* = \mathbb{E}_{x' \sim p} \inf_{z \in \mathcal{Y}} \mathbb{E}[\ell(y, z) x = x']$ | Bayes risk |

Table 2.1: Summary of notions and notations presented in this chapter and used throughout the book.

2.1 From training data to predictions

Main goal. Given some observations $(x_i, y_i) \in \mathcal{X} \times \mathcal{Y}$, $i = 1, \dots, n$, of inputs/outputs, features/labels, covariates/responses (which are referred to as the training data), the main goal of supervised learning is to predict a new $y \in \mathcal{Y}$ given a new previously unseen $x \in \mathcal{X}$. The unobserved data are usually referred to as the testing data.

⚠ There are few fundamental differences between machine learning and the branch of statistics dealing with regression and its various extensions, particularly when it comes to providing theoretical guarantees. The focus on algorithms and computational scalability is arguably stronger within machine learning (but also present in statistics). At the same time, the focus on models and their interpretability beyond their predictive performance is more prominent within statistics (but also present in machine learning).

Examples. Supervised learning is used in many areas of science, engineering, and industry. There are thus many examples where \mathcal{X} and \mathcal{Y} can be very diverse:

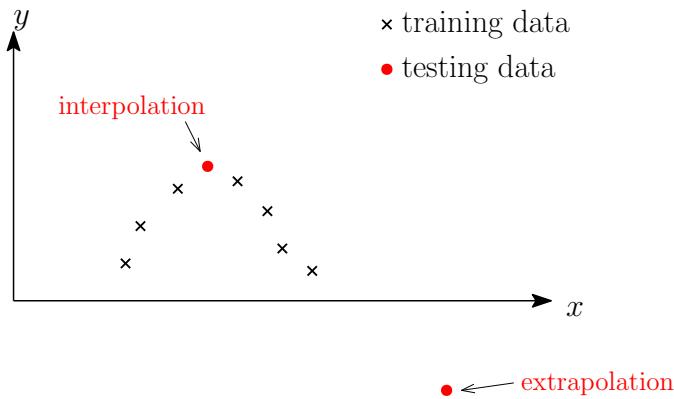
- **Inputs** $x \in \mathcal{X}$: they can be images, sounds, videos, text, proteins, sequences of DNA bases, web pages, social network activities, sensors from industry, financial time series, etc. The set \mathcal{X} may thus have a variety of structures that can be leveraged. All learning methods that we present in this textbook will use at one point a vector space representation of inputs, either by building an explicit mapping from \mathcal{X} to a vector space (such as \mathbb{R}^d) or implicitly by using a notion of pairwise dissimilarity or similarity between pairs of inputs. The choice of these representations is highly domain dependent. However, we note that (a) common topologies are encountered in many diverse areas (such as sequences, two-dimensional or three-dimensional objects), and thus common tools are used, and (b) learning these representations is an active area of research (see discussions in Chapter 7 and Chapter 9).

In this textbook, we will primarily consider that inputs are d -dimensional vectors, with d potentially large (up to 10^6 or 10^9).

- **Outputs** $y \in \mathcal{Y}$: the most classical examples are binary labels $\mathcal{Y} = \{0, 1\}$ or $\mathcal{Y} = \{-1, 1\}$, multiclass classification problems with $\mathcal{Y} = \{1, \dots, k\}$, and classical regression with real responses/outputs $\mathcal{Y} = \mathbb{R}$. These will be the main examples we treat in most of the book. Note, however, that most of the concepts extend to the more general *structured prediction* set-up, where more general structured outputs (e.g., graph prediction, visual scene analysis, source separation) can be considered (see Chapter 15).

Why is it difficult? Supervised learning is difficult (and thus interesting) for a variety of reasons:

- The label y may not be a deterministic function of x : given $x \in \mathcal{X}$, the outputs are noisy, that is, y is not a deterministic function of x . When $y \in \mathbb{R}$, we will often make the simplifying “additive noise” assumption that $y = f(x) + \varepsilon$ with some zero-mean noise ε , but in general, we only assume that there is a conditional distribution of y given x . This stochasticity is typically due to diverging views between labelers or dependence on random external unobserved quantities (that is, $y = f(x, z)$, z random and not observed).
- The prediction function f may be quite complex, highly non-linear when \mathcal{X} is a vector space, and even hard to define when \mathcal{X} is not a vector space.
- Only a few x ’s are observed: we thus need interpolation and potentially extrapolation (see below for an illustration for $\mathcal{X} = \mathcal{Y} = \mathbb{R}$), and therefore overfitting (predicting well on the training data but not as well on the testing data) is always a possibility.



Moreover, the training observations may not be uniformly distributed in \mathcal{X} . In this book, they will be assumed to be random, but some analyses will rely on deterministically located inputs to simplify some theoretical arguments.

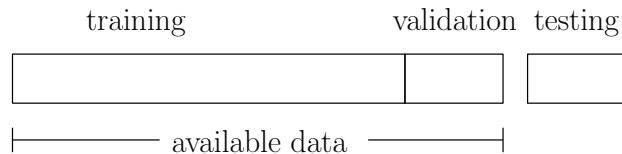
- The input space \mathcal{X} may be very large, that is, with high dimension when this is a vector space. This leads to both computational issues (scalability) and statistical issues (generalization to unseen data). One usually refers to this problem as the *curse of dimensionality*.
- There may be a weak link between training and testing distributions. In other words, the data at training time can have different characteristics than the data at testing time.
- The criterion for performance is not always well defined.

Main formalization. Most modern theoretical analyses of supervised learning rely on a probabilistic formulation, that is, we see (x_i, y_i) as a realization of random variables. The criterion is to maximize the expectation of some “performance” measure with respect to the distribution of the test data (in this book, *maximizing* the performance will be obtained by *minimizing* a loss function). The main assumption is that the random variables (x_i, y_i) are independent and identically distributed (i.i.d.) with the same distribution as the testing distribution. In this course, we will ignore the potential mismatch between train and test distributions (although this is an important research topic, as in most applications, training data are not i.i.d. from the same distribution as the test data).

A machine learning algorithm \mathcal{A} is then a function that goes from a dataset, i.e., an element of $(\mathcal{X} \times \mathcal{Y})^n$, to a function from \mathcal{X} to \mathcal{Y} . In other words, the output of a machine learning algorithm is itself an algorithm!

Practical performance evaluation. In practice, we do not have access to the test distribution but samples from it. In most cases, the data given to the machine learning user are split into three parts:

- the *training set*, on which learning models will be estimated,
- the *validation set*, to estimate hyperparameters (all learning techniques have some),
- the *testing set*, to evaluate the performance of the final chosen model.



In theory, the test set can only be used once! In practice, this is unfortunately only sometimes the case. If the test data are seen multiple times, the estimation of the performance on unseen data is overestimated.

Cross-validation is often preferred to use a maximal amount of training data and reduce the variability of the validation procedure: the available data are divided in k folds (typically $k = 5$ or 10), and all models are estimated k times, each time choosing a different fold as validation data (pink data below), and averaging the k obtained error measures. Cross-validation can be applied to any learning method, and its detailed theoretical analysis is an active area of research (see, [Arlot and Celisse, 2010](#), and the many references therein).



“Debugging” a machine learning implementation is often an art: on top of commonly found bugs, the learning method may not predict well enough on testing data. This is where theory can be useful to understand when a method is supposed to work or not. This is the primary goal of this book.

Random design vs. fixed design. What we have described is often referred to as the “random design” set-up in statistics, where both x and y are assumed random and sampled i.i.d. It is common to simplify the analysis by considering that the input data x_1, \dots, x_n are deterministic, either because they are actually deterministic (i.e., equally spaced in the input space \mathcal{X}), or by conditioning on them if they are actually random. This will be referred to as the “fixed design” setting and studied precisely in the context of least-squares regression in Chapter 3.

2.2 Decision theory

Main question. In this section, we tackle the following question: What is the optimal performance, regardless of the finiteness of the training data? In other words, if we have a perfect knowledge of the underlying probability distribution of the data, what should be done? We will thus introduce the concept of *loss function*, *risk*, and “*Bayes*” *predictor*.

We consider a fixed (testing) distribution $p_{x,y}$ on $\mathcal{X} \times \mathcal{Y}$, with marginal distribution p_x on \mathcal{X} . Note that we make no assumptions at this point on the input space \mathcal{X} .

⚠ We will almost always use the overloaded notation p , to denote $p_{x,y}$ and p_x , where the context can always make the definition unambiguous. For example, when $f : \mathcal{X} \rightarrow \mathbb{R}$ and $g : \mathcal{X} \times \mathcal{Y} \rightarrow \mathbb{R}$, we have $\mathbb{E}[f(x)] = \int_{\mathcal{X}} f(x) dp(x)$ and $\mathbb{E}[g(x, y)] = \int_{\mathcal{X} \times \mathcal{Y}} g(x, y) dp(x, y)$.

⚠ We ignore on-purpose measurability issues. The interested reader can look at the book by [Christmann and Steinwart \(2008\)](#) for a more formal presentation.

2.2.1 Loss functions

We consider a loss function $\ell : \mathcal{Y} \times \mathcal{Y} \rightarrow \mathbb{R}$ (often \mathbb{R}_+), where $\ell(y, z)$ is the loss of predicting z while the true label is y .

-  Some authors swap y and z in the definition above.
-  Some related research communities (e.g., economics) use the concept of “utility”, which is then maximized.

The loss function is only concerned with the output space \mathcal{Y} independently of the input space \mathcal{X} . The main examples are:

- **Binary classification:** $\mathcal{Y} = \{0, 1\}$ (or often $\mathcal{Y} = \{-1, 1\}$), or, less often, when seen as a subcase of the loss below, $\mathcal{Y} = \{1, 2\}$), and $\ell(y, z) = 1_{y \neq z}$ (“0-1” loss), that is, 0 if y is equal to z (no mistake), and 1 otherwise (mistake).



It is very common to mix the two conventions $\mathcal{Y} = \{0, 1\}$ and $\mathcal{Y} = \{-1, 1\}$.

- **Multicategory classification:** $\mathcal{Y} = \{1, \dots, k\}$, and $\ell(y, z) = 1_{y \neq z}$ (“0-1” loss).
- **Regression:** $\mathcal{Y} = \mathbb{R}$ and $\ell(y, z) = (y - z)^2$ (square loss). The absolute loss $\ell(y, z) = |y - z|$ is often used for “robust” estimation (since the penalty for large errors is smaller).
- **Structured prediction:** while this textbook focuses primarily on the examples above, there are many practical problems where \mathcal{Y} is more complicated, with associated algorithms and theoretical results. For example, when $\mathcal{Y} = \{0, 1\}^k$ (leading to multi-label classification), the Hamming loss $\ell(y, z) = \sum_{j=1}^k 1_{y_j \neq z_j}$ is commonly used; also, ranking problems involve losses on permutations. See Chapter 15.

Throughout the textbook, we will assume that the loss function is given to us. Note that in practice, the final user imposes the loss function, as this is how models will be evaluated. Clearly, a single real number may not be enough to characterize the entire prediction behavior. For example, in binary classification, there are two types of errors, false positives and false negatives, which can be considered simultaneously. Since we now have two performance measures, we typically need a curve to characterize the performance of a prediction function. This is precisely what “receiver operating characteristic” (ROC) curves are achieving (see, e.g., [Bach et al., 2006](#), and references therein). For simplicity, in this book, we stick to a single loss function ℓ .

2.2.2 Risks

Given the loss function $\ell : \mathcal{Y} \times \mathcal{Y} \rightarrow \mathbb{R}$, we can define the *expected risk* (also referred to as *generalization performance*, or *testing error*) of a function $f : \mathcal{X} \rightarrow \mathcal{Y}$, as the expectation of the loss function between the output y and the prediction $f(x)$.

Definition 2.1 (Expected risk) *Given a function $f : \mathcal{X} \rightarrow \mathcal{Y}$, a loss function $\ell : \mathcal{Y} \times \mathcal{Y} \rightarrow \mathbb{R}$, and a probability distribution p on $\mathcal{X} \times \mathcal{Y}$, the expected risk of a prediction function $f : \mathcal{X} \rightarrow \mathcal{Y}$ is defined as:*

$$\mathcal{R}(f) = \mathbb{E}[\ell(y, f(x))] = \int_{\mathcal{X} \times \mathcal{Y}} \ell(y, f(x)) dp(x, y).$$

The risk depends on the distribution p on (x, y) . We sometimes use the notation $\mathcal{R}_p(f)$ to make it explicit. The expected risk is our main performance criterion in this textbook.



Be careful with the randomness, or lack thereof, of f : when performing learning from data, f will depend on the random training data and not on the testing data, and thus $\mathcal{R}(f)$ is typically random because of the dependence on the training data. However, as a function on functions, the expected risk \mathcal{R} is deterministic.

Note that sometimes, we consider random predictions, that is, for any x , we output a distribution on y , and then the risk is taken as the expectation over the randomness of the outputs.

Averaging the loss on the training data defines the *empirical risk*, or *training error*.

Definition 2.2 (Empirical risk) *Given a function $f : \mathcal{X} \rightarrow \mathcal{Y}$, a loss function $\ell : \mathcal{Y} \times \mathcal{Y} \rightarrow \mathbb{R}$, and data $(x_i, y_i) \in \mathcal{X} \times \mathcal{Y}$, $i = 1, \dots, n$, the empirical risk of a prediction function $f : \mathcal{X} \rightarrow \mathcal{Y}$ is defined as:*

$$\widehat{\mathcal{R}}(f) = \frac{1}{n} \sum_{i=1}^n \ell(y_i, f(x_i)).$$

Note that $\widehat{\mathcal{R}}$ is a random function on functions (and is often applied to random functions, with dependent randomness as both will depend on the training data).

Special cases. For the classical losses defined earlier, the risks have specific formulations:

- **Binary classification:** $\mathcal{Y} = \{0, 1\}$ (or often $\mathcal{Y} = \{-1, 1\}$), and $\ell(y, z) = 1_{y \neq z}$ (“0-1” loss). We can express the risk as $\mathcal{R}(f) = \mathbb{P}(f(x) \neq y)$. This is simply the probability

of making a mistake on the testing data, while the empirical risk is the proportion of mistakes on the training data.

! In practice, the *accuracy*, which is one minus the error rate, is often reported.

- **Multi-category classification:** $\mathcal{Y} = \{1, \dots, k\}$, and $\ell(y, z) = 1_{y \neq z}$ (“0-1” loss). We can also express the risk as $\mathcal{R}(f) = \mathbb{P}(f(x) \neq y)$. This is also the probability of making a mistake.
- **Regression:** $\mathcal{Y} = \mathbb{R}$ and $\ell(y, z) = (y - z)^2$ (square loss). The risk is then $\mathcal{R}(f) = \mathbb{E}[(y - f(x))^2]$.

2.2.3 Bayes risk and Bayes predictor

Now that we have defined the performance criterion for supervised learning (the expected risk), the main question we tackle here is: what is the best prediction function f (regardless of the training data)?

Using the conditional expectation and its associated law of total expectation, we have

$$\mathcal{R}(f) = \mathbb{E}[\ell(y, f(x))] = \mathbb{E}[\mathbb{E}[\ell(y, f(x))|x]],$$

which we can rewrite

$$\mathcal{R}(f) = \mathbb{E}_{x' \sim p}[\mathbb{E}[\ell(y, f(x))|x = x']] = \int_{\mathcal{X}} \mathbb{E}[\ell(y, f(x))|x = x'] dp(x').$$

! To distinguish between the random variable x and a value it may take, we use the notation x' .

Given the conditional distribution given any $x' \in \mathcal{X}$, that is $y|x = x'$, we can define the *conditional risk* for any $z \in \mathcal{Y}$ (it is a deterministic function):

$$r(z|x') = \mathbb{E}[\ell(y, z)|x = x'],$$

which leads to

$$\mathcal{R}(f) = \mathbb{E}[r(f(x)|x)] = \mathbb{E}_{x' \sim p}[r(f(x')|x')] = \int_{\mathcal{X}} r(f(x')|x') dp(x').$$

A minimizer of $\mathcal{R}(f)$ can be obtained by considering for any $x' \in \mathcal{X}$, the function value $f(x')$ to be equal to a minimizer $z \in \mathcal{Y}$ of $r(z|x') = \mathbb{E}[\ell(y, z)|x = x']$. We can therefore **consider all x' as being treated independently**. This leads to the following proposition.

Proposition 2.1 (Bayes predictor and Bayes risk) *The expected risk is minimized at a Bayes predictor $f^* : \mathcal{X} \rightarrow \mathcal{Y}$ satisfying for all $x' \in \mathcal{X}$,*

$$f^*(x') \in \arg \min_{z \in \mathcal{Y}} \mathbb{E}[\ell(y, z) | x = x'] = \arg \min_{z \in \mathcal{Y}} r(z|x'). \quad (2.1)$$

The Bayes risk \mathcal{R}^ is the risk of all Bayes predictors and is equal to*

$$\mathcal{R}^* = \mathbb{E}_{x' \sim p} \left[\inf_{z \in \mathcal{Y}} \mathbb{E}[\ell(y, z) | x = x'] \right].$$

Note that (a) the Bayes predictor is not always unique, but that all lead to the same Bayes risk (for example, in binary classification when $\mathbb{P}(y = 1|x) = 1/2$), and (b) that the Bayes risk is usually non zero (unless the dependence between x and y is deterministic). Given a supervised learning problem, the Bayes risk is the optimal performance; we define the excess risk as the deviation with respect to the optimal risk.

Definition 2.3 (Excess risk) *The excess risk of a function $f : \mathcal{X} \rightarrow \mathcal{Y}$ is equal to $\mathcal{R}(f) - \mathcal{R}^*$ (it is always non-negative).*

Therefore, machine learning is “trivial”: given the distribution $y|x$ for any x , the optimal predictor is known and given by Eq. (2.1). The difficulty will be that this distribution is unknown.

Special cases. For our usual set of losses, we can compute the Bayes predictors in closed form:

- **Binary classification:** the Bayes predictor for $\mathcal{Y} = \{0, 1\}$ and $\ell(y, z) = 1_{y \neq z}$ is such that

$$\begin{aligned} f^*(x') \in \arg \min_{z \in \{0, 1\}} \mathbb{P}(y \neq z | x = x') &= \arg \min_{z \in \{0, 1\}} 1 - \mathbb{P}(y = z | x = x') \\ &= \arg \max_{z \in \{0, 1\}} \mathbb{P}(y = z | x = x'). \end{aligned}$$

The optimal classifier will select the most likely class given x' . Denoting $\eta(x') = \mathbb{P}(y = 1 | x = x')$, then, if $\eta(x') > 1/2$, $f^*(x') = 1$, while if $\eta(x') < 1/2$, $f^*(x') = 0$. What happens for $\eta(x') = 1/2$ is irrelevant.

The Bayes risk is then equal to $\mathcal{R}^* = \mathbb{E}[\min\{\eta(x), 1 - \eta(x)\}]$, which in general strictly positive (unless $\eta(x) \in \{0, 1\}$ almost surely, that is, y is a deterministic function of x).

This extends directly to multiple categories $\mathcal{Y} = \{1, \dots, k\}$, for $k \geq 2$, where we have $f^*(x') \in \arg \max_{i \in \{1, \dots, k\}} \mathbb{P}(y = i | x = x')$.

! These Bayes predictors and risks are only valid for the 0-1 loss. Less symmetric losses are very common in applications (e.g., for spam detection) and would lead to different formulas (see exercise below).

- **Regression:** the Bayes predictor for $\mathcal{Y} = \mathbb{R}$ and $\ell(y, z) = (y - z)^2$ is such that¹

$$\begin{aligned} f^*(x') &\in \arg \min_{z \in \mathbb{R}} \mathbb{E}[(y - z)^2 | x = x'] \\ &= \arg \min_{z \in \mathbb{R}} \left\{ \mathbb{E}[(y - \mathbb{E}[y|x=x'])^2 | x = x'] + (z - \mathbb{E}[y|x=x'])^2 \right\}. \end{aligned}$$

This leads to the conditional expectation $f^*(x') = \mathbb{E}[y|x=x']$.

Exercise 2.1 We consider binary classification with $\mathcal{Y} = \{-1, 1\}$ with the loss function $\ell(-1, -1) = \ell(1, 1) = 0$ and $\ell(-1, 1) = c_- > 0$ (cost of a false positive), and $\ell(1, -1) = c_+ > 0$ (cost of a false negative). Compute the Bayes estimator at x as a function of $\mathbb{E}[y|x]$.

Exercise 2.2 What is the Bayes predictor for regression with the absolute loss $\ell(y, z) = |y - z|$?

Exercise 2.3 (inverting predictions) We consider the binary classification problem with $\mathcal{Y} = \{-1, 1\}$ and the 0-1 loss. Relate the risk of a prediction f and its opposite $-f$.

Exercise 2.4 (“chance” predictions) We consider the binary classification problem with the 0-1 loss, what is the risk of a random prediction rule where we predict the two classes with equal probabilities independently of the input x ? Same question with multiple categories.

Exercise 2.5 (♦) We consider a random prediction rule where we predict from the probability distribution of y given x' . When is this achieving the Bayes risk?

2.3 Learning from data

The decision theory framework outlined in the previous section gives a test performance criterion and optimal predictors, but it depends on the full knowledge of the test distribution p . We now briefly review how we can obtain good prediction functions from training data, that is, data sampled i.i.d. from the same distribution.

Two main classes of prediction algorithms will be studied in this textbook:

¹We use the law of total variance: $\mathbb{E}[(y - a)^2] = \text{var}(y) + (\mathbb{E}[y] - a)^2$ for any random variable y and constant $a \in \mathbb{R}$, which can be shown by expanding the square.

- (1) Local averaging (Chapter 6).
- (2) Empirical risk minimization (Chapters 3, 4, 7, 8, 9, 11, 15).

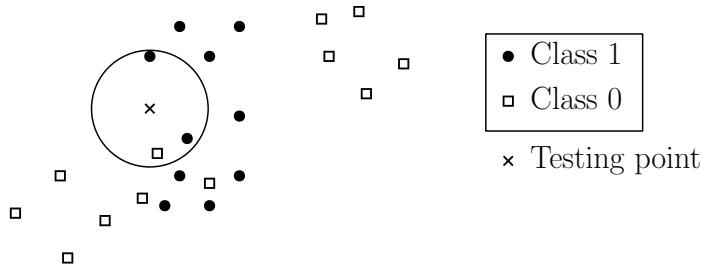
Note that there are prediction algorithms that do not fit exactly into one of these two categories, such as boosting or ensemble classifiers (see Chapter 10). Moreover, some situations do not fit the classical i.i.d. framework, such as in online learning (see Chapter 13). We also consider probabilistic methods in Chapter 14, which rely on a different principle.

2.3.1 Local averaging

The goal here is to try to approximate/emulate the Bayes predictor, e.g., $f^*(x') = \mathbb{E}(y|x = x')$ for least-squares regression, from empirical data. This is often done by explicit/implicit estimation of the conditional distribution by *local averaging* (k -nearest neighbors, which is used as the primary example for this chapter, Nadaraya Watson, or decision trees). We briefly outline here the main properties for one instance of these algorithms; see Chapter 6 for details.

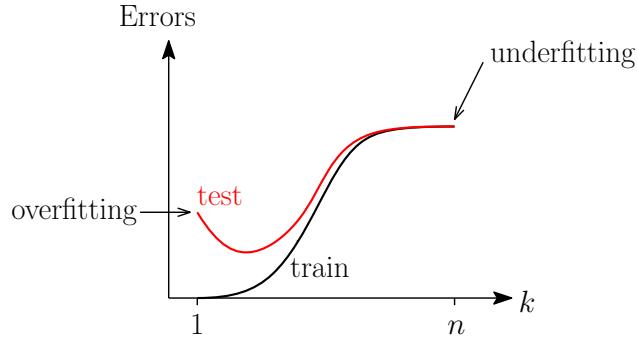
k -nearest-neighbor classification. Given n observations $(x_1, y_1), \dots, (x_n, y_n)$ where \mathcal{X} is a metric space and $\mathcal{Y} \in \{0, 1\}$, a new point x^{test} is classified by a majority vote among the k -nearest neighbors of x^{test} .

Below, we consider the 3-nearest-neighbor classifier on a particular testing point (which will be predicted as 1).



- Pros: (a) no optimization or training, (b) often easy to implement, (c) can get very good performance in low dimensions (in particular for non-linear dependences between x and y).
- Cons: (a) slow at query time: must pass through all training data at each testing point (there are algorithmic tools to reduce complexity, see Chapter 6), (b) bad for high-dimensional data (because of the curse of dimensionality, more on this in Chapter 6), (c) the choice of local distance function is crucial, (d) the choice of “width” hyperparameters (or k) has to be performed.

- Plot of training errors and testing errors as functions of k for a typical problem. When k is too large, there is *underfitting* (the learned function is too close to a constant, which is too simple), while for k too small, there is *overfitting* (there is a strong discrepancy between the testing and training errors).



- **Exercise 2.6** How would the curve move when n increases (assuming the same balance between classes)?

2.3.2 Empirical risk minimization

Consider a parameterized family of prediction functions $f_\theta : \mathcal{X} \rightarrow \mathcal{Y}$ for $\theta \in \Theta$ (typically a subset of a vector space), and minimize the empirical risk with respect to $\theta \in \Theta$:

$$\hat{\mathcal{R}}(f_\theta) = \frac{1}{n} \sum_{i=1}^n \ell(y_i, f_\theta(x_i)).$$

This defines an estimator $\hat{\theta} \in \arg \min_{\theta \in \Theta} \hat{\mathcal{R}}(f_\theta)$, and thus a function $f_{\hat{\theta}} : \mathcal{X} \rightarrow \mathcal{Y}$.

The most classic example is linear least-squares regression (studied at length in Chapter 3), where we minimize

$$\frac{1}{n} \sum_{i=1}^n (y_i - \theta^\top \varphi(x_i))^2,$$

where f is linear in some feature vector $\varphi(x) \in \mathbb{R}^d$ (there is no need for \mathcal{X} to be a vector space). The vector $\varphi(x)$ can be quite large (or even implicit, like in kernel methods, see Chapter 7). Other examples include neural networks (Chapter 9).

- Pros: (a) can be relatively easy to optimize (e.g., least-squares with simple derivation and numerical algebra, see Chapter 3), many algorithms available (primarily based on gradient descent, see Chapter 5), (b) can be applied in any dimension (if a good feature vector is available).

- Cons: (a) can be relatively hard to optimize when the optimization formulation is not convex (e.g., neural networks), (b) need a suitable feature vector for linear methods, (c) the dependence on parameters can be complex (e.g., neural networks), (d) need some capacity control to avoid overfitting, (e) how to parameterize functions with values in $\{0, 1\}$ (see Chapter 4 for the use of convex surrogates)?

Risk decomposition. The material in this section will be studied further in more detail in Chapter 4.

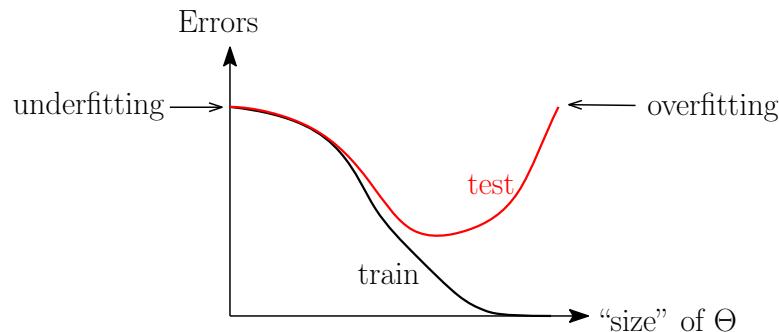
- Risk decomposition in estimation error + approximation error: given any $\hat{\theta} \in \Theta$, we can write the excess risk of $f_{\hat{\theta}}$ as:

$$\begin{aligned}\mathcal{R}(f_{\hat{\theta}}) - \mathcal{R}^* &= \left\{ \mathcal{R}(f_{\hat{\theta}}) - \inf_{\theta' \in \Theta} \mathcal{R}(f_{\theta'}) \right\} + \left\{ \inf_{\theta' \in \Theta} \mathcal{R}(f_{\theta'}) - \mathcal{R}^* \right\} \\ &= \text{estimation error} \quad + \text{approximation error}\end{aligned}$$

The approximation error $\left\{ \inf_{\theta' \in \Theta} \mathcal{R}(f_{\theta'}) - \mathcal{R}^* \right\}$ is always non-negative, does not depend on the chosen $f_{\hat{\theta}}$ and depends only on the class of functions parameterized by $\theta \in \Theta$. It is thus always a deterministic quantity, which characterizes the modeling assumptions made by the chosen class of functions. When Θ grows, the approximation error goes down to zero if arbitrary functions can be approximated arbitrarily well by the functions f_{θ} . It is also independent of n .

The estimation error $\left\{ \mathcal{R}(f_{\hat{\theta}}) - \inf_{\theta' \in \Theta} \mathcal{R}(f_{\theta'}) \right\}$ is also always non-negative and is typically random because the function $f_{\hat{\theta}}$ is random. It typically decreases in n and goes up when Θ grows.

Overall the typical error curves look like this:



- Typically, we will see in later chapters that the estimation error is often decomposed as follows, for θ' a minimizer on Θ of the expected risk $\mathcal{R}(f_{\theta'})$:

$$\begin{aligned}\left\{ \mathcal{R}(f_{\hat{\theta}}) - \mathcal{R}(f_{\theta'}) \right\} &= \left\{ \mathcal{R}(f_{\hat{\theta}}) - \hat{\mathcal{R}}(f_{\hat{\theta}}) \right\} + \left\{ \hat{\mathcal{R}}(f_{\hat{\theta}}) - \hat{\mathcal{R}}(f_{\theta'}) \right\} + \left\{ \hat{\mathcal{R}}(f_{\theta'}) - \mathcal{R}(f_{\theta'}) \right\} \\ &\leq 2 \sup_{\theta \in \Theta} |\hat{\mathcal{R}}(f_{\theta}) - \mathcal{R}(f_{\theta})| + \text{empirical optimization error},\end{aligned}$$

where the “empirical optimization error” is $\{\hat{\mathcal{R}}(f_{\hat{\theta}}) - \hat{\mathcal{R}}(f_{\theta'})\}$ (it is equal to zero for the exact empirical risk minimizer, but in practice, when using optimization algorithms from Chapter 5, it is not). The uniform deviation $\sup_{\theta \in \Theta} |\hat{\mathcal{R}}(f_{\theta}) - \mathcal{R}(f_{\theta})|$ grows with the “size” of Θ , and usually decays with n . See more details in Chapter 4.

Capacity control. To avoid overfitting, we need to make sure that the set of allowed functions is not too large by typically reducing the number of parameters or by restricting the norm of predictors (thus by lowering the “size” of Θ): this typically leads to constrained optimization, and allows for risk decompositions as done above.

Capacity control can also be done by regularization, that is, by minimizing

$$\hat{\mathcal{R}}(f_{\theta}) + \lambda \Omega(\theta) = \frac{1}{n} \sum_{i=1}^n \ell(y_i, f_{\theta}(x_i)) + \lambda \Omega(\theta),$$

where $\Omega(\theta)$ controls the complexity of f_{θ} . The main example is ridge regression:

$$\min_{\theta \in \mathbb{R}^d} \frac{1}{n} \sum_{i=1}^n (y_i - \theta^\top \varphi(x_i))^2 + \lambda \|\theta\|_2^2.$$

This is often easier for optimization but harder to analyze (see Chapter 4 and Chapter 5).



There is a difference between parameters (e.g., θ) learned on the training data and hyperparameters (e.g., λ) estimated on the validation data.

Examples of approximations by polynomials in one-dimensional regression. We consider $(x, y) \in \mathbb{R} \times \mathbb{R}$, with prediction functions which are polynomials of order k , from $k = 0$ (constant functions) to $k = 14$. For each k , the model has $k + 1$ parameters. The training error (using square loss) is minimized with $n = 20$ observations. The data were generated with inputs uniformly distributed on $[-1, 1]$ and outputs as the quadratic function $f(x) = x^2 - \frac{1}{2}$ of the inputs plus some independent additive noise (Gaussian with standard deviation $1/4$). As shown in Figure 2.1 and Figure 2.2, the training error monotonically decreases in k while the testing error goes down and then up.

2.4 Statistical learning theory

The goal of learning theory is to provide some guarantees of performance on unseen data. A common assumption is that the data $\mathcal{D}_n(p) = \{(x_1, y_1), \dots, (x_n, y_n)\}$ is obtained as independent and identically distributed (i.i.d.) observations from some unknown distribution p from a family \mathcal{P} .

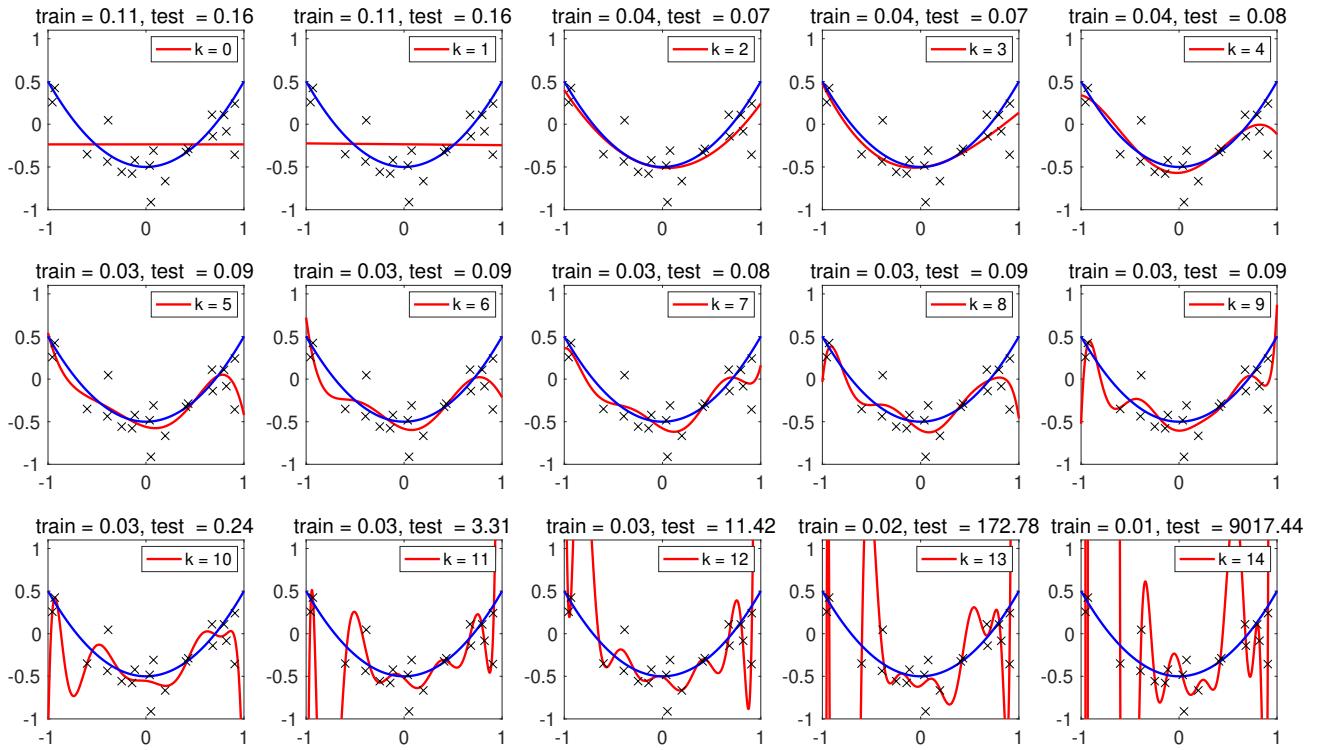


Figure 2.1: Polynomial regression with increasing orders k . Plots of estimated functions, with training and testing errors. The Bayes prediction function $f^*(x) = \mathbb{E}[y|x]$ is plotted in blue.

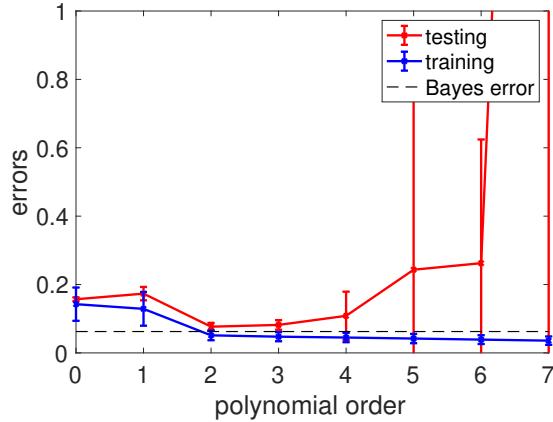


Figure 2.2: Polynomial regression with increasing orders. Plots of training and testing errors with error bars (computed as standard deviations obtained from 32 replications), together with the Bayes error.

An algorithm \mathcal{A} is a mapping from $\mathcal{D}_n(p)$ (for any n) to a function from \mathcal{X} to \mathcal{Y} . The expected risk depends on the probability distribution $p \in \mathcal{P}$, as $\mathcal{R}_p(f)$. The goal is to find \mathcal{A} such that the (expected) risk

$$\mathcal{R}_p(\mathcal{A}(\mathcal{D}_n(p))) - \mathcal{R}_p^*$$

is small, where \mathcal{R}_p^* is the Bayes risk (which depends on the joint distribution p), assuming $\mathcal{D}_n(p)$ is sampled from p , but without knowing which $p \in \mathcal{P}$ is considered. Moreover, the risk is random because $\mathcal{D}_n(p)$ is random.

2.4.1 Measures of performance

There are several ways of dealing with randomness to obtain a criterion.

- *Expected error*: we measure performance as

$$\mathbb{E}\left[\mathcal{R}_p(\mathcal{A}(\mathcal{D}_n(p)))\right],$$

where the expectation is with respect to the training data. An algorithm \mathcal{A} is called *consistent in expectation* for the distribution p , if

$$\mathbb{E}\left[\mathcal{R}_p(\mathcal{A}(\mathcal{D}_n(p)))\right] - \mathcal{R}_p^*$$

goes to zero when n tends to infinity. In this course, we will primarily use this notion of consistency.

- “*Probably approximately correct*” (PAC) learning: for a given $\delta \in (0, 1)$ and $\varepsilon > 0$:

$$\mathbb{P}\left(\left[\mathcal{R}_p(\mathcal{A}(\mathcal{D}_n(p))) - \mathcal{R}_p^*\right] \leq \varepsilon\right) \geq 1 - \delta.$$

The crux is to find ε , which is as small as possible (typically as a function of δ). The notion of PAC consistency corresponds, for any $\varepsilon > 0$, to have such an inequality for each n and a sequence δ_n that tends to zero.

2.4.2 Notions of consistency over classes of problems

An algorithm is called *universally consistent* (in expectation) if for all distributions $p = p_{x,y}$ on (x, y) the algorithm \mathcal{A} is consistent in expectation for the distribution p .

! Be careful with the order of quantifiers: convergence speed will depend on p . See the no-free lunch theorem section below to highlight that having a uniform rate over all distributions is hopeless.

Most often, we want to study uniform consistency within a class \mathcal{P} of distributions satisfying some regularity properties (e.g., the inputs live in a compact space, or the dependence between y and x is at most of some complexity). We thus aim at finding an algorithm \mathcal{A} such that

$$\sup_{p \in \mathcal{P}} \mathbb{E}[\mathcal{R}_p(\mathcal{A}(\mathcal{D}_n(p)))] - \mathcal{R}_p^*$$

is as small as possible. The so-called “minimax risk” is equal to

$$\inf_{\mathcal{A}} \sup_{p \in \mathcal{P}} \mathbb{E}[\mathcal{R}_p(\mathcal{A}(\mathcal{D}_n(p)))] - \mathcal{R}_p^*.$$

This is typically a function of the sample size n and properties of \mathcal{X}, \mathcal{Y} and the allowed set of problems \mathcal{P} (e.g., dimension of \mathcal{X} , number of parameters). To compute estimates of the minimax risk, several techniques exist:

- Upper-bounding the optimal performance: one given algorithm with a convergence proof provides an upper bound. This is the main focus of this book.
- Lower-bounding the optimal performance: in some setups, it is possible to show that the infimum over all algorithms is greater than a certain quantity. See Chapter 12 for a description of techniques to obtain such lower bounds. Machine learners are happy when upper-bounds and lower-bounds match (up to constant factors).

Non-asymptotic vs. asymptotic analysis. The analysis can be “non-asymptotic”, with an upper bound with explicit dependence on all quantities; the bound is then valid for all n , even if sometimes vacuous (e.g., a bound greater than 1 for a loss uniformly bounded by 1).

The analysis can also be “asymptotic”, where for example, n goes to infinity and limits are taken (alternatively, several quantities can be made to grow simultaneously).



What (arguably) matters most here is the dependence of these rates on the problem, not the choice of “in expectation” vs. “in high probability”, or “asymptotic” vs. “non-asymptotic”, as long as the problem parameters explicitly appear.

2.5 No free lunch theorems (♦)

Although it may be tempting to define the optimal learning algorithm that works optimally for all distributions, this is impossible. In other words, learning is only possible with assumptions. See [Devroye et al. \(1996, Chapter 7\)](#) for details.

The following theorem shows that for any algorithm, for a fixed n , there is a data distribution that makes the algorithm useless (with a risk that is the same as the chance level).

Theorem 2.1 (no free lunch - fixed n) Consider the binary classification with 0-1 loss, with \mathcal{X} infinite. Let \mathcal{P} denote the set of all probability distributions on $\mathcal{X} \times \{0, 1\}$. For any $n > 0$ and any learning algorithm \mathcal{A} ,

$$\sup_{p \in \mathcal{P}} \mathbb{E}\left[\mathcal{R}_p(\mathcal{A}(\mathcal{D}_n(p)))\right] - \mathcal{R}_p^* \geq 1/2.$$

Proof (♦♦) Let k be a positive integer. Without loss of generality, we can assume that $\mathbb{N} \subset \mathcal{X}$. The main ideas of the proof are (a) to construct a probability distribution supported on k elements in \mathbb{N} , where k is large compared to n (which is fixed), and to show that the knowledge of n labels does not imply doing well on all k elements, and (b) to choose parameters of this distribution (the vector r below) by comparing to a performance obtained by random parameters.

Given $r \in \{0, 1\}^k$, we define the joint distribution p on (x, y) such that $\mathbb{P}(x = j, y = r_j) = 1/k$ for $j \in \{1, \dots, k\}$; that is, for x , we choose one of the first k elements uniformly at random, and then y is selected deterministically as $y = r_x$. Thus the Bayes risk is zero (because there is a deterministic relationship): $\mathcal{R}_p^* = 0$.

Denoting $\hat{f}_{\mathcal{D}_n} = \mathcal{A}(\mathcal{D}_n(p))$ the classifier, and $S(r) = \mathbb{E}\left[\mathcal{R}_p(\hat{f}_{\mathcal{D}_n})\right]$ the expectation of the expected risk, we want to maximize $S(r)$ with respect to $r \in \{0, 1\}^k$; the maximum is greater than the expectation of $S(r)$ for any probability distribution q on r , in particular the uniform distribution (each r_j being an independent unbiased Bernoulli variable). Then

$$\begin{aligned} \max_{r \in \{0, 1\}^k} S(r) &\geq \mathbb{E}_{r \sim q} S(r) \\ &= \mathbb{P}(\hat{f}_{\mathcal{D}_n}(x) \neq y) = \mathbb{P}(\hat{f}_{\mathcal{D}_n}(x) \neq r_x), \end{aligned}$$

because x is almost surely in $\{1, \dots, k\}$ and $y = r_x$ almost surely. Note that we take expectations and probabilities with respect to x_1, \dots, x_n, x , and r (all being independent of each other).

Then, we get, using that $\mathcal{D}_n(p) = \{x_1, r_{x_1}, \dots, x_n, r_{x_n}\}$:

$$\begin{aligned} \mathbb{E}_{r \sim q} S(r) &= \mathbb{E}\left[\mathbb{P}(\hat{f}_{\mathcal{D}_n}(x) \neq r_x | x_1, \dots, x_n, r_{x_1}, \dots, r_{x_n})\right] \text{ by the law of total expectation,} \\ &\geq \mathbb{E}\left[\mathbb{P}(\hat{f}_{\mathcal{D}_n}(x) \neq r_x \& x \notin \{x_1, \dots, x_n\} | x_1, \dots, x_n, r_{x_1}, \dots, r_{x_n})\right] \\ &\quad \text{by monotonicity of probabilities,} \\ &= \mathbb{E}\left[\frac{1}{2}\mathbb{P}(x \notin \{x_1, \dots, x_n\} | x_1, \dots, x_n, r_{x_1}, \dots, r_{x_n})\right], \end{aligned}$$

because $\mathbb{P}(\hat{f}_{\mathcal{D}_n}(x) \neq r_x | x \notin \{x_1, \dots, x_n\}, x_1, \dots, x_n, r_{x_1}, \dots, r_{x_n}) = 1/2$ (the label $x = r_x$ has the same probability of being 0 or 1, given that it was not observed). Thus,

$$\mathbb{E}_{r \sim q} S(r) \geq \frac{1}{2}\mathbb{P}(x \notin \{x_1, \dots, x_n\}) = \frac{1}{2}\mathbb{E}\left[\prod_{i=1}^n \mathbb{P}(x_i \neq x | x)\right] = \frac{1}{2}(1 - 1/k)^n.$$

Given n , we can let k tend to infinity to conclude. ■

A caveat is that the hard distribution may depend on n (from the proof, it takes k values, with k tending to infinity fast enough compared with n). The following theorem is given without proof and is much “stronger” ([Devroye et al., 1996](#), Theorem 7.2), as it more convincingly shows that learning can be arbitrarily slow without assumption (note that the earlier one is not a corollary of the later one).

Theorem 2.2 (no free lunch - sequence of errors) *Consider a binary classification problem with the 0-1 loss, with \mathcal{X} infinite. Let \mathcal{P} denote the set of all probability distributions on $\mathcal{X} \times \{0, 1\}$. For any decreasing sequence a_n tending to zero and such that $a_1 \leq 1/16$, for any learning algorithm \mathcal{A} , there exists $p \in \mathcal{P}$, such that for all $n \geq 1$:*

$$\mathbb{E}\left[\mathcal{R}_p(\mathcal{A}(\mathcal{D}_n(p)))\right] - \mathcal{R}_p^* \geq a_n.$$

2.6 Quest for adaptivity

As seen in the previous section, no method can be universal and achieve a good convergence rate on all problems. However, such negative results consider classes of problems which are arbitrarily large. In this textbook, we will consider reduced sets of learning problems by considering $\mathcal{X} = \mathbb{R}^d$ and putting restrictions on the target function f^* based on smoothness and/or dependence on an unknown low-dimensional projection. That is, the most general set of functions will be the set of Lipschitz-continuous functions, for which the optimal rate will be essentially proportional to $O(n^{-1/d})$, typical of the curse of dimensionality. No method can beat this, not k -nearest-neighbors, not kernel methods, not even neural networks.

When the target function is smoother, that is, with all derivatives up to order m bounded, then we will see that kernel methods ([Chapter 7](#)) and neural networks ([Chapter 9](#)), with the proper choice of the regularization parameter, will lead to the optimal rate of $O(n^{-m/d})$.

When the target function moreover depends only on a k -dimensional linear projection, neural networks (if the optimization problem is solved correctly) will have the extra ability to lead to rates of the form $O(n^{-m/k})$ instead of $O(n^{-m/d})$, which is not the case for kernel methods (see [Chapter 9](#))

Note that another form of adaptivity, which is often considered, is to situations where the input data lie on a submanifold of \mathbb{R}^d (e.g., an affine subspace), where for most methods presented in this textbook, adaptivity is obtained. In the convergence rate, d can be replaced by the dimension of the subspace (or submanifold) where the data live. See studies by [Kpotufe \(2011\)](#) for k -nearest neighbors, and [Hamm and Steinwart \(2021\)](#) for kernel methods.

See more details in <https://francisbach.com/quest-for-adaptivity/> as well as Chapter 7 and Chapter 9 for detailed results.

Chapter 3

Linear least-squares regression

Chapter summary

- Ordinary least-squares estimator: least-squares regression with linearly parameterized predictors leads to a linear system of size d (the number of predictors).
- Guarantees in the fixed design setting with no regularization: when the inputs are assumed deterministic and $d < n$, the excess risk is equal to $\sigma^2 d/n$.
- Ridge regression: with ℓ_2 -regularization, excess risk bounds become dimension independent and allow high-dimensional feature vectors where $d > n$.
- Guarantees in the random design setting: although they are harder to show, they have a similar form.
- Lower bound of performance: under well-specification, the rate $\sigma^2 d/n$ is unimprovable.

3.1 Introduction

In this chapter, we introduce and analyze linear least-squares regression, a tool that can be traced back to Legendre (1805) and Gauss (1809).¹

Why should we study linear least-squares regression? Has there not been any progress since 1805? A few reasons:

- It already captures many of the concepts in learning theory, such as the bias-variance trade-off, as well as the dependence of generalization performance on the underlying

¹see https://en.wikipedia.org/wiki/Least_squares for an interesting discussion and the claim that Gauss knew about it already in 1795.

dimension of the problem with no regularization or on dimension-less quantities when regularization is added.

- Because of its simplicity, many results can be easily derived without the need for complicated mathematics, both in terms of algorithms and statistical analysis (simple linear algebra for the simplest results).
- Using non-linear features, it can be extended to arbitrary non-linear predictions (see kernel methods in Chapter 7).

In subsequent chapters, we will extend many of these results beyond least-squares.

3.2 Least-squares framework

We recall the goal of supervised machine learning from Chapter 2: given some observations $(x_i, y_i) \in \mathcal{X} \times \mathcal{Y}$, $i = 1, \dots, n$, of inputs/outputs, features/variables (training data), given a new $x \in \mathcal{X}$, predict $y \in \mathcal{Y}$ (testing data) with a *regression* function f such that $y \approx f(x)$. We assume that $\mathcal{Y} = \mathbb{R}$ and we use the square loss $\ell(y, z) = (y - z)^2$, for which we know from the previous chapter that the optimal predictor is $f^*(x) = \mathbb{E}(y|x)$.

In this chapter, we consider empirical risk minimization. We choose a parameterized family of prediction functions $f_\theta : \mathcal{X} \rightarrow \mathcal{Y} = \mathbb{R}$ for $\theta \in \Theta$ and minimize the empirical risk

$$\frac{1}{n} \sum_{i=1}^n (y_i - f_\theta(x_i))^2,$$

leading to the estimator $\hat{\theta} \in \arg \min_{\theta \in \Theta} \frac{1}{n} \sum_{i=1}^n (y_i - f_\theta(x_i))^2$. Note that in most cases, the Bayes predictor f^* does not belong to the class of functions $\{f_\theta, \theta \in \Theta\}$, that is, the model is said *misspecified*.

Least-squares regression can be carried out with parameterizations of the function f_θ , which may be non-linear in the parameter θ (such as for neural networks in Chapter 9). In this chapter, we will consider only situations where $f_\theta(x)$ is linear in θ , which is thus assumed to live in a vector space, and which we take to be \mathbb{R}^d for simplicity.



Being linear in x or linear θ is different!

While we assume linearity in the parameter θ , nothing forces $f_\theta(x)$ to be linear in the input x . In fact, even the concept of linearity may be meaningless if \mathcal{X} is not a vector space. If $f_\theta(x)$ is linear in $\theta \in \mathbb{R}^d$, then it has to be a linear combination of the form

$f_\theta(x) = \sum_{i=1}^d \alpha_i(x)\theta_i$, where $\alpha_i : \mathcal{X} \rightarrow \mathbb{R}$, $i = 1, \dots, d$, are d functions. By concatenating them in a vector $\varphi(x) \in \mathbb{R}^d$ where $\varphi(x)_i = \alpha_i(x)$, we get the representation

$$f_\theta(x) = \varphi(x)^\top \theta.$$

The vector $\varphi(x) \in \mathbb{R}^d$ is typically called the *feature vector*, which we assume to be known (in other words, it is given to us and can be computed explicitly when needed). We thus consider minimizing

$$\hat{\mathcal{R}}(\theta) := \frac{1}{n} \sum_{i=1}^n (y_i - \varphi(x_i)^\top \theta)^2. \quad (3.1)$$

When $\mathcal{X} \subset \mathbb{R}^d$, we can make the extra assumptions that f_θ is an affine function, which could be obtained through $\varphi(x) = \begin{pmatrix} x \\ 1 \end{pmatrix} \in \mathbb{R}^{d+1}$. Other classical assumptions are $\varphi(x)$ composed of monomials (so that prediction functions are polynomials). We will see in Chapter 7 (kernel methods) that we can consider infinite-dimensional features.

Matrix notation. The cost function above in Eq. (3.1) can be rewritten in matrix notations. Let $y = (y_1, \dots, y_n)^\top \in \mathbb{R}^n$ be the vector of outputs (sometimes called the *response vector*), and $\Phi \in \mathbb{R}^{n \times d}$ the matrix of inputs, whose rows are $\varphi(x_i)^\top$. It is called the *design matrix* or *data matrix*. In these notations, the empirical risk is

$$\hat{\mathcal{R}}(\theta) = \frac{1}{n} \|y - \Phi\theta\|_2^2, \quad (3.2)$$

where $\|\alpha\|_2^2 = \sum_{j=1}^d \alpha_j^2$ is the squared ℓ_2 -norm of α .

⚠ It is sometimes tempting at first to avoid matrix notations. We strongly advise against it as it leads to long and error-prone formulas.

3.3 Ordinary least-squares (OLS) estimator

We assume that the matrix $\Phi \in \mathbb{R}^{n \times d}$ has full column rank (i.e., the rank of Φ is d). In particular, the problem is said to be “over-determined,” and we must have $d \leq n$. Equivalently, we assume that $\Phi^\top \Phi \in \mathbb{R}^{d \times d}$ is invertible.

Definition 3.1 When Φ has full column rank, the minimizer of Eq. (3.2) is unique and called the ordinary least-squares (OLS) estimator.

3.3.1 Closed-form solution

Since the objective function is quadratic, the gradient will be linear and zeroing it will lead to a closed-form solution.

Proposition 3.1 *When Φ has full column rank, the OLS estimator exists and is unique. It is given by*

$$\hat{\theta} = (\Phi^\top \Phi)^{-1} \Phi^\top y.$$

Denote the (non-centered)² empirical covariance matrix by $\widehat{\Sigma} := \frac{1}{n} \Phi^\top \Phi \in \mathbb{R}^{d \times d}$; we have $\hat{\theta} = \frac{1}{n} \widehat{\Sigma}^{-1} \Phi^\top y$.

Proof Since the function $\hat{\mathcal{R}}$ is coercive (i.e., going to infinity at infinity) and continuous, it admits at least a minimizer. Moreover, it is differentiable, so a minimizer $\hat{\theta}$ must satisfy $\hat{\mathcal{R}}'(\hat{\theta}) = 0$ where $\hat{\mathcal{R}}'(\theta) \in \mathbb{R}^d$ is the gradient of $\hat{\mathcal{R}}$ at θ . For all $\theta \in \mathbb{R}^d$, we have, by expanding the square and computing the gradient:

$$\hat{\mathcal{R}}(\theta) = \frac{1}{n} (\|y\|_2^2 - 2\theta^\top \Phi^\top y + \theta^\top \Phi^\top \Phi \theta) \quad \text{and} \quad \hat{\mathcal{R}}'(\theta) = \frac{2}{n} (\Phi^\top \Phi \theta - \Phi^\top y).$$

The condition $\hat{\mathcal{R}}'(\hat{\theta}) = 0$ gives the so-called *normal equations*:

$$\Phi^\top \Phi \hat{\theta} = \Phi^\top y.$$

The normal equations have a unique solution $\hat{\theta} = (\Phi^\top \Phi)^{-1} \Phi^\top y$. This shows the uniqueness of the minimizer of $\hat{\mathcal{R}}$ as well as its closed-form expression. ■

Another way to show the uniqueness of the minimizer is by showing that $\hat{\mathcal{R}}$ is strongly convex since $\hat{\mathcal{R}}''(\theta) = 2\widehat{\Sigma}$ is invertible for all $\theta \in \mathbb{R}^d$ (convexity will be studied in Chapter 5).

⚠ For readers worried about carrying a factor of two in the gradients, we will use an additional factor 1/2 in chapters on optimization (e.g., Chapter 5).

3.3.2 Geometric interpretation

Proposition 3.2 *The vector of predictions $\Phi \hat{\theta} = \Phi(\Phi^\top \Phi)^{-1} \Phi^\top y$ is the orthogonal projection of $y \in \mathbb{R}^n$ onto $\text{im}(\Phi) \subset \mathbb{R}^n$, the column space of Φ .*

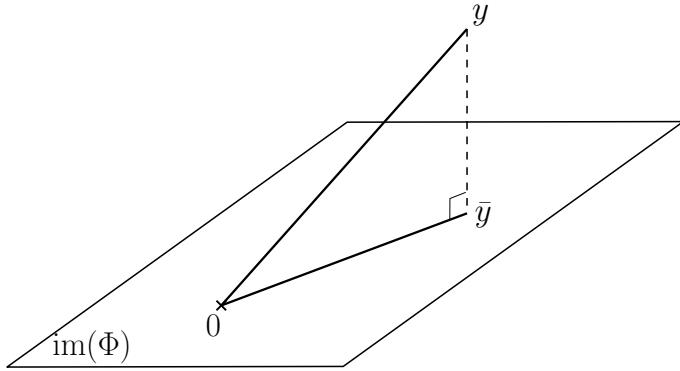
Proof Let us show that $P := \Phi(\Phi^\top \Phi)^{-1} \Phi^\top \in \mathbb{R}^{n \times n}$ is the orthogonal projection on $\text{im}(\Phi)$. For any $a \in \mathbb{R}^d$, it holds $P \Phi a = \Phi(\Phi^\top \Phi)^{-1} \Phi^\top \Phi a = \Phi a$, so $P u = u$ for all $u \in \text{im}(\Phi)$. Also,

²The “centered” covariance matrix would be $\frac{1}{n} \sum_{i=1}^n [\varphi(x_i) - \mu][\varphi(x_i) - \mu]^\top$ where $\mu = \frac{1}{n} \sum_{i=1}^n \varphi(x_i) \in \mathbb{R}^d$ is the empirical mean, while we consider $\widehat{\Sigma} = \frac{1}{n} \sum_{i=1}^n \varphi(x_i) \varphi(x_i)^\top$.

since $\text{im}(\Phi)^\perp = \text{null}(\Phi^\top)$, $Pu' = 0$ for all $u' \in \text{im}(\Phi)^\perp$. These properties characterize the orthogonal projection on $\text{im}(\Phi)$. \blacksquare

Thus we can interpret the OLS estimation as doing the following (see below for an illustration):

1. compute \bar{y} the projection of y on the image of Φ ,
2. solve the linear system $\Phi\theta = \bar{y}$ which has a unique solution.



3.3.3 Numerical resolution

While the closed-form $\hat{\theta} = (\Phi^\top \Phi)^{-1} \Phi^\top y$ is convenient for analysis, inverting $\Phi^\top \Phi$ is sometimes unstable and has a large computational cost when d is large. The following methods are usually preferred.

QR factorization. The QR decomposition factorizes the matrix Φ as $\Phi = QR$ where $Q \in \mathbb{R}^{n \times d}$ has orthonormal columns and $R \in \mathbb{R}^{d \times d}$ is upper triangular (see [Golub and Loan, 1996](#)). Computing a QR decomposition is faster and more stable than inverting a matrix. We then have $\Phi^\top \Phi = R^\top R$, and R is thus the Cholesky factor of $\Phi^\top \Phi$. One then has

$$(\Phi^\top \Phi)\hat{\theta} = \Phi^\top y \Leftrightarrow R^\top Q^\top QR\hat{\theta} = R^\top Q^\top y \Leftrightarrow R^\top R\hat{\theta} = R^\top Q^\top y \Leftrightarrow R\hat{\theta} = Q^\top y.$$

It only remains to solve a triangular linear system, which is easy. The overall running time complexity remains $O(d^3)$. The conjugate gradient algorithm can also be used (see [Golub and Loan, 1996](#), for details).

Gradient descent. We can altogether bypass the need for matrix inversion or factorization using gradient descent. It consists in approximately minimizing $\hat{\mathcal{R}}$ by taking an initial point $\theta_0 \in \mathbb{R}^d$ and iteratively going towards the minimizer by following the opposite of the gradient

$$\theta_t = \theta_{t-1} - \gamma \hat{\mathcal{R}}'(\theta_{t-1}) \quad \text{for } t \geq 1,$$

where $\gamma > 0$ is the step-size. When these iterates converge, it is towards the OLS estimator since a fixed-point θ satisfies $\hat{\mathcal{R}}'(\theta) = 0$. We will study such algorithms in Chapter 5, with running-time complexities going down to linear in d .

3.4 Statistical analysis of OLS

We now prove guarantees on the performance of the OLS estimator. There are two settings of analysis for least-squares:

- *Random design.* In this setting, both the inputs and the outputs are random. This is the classical setting of supervised machine learning, where the goal is *generalization* to unseen data (as in the last chapter). Since it is a bit more complicated, it will be done after the fixed design setting.
- *Fixed design.* In this setting, we assume that the input data (x_1, \dots, x_n) are *not* random, and we are interested in obtaining a small prediction error *on those input points only*. Alternatively, this can be seen as a prediction problem where the input distribution p_x is the empirical distribution of (x_1, \dots, x_n) .

Our goal is thus to minimize the fixed design risk (where thus Φ is deterministic):

$$\mathcal{R}(\theta) = \mathbb{E}_y \left[\frac{1}{n} \sum_{i=1}^n (y_i - \varphi(x_i)^\top \theta)^2 \right] = \mathbb{E}_y \left[\frac{1}{n} \|y - \Phi\theta\|_2^2 \right]. \quad (3.3)$$

This assumption allows a complete analysis with basic linear algebra. It is justified in some settings, e.g., when the inputs are equally spaced along a fixed grid, but is otherwise just a simplifying assumption. It can also be understood as learning the optimal vector $\Phi\theta_* \in \mathbb{R}^n$ of best predictions instead of a function from \mathcal{X} to \mathbb{R} .

In the fixed design setting, no attempts are made to generalize to unseen input points $x \in \mathcal{X}$, and we want to estimate well a label vector y resampled from the same distribution as the observed y . The risk in Eq. (3.3) is often called the *in-sample prediction error*.

We will first consider below the fixed design setting, where the celebrated rate $\sigma^2 d/n$ will appear naturally.

Relationship to maximum likelihood estimation. If in the fixed design setting, we make the stronger assumption that the noise is Gaussian with mean zero and variance σ^2 , i.e., $\varepsilon_i = y_i - \varphi(x_i)^\top \theta_* \sim \mathcal{N}(0, \sigma^2)$, then the least mean-squares estimator of θ_* coincides with the maximum likelihood estimator (where Φ is assumed fixed). Indeed, the density/likelihood

of y is, using independence and the density of the normal distribution:

$$p(y|\theta, \sigma^2) = \prod_{i=1}^n \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{(y_i - \varphi(x_i)^\top \theta)^2}{2\sigma^2}\right).$$

Taking the logarithm and removing constants, the maximum likelihood estimator $(\tilde{\theta}, \tilde{\sigma}^2)$ minimizes

$$\frac{1}{2\sigma^2} \sum_{i=1}^n (y_i - \varphi(x_i)^\top \theta)^2 + \frac{n}{2} \log(\sigma^2).$$

We immediately see that $\tilde{\theta} = \hat{\theta}$, that is, OLS corresponds to maximum likelihood.

! While maximum likelihood under a Gaussian model provides an interesting interpretation, the Gaussian assumption is not needed for the forthcoming analysis.

Exercise 3.1 In the Gaussian model above, compute $\tilde{\sigma}^2$ the maximum likelihood estimator of σ^2 .

3.5 Fixed design setting

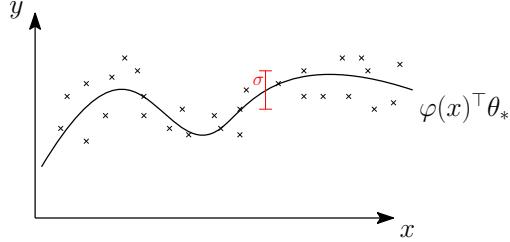
We now assume that Φ is deterministic, and as before, we assume that $\widehat{\Sigma} = \frac{1}{n}\Phi^\top\Phi$ is invertible. Any guarantee requires assumptions about how the data are generated. We assume that:

- There exists a vector $\theta_* \in \mathbb{R}^d$ such that the relationship between input and output is for $i \in \{1, \dots, n\}$

$$y_i = \varphi(x_i)^\top \theta_* + \varepsilon_i. \quad (3.4)$$

- All $\varepsilon_i, i \in \{1, \dots, n\}$, are independent of expectation $\mathbb{E}[\varepsilon_i] = 0$ and variance $\mathbb{E}[\varepsilon_i^2] = \sigma^2$.

The vector $\varepsilon \in \mathbb{R}^n$ accounts for variabilities in the output due to unobserved factors or noise. The “homoscedasticity” assumption above, where the noise variances are uniform, is made for simplicity (and allows for the later bound $\sigma^2 d/n$ to be an equality). Note that to prove upper-bounds in performance, we could also only assume that $\mathbb{E}[\varepsilon_i^2] \leq \sigma^2$ for each $i \in \{1, \dots, n\}$. The noise variance σ^2 is the expected squared error between the observations y_i and the model $\varphi(x_i)^\top \theta_*$.



⚠ In Eq. (3.4), we assume the model is *well-specified*, that is the target function is a linear function of $\varphi(x)$. In general, an additional approximation error is incurred because of a misspecified model (see Chapter 4).

Denoting by \mathcal{R}^* the minimum value of $\mathcal{R}(\theta) = \mathbb{E}_y \left[\frac{1}{n} \|y - \Phi\theta\|_2^2 \right]$ over \mathbb{R}^d , the following proposition shows that it is attained at θ_* , and that is equal to σ^2 .

Proposition 3.3 (Risk decomposition for OLS - fixed design) *Under the linear model and fixed design assumptions above, for any $\theta \in \mathbb{R}^d$, we have $\mathcal{R}^* = \sigma^2$ and*

$$\mathcal{R}(\theta) - \mathcal{R}^* = \|\theta - \theta_*\|_{\widehat{\Sigma}}^2,$$

where $\widehat{\Sigma} := \frac{1}{n} \Phi^\top \Phi$ is the input covariance matrix and $\|\theta\|_{\widehat{\Sigma}}^2 := \theta^\top \widehat{\Sigma} \theta$. If $\hat{\theta}$ is now a random variable (such as an estimator of θ_*), then

$$\mathbb{E}[\mathcal{R}(\hat{\theta})] - \mathcal{R}^* = \underbrace{\|\mathbb{E}[\hat{\theta}] - \theta_*\|_{\widehat{\Sigma}}^2}_{\text{Bias}} + \underbrace{\mathbb{E}\left[\|\hat{\theta} - \mathbb{E}[\hat{\theta}]\|_{\widehat{\Sigma}}^2\right]}_{\text{Variance}}.$$

Proof We have, using $y = \Phi\theta_* + \varepsilon$, with $\mathbb{E}[\varepsilon] = 0$ and $\mathbb{E}[\|\varepsilon\|_2^2] = n\sigma^2$:

$$\begin{aligned} \mathcal{R}(\theta) &= \mathbb{E}_y \left[\frac{1}{n} \|y - \Phi\theta\|_2^2 \right] = \mathbb{E}_\varepsilon \left[\frac{1}{n} \|\Phi\theta_* + \varepsilon - \Phi\theta\|_2^2 \right] \\ &= \frac{1}{n} \mathbb{E}_y \left[\|\Phi(\theta_* - \theta)\|_2^2 + \|\varepsilon\|_2^2 + 2[\Phi(\theta_* - \theta)]^\top \varepsilon \right] \\ &= \sigma^2 + \frac{1}{n} (\theta - \theta_*)^\top \Phi^\top \Phi (\theta - \theta_*). \end{aligned}$$

Since $\widehat{\Sigma} = \frac{1}{n} \Phi^\top \Phi$ is invertible, this shows that θ_* is the unique global minimizer of $\mathcal{R}(\theta)$, and that the minimum value \mathcal{R}^* is equal to σ^2 . This shows the first claim.

Now if θ is random, we perform the usual bias/variance decomposition:

$$\begin{aligned} \mathbb{E}[\mathcal{R}(\hat{\theta})] - \mathcal{R}^* &= \mathbb{E}\left[\|\hat{\theta} - \mathbb{E}[\hat{\theta}] + \mathbb{E}[\hat{\theta}] - \theta_*\|_{\widehat{\Sigma}}^2\right] \\ &= \mathbb{E}\left[\|\hat{\theta} - \mathbb{E}[\hat{\theta}]\|_{\widehat{\Sigma}}^2\right] + 2\mathbb{E}\left[(\hat{\theta} - \mathbb{E}[\hat{\theta}])^\top \widehat{\Sigma} (\mathbb{E}[\hat{\theta}] - \theta_*)\right] + \mathbb{E}\left[\|\mathbb{E}[\hat{\theta}] - \theta_*\|_{\widehat{\Sigma}}^2\right] \\ &= \mathbb{E}\left[\|\hat{\theta} - \mathbb{E}[\hat{\theta}]\|_{\widehat{\Sigma}}^2\right] + 0 + \|\mathbb{E}[\hat{\theta}] - \theta_*\|_{\widehat{\Sigma}}^2. \end{aligned}$$

(note that this is also a simple application of the law of total variance for vectors, that is, $\mathbb{E}\|z - a\|_M^2 = \|\mathbb{E}z - a\|_M^2 + \mathbb{E}\|z - \mathbb{E}[z]\|_M^2$ to $a = \theta_*$, $M = \widehat{\Sigma}$ and $z = \hat{\theta}$). ■

Note that the quantity $\|\cdot\|_{\widehat{\Sigma}}$ is called the Mahalanobis distance norm (it is a “true” norm whenever $\widehat{\Sigma}$ is positive definite). It is the norm on the parameter space induced by the input data.

3.5.1 Statistical properties of the OLS estimator

We can now analyze the properties of the OLS estimator, which has a closed form $\hat{\theta} = (\Phi^\top \Phi)^{-1} \Phi^\top y = \hat{\Sigma}^{-1} (\frac{1}{n} \Phi^\top y)$, with the model $y = \Phi \theta_* + \varepsilon$. The only randomness comes from ε , and we thus need to compute the expectation of linear and quadratic forms in ε .

Proposition 3.4 (Estimation properties of OLS) *The OLS estimator $\hat{\theta}$ has the following properties:*

1. it is unbiased, that is, $\mathbb{E}[\hat{\theta}] = \theta_*$,
2. its variance is $\text{var}(\hat{\theta}) = \mathbb{E}[(\hat{\theta} - \theta_*)(\hat{\theta} - \theta_*)^\top] = \frac{\sigma^2}{n} \hat{\Sigma}^{-1}$, where $\hat{\Sigma}^{-1}$ is often called the precision matrix.

Proof

1. Since $\mathbb{E}[y] = \Phi \theta_*$, we have directly $\mathbb{E}[\hat{\theta}] = (\Phi^\top \Phi)^{-1} \Phi^\top \Phi \theta_* = \theta_*$.
2. It follows that $\hat{\theta} - \theta_* = (\Phi^\top \Phi)^{-1} \Phi^\top (\Phi \theta_* + \varepsilon) - \theta_* = (\Phi^\top \Phi)^{-1} \Phi^\top \varepsilon$. Thus, using that $\mathbb{E}[\varepsilon \varepsilon^\top] = \sigma^2 I$, we get

$$\text{var}(\hat{\theta}) = \mathbb{E}[(\Phi^\top \Phi)^{-1} \Phi^\top \varepsilon \varepsilon^\top \Phi (\Phi^\top \Phi)^{-1}] = \sigma^2 (\Phi^\top \Phi)^{-1} (\Phi^\top \Phi) (\Phi^\top \Phi)^{-1} = \sigma^2 (\Phi^\top \Phi)^{-1},$$

which leads to the desired result $\frac{\sigma^2}{n} \hat{\Sigma}^{-1}$.

■

We can now put back the expression of the variance in the risk.

Proposition 3.5 (Risk of OLS) *The excess risk of the OLS estimator is equal to*

$$\mathbb{E}[\mathcal{R}(\hat{\theta})] - \mathcal{R}^* = \frac{\sigma^2 d}{n}. \quad (3.5)$$

Proof Note here that the expectation is over ε only as we are in the fixed design setting. Using the risk decomposition of Proposition 3.3 and the fact that $\mathbb{E}[\hat{\theta}] = \theta_*$, we have

$$\mathbb{E}[\mathcal{R}(\hat{\theta})] - \mathcal{R}^* = \mathbb{E}\|\hat{\theta} - \theta_*\|_{\hat{\Sigma}}^2.$$

We have: $\mathbb{E}[\mathcal{R}(\hat{\theta})] - \mathcal{R}^* = \text{tr}[\text{var}(\hat{\theta}) \hat{\Sigma}] = \text{tr}[\frac{\sigma^2}{n} \hat{\Sigma}^{-1} \hat{\Sigma}] = \frac{\sigma^2}{n} \text{tr}(I) = \frac{\sigma^2 d}{n}$.

We can also give a direct proof. Using the identity $\hat{\theta} - \theta_* = (\Phi^\top \Phi)^{-1} \Phi^\top \varepsilon$, we get

$$\begin{aligned}\mathbb{E}[\mathcal{R}(\hat{\theta})] - \mathcal{R}^* &= \mathbb{E}\|(\Phi^\top \Phi)^{-1} \Phi^\top \varepsilon\|_\Sigma^2 \\ &= \frac{1}{n} \mathbb{E}[\varepsilon^\top \Phi(\Phi^\top \Phi)^{-1} \Phi^\top \Phi(\Phi^\top \Phi)^{-1} \Phi^\top \varepsilon] = \frac{1}{n} \mathbb{E}[\varepsilon^\top \Phi(\Phi^\top \Phi)^{-1} \Phi^\top \varepsilon] \\ &= \frac{1}{n} \mathbb{E}[\varepsilon^\top P\varepsilon] = \frac{1}{n} \mathbb{E}[\text{tr}(P\varepsilon\varepsilon^\top)] = \frac{\sigma^2}{n} \text{tr}(P) = \frac{\sigma^2 d}{n},\end{aligned}$$

where we used that $P = \Phi(\Phi^\top \Phi)^{-1} \Phi^\top$ is the orthogonal projection on $\text{im}(\Phi)$, which is d -dimensional. ■

We can make the following observations:

- ! In the fixed design setting, the expectation over ε appears twice: (1) in the definition of the risk of some θ in Eq. (3.3), and when taking an expectation over the data in Eq. (3.5).

Exercise 3.2 Show that the expected empirical risk $\mathbb{E}[\hat{\mathcal{R}}(\hat{\theta})]$ is equal to $\mathbb{E}[\hat{\mathcal{R}}(\hat{\theta})] = \frac{n-d}{n} \sigma^2$. In particular, when $n > d$, deduce that an unbiased estimator of the noise variance σ^2 is given by $\frac{\|Y - \Phi\hat{\theta}\|_2^2}{n-d}$.

- In the exercise above, we have an expression of the expected training error, which is equal to $\frac{n-d}{n} \sigma^2 = \sigma^2 - \frac{d}{n} \sigma^2$, while the expected testing error is $\sigma^2 + \frac{d}{n} \sigma^2$. We thus see that in the context of least-squares, the training error underestimates (in expectation) the testing error by a factor of $2\sigma^2 d/n$, which characterizes the amount of overfitting. This difference can be used to perform model selection.³
- In the fixed design setting, OLS thus leads to unbiased estimation, with an excess risk of $\sigma^2 d/n$.
- On the positive side, the math is very simple, and as we will show in Section 3.7, the obtained convergence rate is optimal.
- On the negative side, for the excess risk being small compared to σ^2 , we need d/n to be small, which seems to exclude high-dimensional problems where d is close to n (let alone problems where $d > n$ or d much larger than n). Regularization (ridge in this chapter or with the ℓ_1 -norm in Chapter 8) will come to the rescue.
- This is only for the fixed design setting. We consider the random design setting below, which is a bit more involved mathematically, mostly because of the presence of $\hat{\Sigma}^{-1}$ which does not cancel anymore (leading to the term $\hat{\Sigma}^{-1} \Sigma$).

³See https://en.wikipedia.org/wiki/Mallows%27s_Cp.

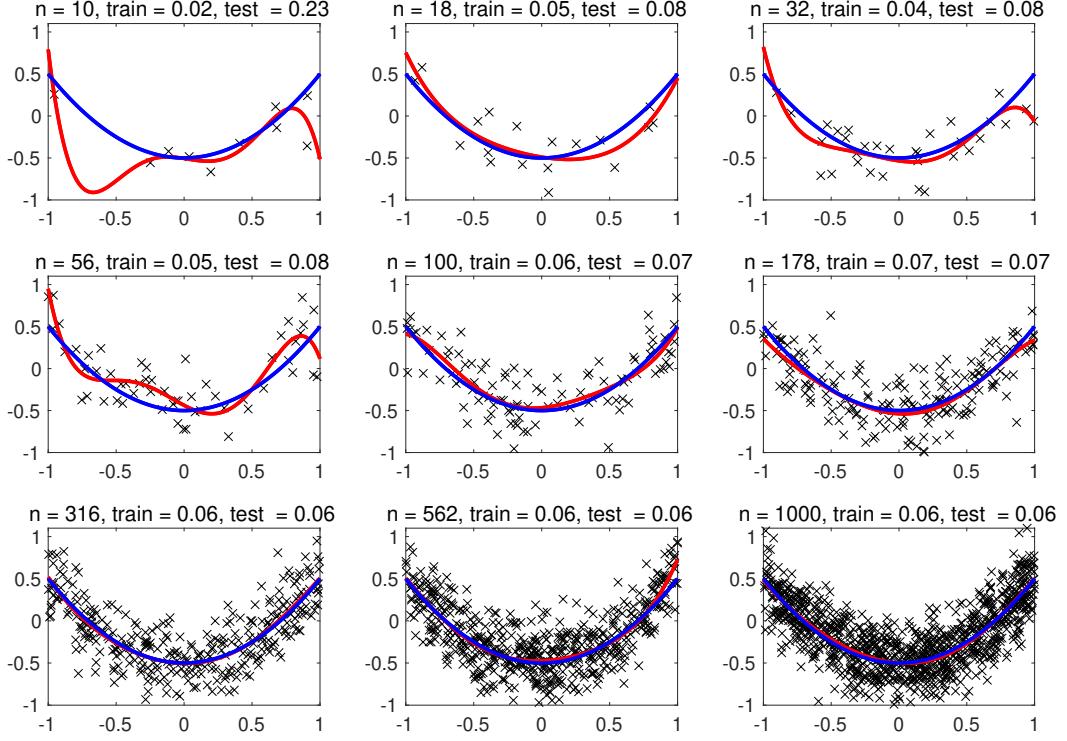


Figure 3.1: Polynomial regression with a varying number of observations. Blue: Optimal prediction, red: estimated prediction by ordinary least-squares with degree 5 polynomials.

Exercise 3.3 (general noise) We consider the fixed design regression model $y = \Phi\theta_* + \varepsilon$ with ε with zero mean and covariance matrix equal to C (not anymore $\sigma^2 I$). Show that the expected excess risk of the OLS estimator is equal to $\frac{1}{n} \text{tr} [\Phi(\Phi^\top \Phi)^{-1} \Phi^\top C]$.

Exercise 3.4 (♦) (multivariate regression) We consider $\mathcal{Y} = \mathbb{R}^k$ and the multivariate regression model $y = \theta_*^\top \varphi(x) + \varepsilon \in \mathbb{R}^k$, where $\theta_* \in \mathbb{R}^{d \times k}$, and ε has zero-mean with covariance matrix $C \in \mathbb{R}^{k \times k}$. In the fixed regression setting with design matrix $\Phi \in \mathbb{R}^{n \times d}$ and $Y \in \mathbb{R}^{n \times k}$ the matrix of responses, derive the OLS estimator and its excess risk.

3.5.2 Experiments

To illustrate the bound $\sigma^2 d/n$, we consider polynomial regression in one dimension, with $x \in \mathbb{R}$, $\varphi(x) = (1, x, x^2, \dots, x^k)^\top \in \mathbb{R}^{k+1}$, so $d = k + 1$. The inputs are sampled from the uniform distribution in $[-1, 1]$, while the optimal regression function is a degree 2 polynomial $f(x) = x^2 - \frac{1}{2}$ (blue curve in Figure 3.1). Gaussian noise with standard deviation $\frac{1}{4}$ is added to generate the outputs (black crosses). The ordinary least-squares estimator is plotted in red, for various values of n , from $n = 10$ to $n = 1000$, for $k = 5$.

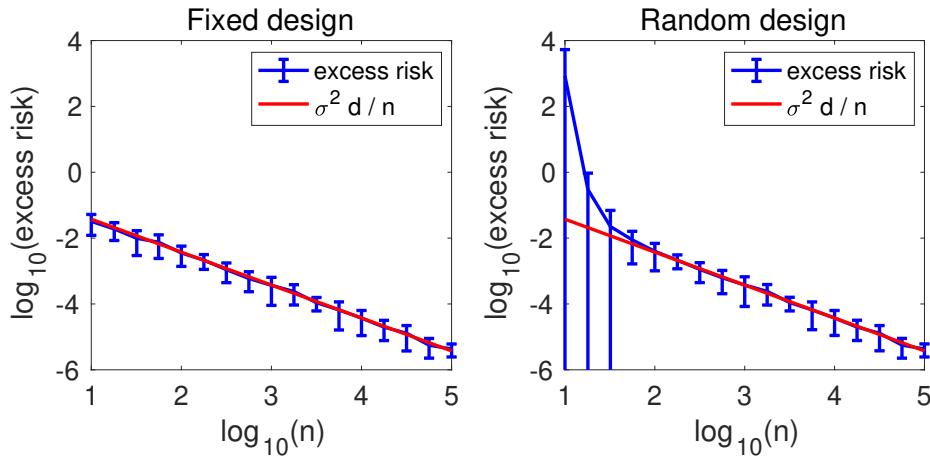


Figure 3.2: Convergence rate for polynomial regression with error bars (obtained from 32 replications by adding/subtracting standard deviations), plotted in logarithmic scale, with fixed design (left plot) and random design (right plot). The large error bars for small n in the right plot are due to the lower error bar being negative before taking the logarithm.

We can now plot in Figure 3.2 the expected excess risk as a function of n , estimated by 32 replications of the experiment, together with the bound. In the right plot, we consider the random design setting (generalization error, considered in Section 3.8), while in the left plot, we consider the fixed design setting (in-sample error). Notice the closeness of the bound for all n for the fixed design (as predicted by our bounds), while this is only valid for n large enough in the random design setting.

3.6 Ridge least-squares regression

Least-squares in high dimensions. When d/n approaches 1, we are essentially memorizing the observations y_i (that is, for example, when $d = n$ and Φ is a square invertible matrix, $\theta = \Phi^{-1}y$ leads to $y = \Phi\theta$, that is, ordinary least-squares will lead to a perfect fit, which is typically not good for generalization to unseen data, see more details in Chapter 11). Also, when $d > n$, then $\Phi^\top\Phi$ is not invertible, and the normal equations admit a linear subspace of solutions. These behaviors of OLS in high dimension (d large) are often undesirable.

Several solutions exist to fix these issues. The most common is to regularize the least-squares objective, either by adding an ℓ_1 -penalty $\|\theta\|_1$ to the empirical risk (leading to “*Lasso*” regression, see Chapter 8) or $\|\theta\|_2^2$ (leading to *ridge* regression, as done in this chapter and also in Chapter 7).

Definition 3.2 (Ridge least-squares regression) For a regularization parameter $\lambda > 0$, we define the ridge least-squares estimator $\hat{\theta}_\lambda$ as the minimizer of

$$\min_{\theta \in \mathbb{R}^d} \frac{1}{n} \|y - \Phi\theta\|_2^2 + \lambda \|\theta\|_2^2.$$

The ridge regression estimator can be obtained in closed form, and we do not require anymore $\Phi^\top \Phi$ to be invertible.

Proposition 3.6 We recall that $\hat{\Sigma} = \frac{1}{n} \Phi^\top \Phi \in \mathbb{R}^{d \times d}$. We have $\hat{\theta}_\lambda = \frac{1}{n} (\hat{\Sigma} + \lambda I)^{-1} \Phi^\top y$.

Proof As for the proof of Proposition 3.1, we can compute the gradient of the objective function, which is equal to $\frac{2}{n} (\Phi^\top \Phi \theta - \Phi^\top y) + 2\lambda\theta$. Setting it to zero leads to the estimator. Note that when $\lambda > 0$, the linear system always has a unique solution regardless of the invertibility of $\hat{\Sigma}$. \blacksquare

Exercise 3.5 Show that the estimator above can be written $\hat{\theta}_\lambda = (\Phi^\top \Phi + n\lambda I)^{-1} \Phi^\top y = \Phi^\top (\Phi \Phi^\top + n\lambda I)^{-1} y$. What could be the computational benefits?

As for the OLS estimator, we can analyze the statistical properties of this estimator under the linear model and fixed design assumptions. See Chapter 7 for an analysis of random design and potentially infinite-dimensional features.

Proposition 3.7 Under the linear model assumption (and for the fixed design setting), the ridge least-squares estimator $\hat{\theta}_\lambda = \frac{1}{n} (\hat{\Sigma} + \lambda I)^{-1} \Phi^\top y$ has the following excess risk

$$\mathbb{E}[\mathcal{R}(\hat{\theta}_\lambda)] - \mathcal{R}^* = \lambda^2 \theta_*^\top (\hat{\Sigma} + \lambda I)^{-2} \hat{\Sigma} \theta_* + \frac{\sigma^2}{n} \text{tr} [\hat{\Sigma}^2 (\hat{\Sigma} + \lambda I)^{-2}].$$

Proof We use the risk decomposition of Proposition 3.3 into a bias term B and a variance term V . Since we have $\mathbb{E}[\hat{\theta}_\lambda] = \frac{1}{n} (\hat{\Sigma} + \lambda I)^{-1} \Phi^\top \Phi \theta_* = (\hat{\Sigma} + \lambda I)^{-1} \hat{\Sigma} \theta_* = \theta_* - \lambda (\hat{\Sigma} + \lambda I)^{-1} \theta_*$, it follows

$$\begin{aligned} B &= \|\mathbb{E}[\hat{\theta}_\lambda] - \theta_*\|_{\hat{\Sigma}}^2 \\ &= \lambda^2 \theta_*^\top (\hat{\Sigma} + \lambda I)^{-2} \hat{\Sigma} \theta_*. \end{aligned}$$

For the variance term, using the fact that $\mathbb{E}[\varepsilon \varepsilon^\top] = \sigma^2 I$, we have

$$\begin{aligned} V &= \mathbb{E} \left[\|\hat{\theta}_\lambda - \mathbb{E}[\hat{\theta}_\lambda]\|_{\hat{\Sigma}}^2 \right] = \mathbb{E} \left[\left\| \frac{1}{n} (\hat{\Sigma} + \lambda I)^{-1} \Phi^\top \varepsilon \right\|_{\hat{\Sigma}}^2 \right] \\ &= \mathbb{E} \left[\frac{1}{n^2} \text{tr} \left(\varepsilon^\top \Phi (\hat{\Sigma} + \lambda I)^{-1} \hat{\Sigma} (\hat{\Sigma} + \lambda I)^{-1} \Phi^\top \varepsilon \right) \right] \\ &= \mathbb{E} \left[\frac{1}{n^2} \text{tr} \left(\Phi^\top \varepsilon \varepsilon^\top \Phi (\hat{\Sigma} + \lambda I)^{-1} \hat{\Sigma} (\hat{\Sigma} + \lambda I)^{-1} \right) \right] = \frac{\sigma^2}{n} \text{tr} \left(\hat{\Sigma} (\hat{\Sigma} + \lambda I)^{-1} \hat{\Sigma} (\hat{\Sigma} + \lambda I)^{-1} \right). \end{aligned}$$

The proposition follows by summing the bias and variance terms. ■

We can make the following observations:

- The result above is also a bias/variance decomposition with the bias term equal to $B = \lambda^2 \theta_*^\top (\widehat{\Sigma} + \lambda I)^{-2} \widehat{\Sigma} \theta_*$, and the variance term equal to $V = \frac{\sigma^2}{n} \text{tr} [\widehat{\Sigma}^2 (\widehat{\Sigma} + \lambda I)^{-2}]$. They are plotted in Figure 3.3.
- The bias term is increasing in λ and equal to zero for $\lambda = 0$ if $\widehat{\Sigma}$ is invertible, while when λ goes to infinity, the bias goes to $\theta_*^\top \widehat{\Sigma} \theta_*$. It is independent of n and plays the role of the approximation error in the risk decomposition.
- The variance term is decreasing in λ , and equal to $\sigma^2 d/n$ for $\lambda = 0$ if $\widehat{\Sigma}$ is invertible, and converging to zero when λ goes to infinity. It depends on n and plays the role of the estimation error in the risk decomposition.
- The quantity $\text{tr} [\widehat{\Sigma}^2 (\widehat{\Sigma} + \lambda I)^{-2}]$ is called the “degrees of freedom”, and is often considered as an implicit number of parameters. It can be expressed as $\sum_{j=1}^d \frac{\lambda_j^2}{(\lambda_j + \lambda)^2}$, where $(\lambda_j)_{j \in \{1, \dots, d\}}$ are the eigenvalues of $\widehat{\Sigma}$. This quantity will be very important in the analysis of kernel methods in Chapter 7.
- Observe how this converges to the OLS estimator (when defined) as $\lambda \rightarrow 0$.
- In most cases, $\lambda = 0$ is not the optimal choice, that is, biased estimation (with controlled bias) is preferable to unbiased estimation. In other words, the mean square error is minimized for a biased estimator.

3.6.1 Choice of λ

Based on the expression for the risk, we can tune the regularization parameter λ to obtain a potentially better bound than with the OLS (which corresponds to $\lambda = 0$ and the excess risk $\sigma^2 d/n$).

Proposition 3.8 (choice of regularization parameter) *With the choice $\lambda^* = \frac{\sigma \text{tr}(\widehat{\Sigma})^{1/2}}{\|\theta_*\|_2 \sqrt{n}}$, we have*

$$\mathbb{E}[\mathcal{R}(\hat{\theta}_{\lambda^*})] - \mathcal{R}^* \leq \frac{\sigma \text{tr}(\widehat{\Sigma})^{1/2} \|\theta_*\|_2}{\sqrt{n}}.$$

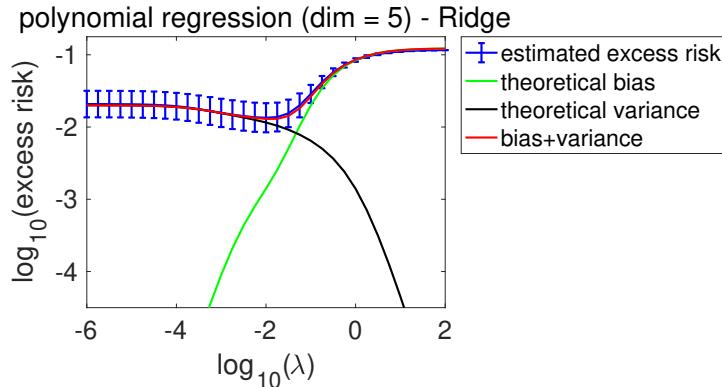


Figure 3.3: Polynomial regression (same set-up as Figure 3.2, with $n = 300$), with $k = 5$: bias/variance trade-offs for ridge regression as a function of λ . We can see the monotonicity of bias and variance with respect to λ and the presence of an optimal choice of λ .

Proof We have, using the fact that the eigenvalues of $(\widehat{\Sigma} + \lambda I)^{-2}\lambda\widehat{\Sigma}$ are less than $1/2$ (which is a simple consequence of $(\mu + \lambda)^{-2}\mu\lambda \leq 1/2 \Leftrightarrow (\mu + \lambda)^2 \geq 2\lambda\mu$ for all eigenvalues μ of $\widehat{\Sigma}$):

$$B = \lambda^2\theta_*^\top(\widehat{\Sigma} + \lambda I)^{-2}\widehat{\Sigma}\theta_* = \lambda\theta_*^\top(\widehat{\Sigma} + \lambda I)^{-2}\lambda\widehat{\Sigma}\theta_* \leq \frac{\lambda}{2}\|\theta_*\|_2^2.$$

Similarly, we have $V = \frac{\sigma^2}{n}\text{tr}[\widehat{\Sigma}^2(\widehat{\Sigma} + \lambda I)^{-2}] = \frac{\sigma^2}{\lambda n}\text{tr}[\widehat{\Sigma}\lambda\widehat{\Sigma}(\widehat{\Sigma} + \lambda I)^{-2}] \leq \frac{\sigma^2\text{tr}\widehat{\Sigma}}{2\lambda n}$. This leads to

$$\mathbb{E}[\mathcal{R}(\widehat{\theta}_{\lambda^*})] - \mathcal{R}^* \leq \frac{\lambda}{2}\|\theta_*\|_2^2 + \frac{\sigma^2\text{tr}\widehat{\Sigma}}{2\lambda n}. \quad (3.6)$$

Plugging in λ^* (which was chosen to minimize the upper bound on $B + V$) gives the result.⁴

■

We can make the following observations:

- If we write $R = \max_{i \in \{1, \dots, n\}} \|\varphi(x_i)\|_2$, then we have

$$\text{tr}(\widehat{\Sigma}) = \sum_{j=1}^d \widehat{\Sigma}_{jj} = \frac{1}{n} \sum_{i=1}^n \sum_{j=1}^d \varphi(x_i)_j^2 = \frac{1}{n} \sum_{i=1}^n \|\varphi(x_i)\|_2^2 \leq R^2.$$

Thus in the excess risk bound, the dimension d plays no explicit role and could even be infinite (given that R and $\|\theta_*\|_2$ remain finite). This type of bounds is called *dimension-free* bounds (see more details in Chapter 7).

 The number of parameters is not the only way to measure the generalization capabilities of a learning method.

⁴We have used the property that for any vector u , any symmetric matrix M , and any symmetric positive semi-definite matrix A , $u^\top Mu \leq \|u\|_2^2 \cdot \lambda_{\max}(M)$ and $\text{tr}(AM) \leq \text{tr}(A) \cdot \lambda_{\max}(M)$.

- Comparing this bound with that of the OLS estimator, we see that it converges slower to 0 as a function of n (from n^{-1} to $n^{-1/2}$), but it has a milder dependence on the noise (from σ^2 to σ). The presence of a “fast” rate in $O(n^{-1})$ with a potentially large constant and of a “slow” rate $O(n^{-1/2})$ with a smaller constant will appear several times in this book.



Depending on n and the constants, the “fast” rate result is not always the best.

- The value of λ^* involves quantities that we typically do not know in practice (such as σ and $\|\theta_*\|_2$). This is still useful to highlight the existence of some λ with good predictions (which can be found by cross-validation, as presented in Section 2.1).
- Note here that the choice of $\lambda^* = \frac{\sigma\sqrt{\text{tr}(\widehat{\Sigma})}}{\|\theta_*\|_2\sqrt{n}}$ is optimizing the *upper-bound* $\frac{\lambda}{2}\|\theta_*\|_2^2 + \frac{\sigma^2 \text{tr}(\widehat{\Sigma})}{2\lambda n}$, and is thus typically not optimal for the true expected risk.
- We can check the homogeneity of the various formula by a basic dimensional analysis. We use the bracket notation to denote the unit. Then $[\lambda] \times [\theta]^2 = [y^2] = [\sigma^2]$ since $\lambda\|\theta\|_2^2$ appears in the same objective function as y^2 (or σ^2). Moreover, we have $[y] = [\sigma] = [\varphi][\theta]$, leading to $[\lambda] = [\varphi]^2$. The value of λ suggested above has the dimension $\frac{[\varphi] \times [\sigma]}{[\theta]}$, which is indeed equal to $[\varphi]^2$. Similarly, we can check that the bias and variance terms have the correct dimensions.

Choosing λ in practice. The regularization λ is an example of a *hyper-parameter*. This term broadly refers to any quantity that influences the behavior of a machine learning algorithm, and that is left to choose by the practitioner. While theory often offers guidelines and qualitative understanding on best choosing the hyper-parameters, their precise numerical value depends on quantities that are often difficult to know or even guess. In practice, we typically resort to validation and cross-validation.

Exercise 3.6 Compute the expected risk of the estimators obtained by regularizing by $\theta^\top \Lambda \theta$ instead of $\lambda\|\theta\|_2^2$, where $\Lambda \in \mathbb{R}^{d \times d}$ is a positive definite matrix.

Exercise 3.7 (♦) We consider the leave-one-out estimator $\theta_\lambda^{-i} \in \mathbb{R}^d$ obtained, for each $i \in \{1, \dots, n\}$, by minimizing $\frac{1}{n} \sum_{j \neq i} (y_j - \theta^\top \varphi(x_j))^2 + \lambda\|\theta\|_2^2$. Given the matrix $H = \Phi(\Phi^\top \Phi + n\lambda I)^{-1} \Phi^\top \in \mathbb{R}^{n \times n}$, and its diagonal $h = \text{diag}(H) \in \mathbb{R}^n$, show that

$$\frac{1}{n} \sum_{i=1}^n (y_i - \varphi(x_i)^\top \theta_\lambda^{-i})^2 = \frac{1}{n} \|(I - \text{Diag}(h))^{-1} (I - H)^\top y\|_2^2.$$

3.7 Lower-bound (♦)

To show a lower bound in the fixed design setting, we will consider only Gaussian noise, that is, ε has a joint Gaussian distribution with mean zero and covariance matrix $\sigma^2 I$ (adding an extra assumption can only make the lower bound smaller). We follow the elegant and simple proof technique outlined by [Mourtada \(2019\)](#).

The only unknown in the model is the location of θ_* . To make the dependence on θ_* explicit, we denote by $\mathcal{R}_{\theta_*}(\theta)$ the excess risk (in the previous chapter, we were using the notation \mathcal{R}_p to make the dependence on the distribution p explicit), which is equal to

$$\mathcal{R}_{\theta_*}(\theta) = \|\theta - \theta_*\|_{\hat{\Sigma}}^2.$$

Our goal is to lower bound

$$\sup_{\theta_* \in \mathbb{R}^d} \mathbb{E}_{\varepsilon \sim \mathcal{N}(0, \sigma^2 I)} \mathcal{R}_{\theta_*}(\mathcal{A}(\Phi\theta_* + \varepsilon)),$$

over all functions \mathcal{A} from \mathbb{R}^n to \mathbb{R}^d (these functions are allowed to depend on the observed deterministic quantities such as Φ). Indeed, algorithms take $y = \Phi\theta_* + \varepsilon \in \mathbb{R}^n$ as an input and output a vector of parameters in \mathbb{R}^d .

The main idea, which is classical in the Bayesian analysis of learning algorithms, is to lower bound the supremum by the expectation with respect to some probability on θ_* , called the prior distribution in Bayesian statistics. That is, we have, for any algorithm/estimator \mathcal{A} :

$$\sup_{\theta_* \in \mathbb{R}^d} \mathbb{E}_{\varepsilon \sim \mathcal{N}(0, \sigma^2 I)} \mathcal{R}_{\theta_*}(\mathcal{A}(\Phi\theta_* + \varepsilon)) \geq \mathbb{E}_{\theta_* \sim \mathcal{N}(0, \frac{\sigma^2}{\lambda n} I)} \mathbb{E}_{\varepsilon \sim \mathcal{N}(0, \sigma^2 I)} \mathcal{R}_{\theta_*}(\mathcal{A}(\Phi\theta_* + \varepsilon)). \quad (3.7)$$

Here, we choose the normal distribution with mean 0 and covariance matrix $\frac{\sigma^2}{\lambda n} I$ as a prior distribution since this will lead to closed-form computations.

Using the expression of the excess risk (and ignoring the additive constant $\sigma^2 = \mathcal{R}^*$), we thus get the lower bound

$$\mathbb{E}_{\theta_* \sim \mathcal{N}(0, \frac{\sigma^2}{\lambda n} I)} \mathbb{E}_{\varepsilon \sim \mathcal{N}(0, \sigma^2 I)} \|\mathcal{A}(\Phi\theta_* + \varepsilon) - \theta_*\|_{\hat{\Sigma}}^2,$$

which we need to minimize with respect to \mathcal{A} . By making θ_* random, we now have a joint Gaussian distribution for (θ_*, ε) . The joint distribution of $(\theta_*, y) = (\theta_*, \Phi\theta_* + \varepsilon)$ is also Gaussian with mean zero and covariance matrix

$$\begin{pmatrix} \frac{\sigma^2}{\lambda n} I & \frac{\sigma^2}{\lambda n} \Phi^\top \\ \frac{\sigma^2}{\lambda n} \Phi & \frac{\sigma^2}{\lambda n} \Phi \Phi^\top + \sigma^2 I \end{pmatrix} = \frac{\sigma^2}{\lambda n} \begin{pmatrix} I & \Phi^\top \\ \Phi & \Phi \Phi^\top + n\lambda I \end{pmatrix}.$$

We need to perform an operation similar to computing the Bayes predictor in Chapter 2. This will be done by conditioning on y by writing

$$\begin{aligned} \mathbb{E}_{\theta_* \sim \mathcal{N}(0, \frac{\sigma^2}{\lambda n} I)} \mathbb{E}_{\varepsilon \sim \mathcal{N}(0, \sigma^2 I)} \|\mathcal{A}(\Phi\theta_* + \varepsilon) - \theta_*\|_{\hat{\Sigma}}^2 &= \mathbb{E}_{(\theta_*, y)} \|\mathcal{A}(y) - \theta_*\|_{\hat{\Sigma}}^2 \\ &= \int_{\mathbb{R}^n} \left(\int_{\mathbb{R}^d} \|\mathcal{A}(y) - \theta_*\|_{\hat{\Sigma}}^2 d\mu(\theta_* | y) \right) dp(y). \end{aligned}$$

Thus, for each y , the optimal $\mathcal{A}(y)$ has to minimize $\int_{\mathbb{R}^d} \|\mathcal{A}(y) - \theta_*\|_{\widehat{\Sigma}}^2 dp(\theta_*|y)$, which is exactly the posterior mean of θ_* given y . Indeed, the vector that minimizes the expected squared deviation is the expectation (exactly like when we computed the Bayes predictor for regression), here applied to the distribution $dp(\theta_*|y)$.

Since the joint distribution of (θ_*, y) is Gaussian with known parameters, we could use classical results about conditioning for Gaussian vectors (see Section 1.1.3). Still, we can also use the property that for Gaussian variables, the posterior mean given y is equal to the posterior mode given y , that is, it can be obtained by maximizing the log-likelihood $\log p(\theta_*, y)$ with respect to θ_* . Up to constants and using independence of ε and θ_* , this log-likelihood is

$$-\frac{1}{2\sigma^2}\|\varepsilon\|^2 - \frac{\lambda n}{2\sigma^2}\|\theta_*\|_2^2 = -\frac{1}{2\sigma^2}\|y - \Phi\theta_*\|^2 - \frac{\lambda n}{2\sigma^2}\|\theta_*\|_2^2,$$

which is exactly (up to a sign and a constant) the ridge regression cost function. Thus, we have $\mathcal{A}^*(y) = (\Phi^\top \Phi + n\lambda I)^{-1}\Phi^\top y$, which is exactly the ridge regression estimator $\hat{\theta}_\lambda$, and we can compute the corresponding optimal risk, to get:

$$\begin{aligned} & \inf_{\mathcal{A}} \sup_{\theta_* \in \mathbb{R}^d} \mathbb{E}_{\varepsilon \sim \mathcal{N}(0, \sigma^2 I)} \mathcal{R}_{\theta_*}(\mathcal{A}(\Phi\theta_* + \varepsilon)) - \mathcal{R}^* \\ & \geq \inf_{\mathcal{A}} \mathbb{E}_{\theta_* \sim \mathcal{N}(0, \frac{\sigma^2}{\lambda n} I)} \mathbb{E}_{\varepsilon \sim \mathcal{N}(0, \sigma^2 I)} \mathcal{R}_{\theta_*}(\mathcal{A}(\Phi\theta_* + \varepsilon)) - \mathcal{R}^* \text{ using Eq. (3.7),} \\ & = \mathbb{E}_{\theta_* \sim \mathcal{N}(0, \frac{\sigma^2}{\lambda n} I)} \mathbb{E}_{\varepsilon \sim \mathcal{N}(0, \sigma^2 I)} \mathcal{R}_{\theta_*}(\mathcal{A}^*(\Phi\theta_* + \varepsilon)) - \mathcal{R}^* \text{ using the reasoning above,} \\ & = \mathbb{E}_{\theta_* \sim \mathcal{N}(0, \frac{\sigma^2}{\lambda n} I)} \mathbb{E}_{\varepsilon \sim \mathcal{N}(0, \sigma^2 I)} \|\mathcal{A}^*(\Phi\theta_* + \varepsilon) - \theta_*\|_{\widehat{\Sigma}}^2 \text{ using the expression of the risk,} \\ & = \mathbb{E}_{\theta_* \sim \mathcal{N}(0, \frac{\sigma^2}{\lambda n} I)} \mathbb{E}_{\varepsilon \sim \mathcal{N}(0, \sigma^2 I)} \|(\Phi^\top \Phi + n\lambda I)^{-1}\Phi^\top(\Phi\theta_* + \varepsilon) - \theta_*\|_{\widehat{\Sigma}}^2 \text{ using the closed-form expression,} \\ & = \mathbb{E}_{\theta_* \sim \mathcal{N}(0, \frac{\sigma^2}{\lambda n} I)} \mathbb{E}_{\varepsilon \sim \mathcal{N}(0, \sigma^2 I)} \|(\Phi^\top \Phi + n\lambda I)^{-1}\Phi^\top\varepsilon - n\lambda(\Phi^\top \Phi + n\lambda I)^{-1}\theta_*\|_{\widehat{\Sigma}}^2 \\ & = \mathbb{E}_{\theta_* \sim \mathcal{N}(0, \frac{\sigma^2}{\lambda n} I)} \| -n\lambda(\Phi^\top \Phi + n\lambda I)^{-1}\theta_* \|_{\widehat{\Sigma}}^2 + \mathbb{E}_{\varepsilon \sim \mathcal{N}(0, \sigma^2 I)} \|(\Phi^\top \Phi + n\lambda I)^{-1}\Phi^\top\varepsilon\|_{\widehat{\Sigma}}^2 \text{ by independence,} \\ & = \frac{\sigma^2}{n\lambda}(n\lambda)^2 \frac{1}{n^2} \text{tr}[(\widehat{\Sigma} + \lambda I)^{-2}\widehat{\Sigma}] + \frac{\sigma^2}{n} \text{tr}(\widehat{\Sigma} + \lambda I)^{-2}\widehat{\Sigma}^2 \\ & = \frac{\sigma^2}{n} \text{tr}[(\widehat{\Sigma} + \lambda I)^{-1}\widehat{\Sigma}]. \end{aligned}$$

When Φ (and thus $\widehat{\Sigma}$) has full rank, this last expression tends to $\frac{\sigma^2}{n} \text{tr}(I) = \frac{\sigma^2 d}{n}$ when λ tends to zero (otherwise, it tends to $\frac{\sigma^2}{n} \text{rank}(\Phi)$). This such shows that

$$\inf_{\mathcal{A}} \sup_{\theta_* \in \mathbb{R}^d} \mathbb{E}_{\varepsilon \sim \mathcal{N}(0, \sigma^2 I)} \mathcal{R}_{\theta_*}(\mathcal{A}(\Phi\theta_* + \varepsilon)) \geq \frac{\sigma^2 d}{n}.$$

This gives us a lower bound on performance, which exactly matches the upper bound obtained by OLS. In the general non-least-squares case, such results are significantly harder to show. See more general lower bounds in Chapter 12.

3.8 Random design analysis

In this section, we consider the regular random design setting, that is, both x and y are considered random, and each pair (x_i, y_i) is assumed independent and identically distributed from a probability distribution p on $\mathcal{X} \times \mathbb{R}$. Our goal is to show that the bound on the excess risk we have shown for the fixed design setting, namely $\sigma^2 d/n$, is still valid. We will make the following assumptions regarding the joint distribution p , transposed from the fixed design setting to the random design setting:

- There exists a vector $\theta_* \in \mathbb{R}^d$ such that the relationship between input and output is for all i ,

$$y_i = \varphi(x_i)^\top \theta_* + \varepsilon_i.$$

- The noise distribution of $\varepsilon_i \in \mathbb{R}$ is independent from x_i , and $\mathbb{E}[\varepsilon_i] = 0$ and with variance $\mathbb{E}[\varepsilon_i^2] = \sigma^2$ (and is the same for all i , as observations are i.i.d.).

With the assumption above, $\mathbb{E}[y_i|x_i] = \varphi(x_i)^\top \theta_*$, and thus, we perform empirical risk minimization where our class of functions includes the Bayes predictor, a situation that is often referred to as the *well-specified* setting. The risk also has a simple expression:

Proposition 3.9 (Excess risk for random design least-squares regression) *Under the linear model above, for any $\theta \in \mathbb{R}^d$, the excess risk is equal to:*

$$\mathcal{R}(\theta) - \mathcal{R}^* = \|\theta - \theta_*\|_\Sigma^2,$$

where $\Sigma := \mathbb{E}[\varphi(x)\varphi(x)^\top]$ is the (non-centered) covariance matrix, and $\mathcal{R}^* = \sigma^2$.

Proof We have, for a pair (x_0, y_0) sampled from the same distribution as all (x_i, y_i) , $i = 1, \dots, n$, with ε_0 the corresponding noise variable:

$$\begin{aligned} \mathcal{R}(\theta) &= \mathbb{E}[(y_0 - \theta^\top \varphi(x_0))^2] = \mathbb{E}[(\varphi(x_0)^\top \theta_* + \varepsilon_0 - \theta^\top \varphi(x_0))^2] \\ &= \mathbb{E}[(\varphi(x_0)^\top \theta_* - \theta^\top \varphi(x_0))^2] + \mathbb{E}[\varepsilon_0^2] = (\theta - \theta_*)^\top \Sigma (\theta - \theta_*) + \sigma^2, \end{aligned}$$

which leads to the desired result. ■

Note that the only difference with the fixed design setting is the replacement of $\widehat{\Sigma}$ by Σ . We can now express the risk of the OLS estimator.

Proposition 3.10 *Under the linear model above, assuming $\widehat{\Sigma}$ is invertible, the expected excess risk of the OLS estimator is equal to*

$$\frac{\sigma^2}{n} \mathbb{E}[\text{tr}(\Sigma \widehat{\Sigma}^{-1})].$$

Proof Since the OLS estimator is equal to $\hat{\theta} = \frac{1}{n}\widehat{\Sigma}^{-1}\Phi^\top y = \frac{1}{n}\widehat{\Sigma}^{-1}\Phi^\top(\Phi\theta_* + \varepsilon) = \theta_* + \frac{1}{n}\widehat{\Sigma}^{-1}\Phi^\top\varepsilon$, we have:

$$\begin{aligned}\mathbb{E}[\mathcal{R}(\hat{\theta})] - \mathcal{R}^* &= \mathbb{E}\left[\left(\frac{1}{n}\widehat{\Sigma}^{-1}\Phi^\top\varepsilon\right)^\top\Sigma\left(\frac{1}{n}\widehat{\Sigma}^{-1}\Phi^\top\varepsilon\right)\right] \\ &= \mathbb{E}\left[\text{tr}\left(\Sigma\left(\frac{1}{n}\widehat{\Sigma}^{-1}\Phi^\top\varepsilon\right)\left(\frac{1}{n}\widehat{\Sigma}^{-1}\Phi^\top\varepsilon\right)^\top\right)\right] = \frac{1}{n^2}\mathbb{E}\left[\text{tr}\left(\Sigma\widehat{\Sigma}^{-1}\Phi^\top\varepsilon\varepsilon^\top\Phi\widehat{\Sigma}^{-1}\right)\right] \\ &= \frac{1}{n^2}\mathbb{E}\left[\text{tr}\left(\Sigma\widehat{\Sigma}^{-1}\Phi^\top\mathbb{E}[\varepsilon\varepsilon^\top]\Phi\widehat{\Sigma}^{-1}\right)\right] = \mathbb{E}\left[\frac{\sigma^2}{n^2}\text{tr}\left(\Sigma\widehat{\Sigma}^{-1}\Phi^\top\Phi\widehat{\Sigma}^{-1}\right)\right] \\ &= \mathbb{E}\left[\frac{\sigma^2}{n}\text{tr}(\Sigma\widehat{\Sigma}^{-1})\right].\end{aligned}$$

■

Thus, to compute the expected risk of the OLS estimator, we need to compute $\mathbb{E}[\text{tr}(\Sigma\widehat{\Sigma}^{-1})]$. One difficulty here is the potential non-invertibility of $\widehat{\Sigma}$. Under simple assumptions (e.g., $\varphi(x)$ has a density on \mathbb{R}^d), as soon as $n > d$, $\widehat{\Sigma}$ is almost surely invertible. However, its smallest eigenvalue can be very small. Additional assumptions are then needed to control it (see, e.g., [Mourtada, 2019](#), Section 3).

Exercise 3.8 Show that for the random design setting with the same assumptions as Prop. [3.10](#), the expected risk of the ridge regression estimator is

$$\mathbb{E}[\mathcal{R}(\hat{\theta}_\lambda) - \mathcal{R}^*] = \lambda^2\mathbb{E}\left[\theta_*^\top(\widehat{\Sigma} + \lambda I)^{-1}\Sigma(\widehat{\Sigma} + \lambda I)^{-1}\theta_* + \frac{\sigma^2}{n}\text{tr}\left[(\widehat{\Sigma} + \lambda I)^{-2}\widehat{\Sigma}\Sigma\right]\right].$$

3.8.1 Gaussian designs

If we assume that $\varphi(x)$ is normally distributed with mean 0 and covariance matrix Σ , then we can directly compute the desired expectation by first considering $z = \Sigma^{-1/2}\varphi(x)$, which has a standard normal distribution (that is, with mean zero and identity covariance matrix), with the corresponding normalized design matrix $Z \in \mathbb{R}^{n \times d}$, and compute $\mathbb{E}[\text{tr}(\Sigma\widehat{\Sigma}^{-1})] = n\mathbb{E}[\text{tr}(Z^\top Z)^{-1}]$.

Note that $\mathbb{E}[Z^\top Z] = nI$, and by convexity of the function $M \mapsto \text{tr}(M^{-1})$ on the cone of positive definite matrices, and using Jensen's inequality, we see that $\mathbb{E}[\text{tr}(Z^\top Z)^{-1}] \geq \frac{d}{n}$ (here we have not used the Gaussian assumption). However, this bound is in the wrong direction (this happens a lot with Jensen's inequality).

It turns out that for Gaussians, the matrix $(Z^\top Z)^{-1}$ has a specific distribution, called the inverse Wishart distribution⁵, with an expectation that can be computed exactly as

⁵See https://en.wikipedia.org/wiki/Inverse-Wishart_distribution.

$\mathbb{E}[(Z^\top Z)^{-1}] = \frac{1}{n-d-1}I$. Thus, we have: $\mathbb{E}[\text{tr}(Z^\top Z)^{-1}] = \frac{d}{n-d-1}$ if $n > d + 1$, thus leading to the expected excess risk of

$$\frac{\sigma^2 d}{n-d-1} = \frac{\sigma^2 d}{n} \frac{1}{1 - (d+1)/n}.$$

See [Breiman and Freedman \(1983\)](#) for further details. Note here that for Gaussian designs, the expected risk is precisely equal to the expression above and that later in this book, we will only consider upper bounds. See also a further analysis in Section [11.2.3](#).

Overall, we see that in the Gaussian case, we have an explicit non-asymptotic bound on the risk, which is equivalent to $\sigma^2 d/n$ when n goes to infinity.

3.8.2 General designs (♦♦)

In this last more technical section, we highlight how the Gaussian assumption can be avoided. The main idea is to show that with high probability, the lowest eigenvalue of $\Sigma^{-1/2}\widehat{\Sigma}\Sigma^{-1/2}$ is larger than some $1 - t$, for some $t \in (0, 1)$. Since the excess risk is $\frac{\sigma^2}{n} \text{tr}(\Sigma\widehat{\Sigma}^{-1})$, this immediately shows that with high probability, the excess risk is less than $\frac{\sigma^2 d}{n} \frac{1}{1-t}$.

To obtain such results, more refined concentration inequalities are needed, such as described by [Tropp \(2012\)](#), [Hsu et al. \(2012\)](#), [Oliveira \(2013\)](#), and [Lecué and Mendelson \(2016\)](#). The sharpest known results for least-squares regression are shown by [Mourtada \(2019\)](#).

Matrix concentration inequality. We will use the matrix Bernstein bound, adapted from [\(Tropp, 2012, Theorem 1.4\)](#), already discussed in Section [1.2.6](#) and recalled here.

Proposition 3.11 (Matrix Bernstein bound) *Given n independent symmetric matrices $M_i \in \mathbb{R}^{d \times d}$, such that for all $i \in \{1, \dots, n\}$, $\mathbb{E}[M_i] = 0$, $\lambda_{\max}(M_i) \leq b$ almost surely, for all $t \geq 0$, we have:*

$$\mathbb{P}\left(\lambda_{\max}\left(\frac{1}{n} \sum_{i=1}^n M_i\right) \geq t\right) \leq d \cdot \exp\left(-\frac{nt^2/2}{\tau^2 + bt/3}\right),$$

for $\tau^2 = \lambda_{\max}\left(\frac{1}{n} \sum_{i=1}^n \mathbb{E}[M_i^2]\right)$.

Application to re-scaled covariance matrices. We can now prove the following proposition that will give the desired high-probability bound for the excess risk with one extra assumption. Below, we will use the order between symmetric matrices, defined as $A \succ B \Leftrightarrow B \preccurlyeq A \Leftrightarrow A - B$ positive semi-definite.

Proposition 3.12 Given $\Sigma = \mathbb{E}[\varphi(x)\varphi(x)^\top] \in \mathbb{R}^{d \times d}$, and i.i.d. observations $\varphi(x_1), \dots, \varphi(x_n)$, assume that, for some $\rho > 0$,

$$\mathbb{E}\left[\varphi(x)^\top \Sigma^{-1} \varphi(x) \varphi(x) \varphi(x)^\top\right] \preceq \rho d \Sigma. \quad (3.8)$$

For $\delta \in (0, 1)$, if $n \geq 5\rho d \log \frac{d}{\delta}$, then with probability greater than $1 - \delta$,

$$\Sigma^{-1/2} \widehat{\Sigma} \Sigma^{-1/2} \succcurlyeq \frac{1}{4} I. \quad (3.9)$$

Before giving the proof, note that from the discussion earlier, the bound in Eq. (3.9) leads to an excess risk less than $\frac{\sigma^2 d}{n} \frac{1}{1-t} = 4 \frac{\sigma^2 d}{n}$ for $t = 3/4$. Moreover, without surprise, the bound is non-vacuous only for $n \geq d$. The extra assumption in Eq. (3.8) can be interpreted as follows. We consider the random vector $z = \Sigma^{-1/2} \varphi(x) \in \mathbb{R}^d$, which is such that $\mathbb{E}[zz^\top] = I$ and $\mathbb{E}[\|z\|_2^2] = d$. The assumption in Eq. (3.8) is then equivalent to

$$\lambda_{\max}\left(\mathbb{E}\left[\|z\|^2 zz^\top\right]\right) \leq \rho d.$$

A sufficient condition is that almost surely $\|z\|_2^2 \leq \rho d$, that is, $\varphi(x)^\top \Sigma^{-1} \varphi(x) \leq \rho d$. Moreover, for a Gaussian distribution with zero mean for z , one can check as an exercise that $\rho = (1 + 2/d)$. Similar results will be obtained for ridge regression in Chapter 7.

Proof We consider the random symmetric matrix $M_i = I - z_i z_i^\top$, which is such that $\mathbb{E}[M_i] = 0$, $\lambda_{\max}(M_i) \leq 1$ almost surely, and $\mathbb{E}[M_i^2] = \mathbb{E}[\|z_i\|^2 z_i z_i^\top] - I$ with largest eigenvalue less than ρd . We thus have for any $t \geq 0$, using Prop. 3.11:

$$\mathbb{P}\left(\lambda_{\max}(I - \frac{1}{n} Z^\top Z) \geq t\right) \leq d \cdot \exp\left(-\frac{nt^2/2}{\rho d + t/3}\right).$$

Thus, if t is such that $\frac{nt^2}{2\rho d + 2t/3} \geq \log \frac{d}{\delta}$, then, with probability greater than $1 - \delta$, we have $I - \Sigma^{-1/2} \widehat{\Sigma} \Sigma^{-1/2} \preceq tI$, that is, the desired result $\Sigma^{-1/2} \widehat{\Sigma} \Sigma^{-1/2} \succcurlyeq (1 - t)I$.

For $t = 3/4$, the condition becomes $n \geq (32\rho d/9 + 8/3) \log \frac{d}{\delta}$, which is implied by $n \geq 5\rho d \log \frac{d}{\delta}$ since we always $\rho \geq 1$. ■

Part II

Generalization bounds for learning algorithms

Chapter 4

Empirical risk minimization

Chapter summary

- Convexification of the risk: for binary classification, optimal predictions can be achieved with convex surrogates.
- Risk decomposition: the risk can be decomposed into the sum of the approximation error and the estimation error.
- Rademacher complexity: To study estimation errors and compute expected uniform deviations of real-valued outputs, Rademacher complexities are a very flexible and powerful tool that allows obtaining dimension-independent concentration inequalities.
- Relationship with asymptotic statistics: classical asymptotic results provide a finer picture of the behavior of empirical risk minimization as they provide asymptotic limits of performance as a well-defined constant times $1/n$, but they may not, in general, characterize small-sample effects.

As outlined in Chapter 2, given a joint distribution p on $\mathcal{X} \times \mathcal{Y}$, and n independent and identically distributed observations from p , our goal is to learn a function $f : \mathcal{X} \rightarrow \mathcal{Y}$ with minimum risk $\mathcal{R}(f) = \mathbb{E}[\ell(y, f(x))]$, or equivalently minimum expected excess risk:

$$\mathcal{R}(f) - \mathcal{R}^* = \mathcal{R}(f) - \inf_{g \text{ measurable}} \mathcal{R}(g).$$

In this chapter, we will consider methods based on empirical risk minimization. Before looking at the necessary probabilistic tools, we will first show how problems where the output space is not a vector space, such as binary classification with $\mathcal{Y} = \{-1, 1\}$, can be reformulated as real-valued outputs, with so-called “convex surrogates” of loss functions.

4.1 Convexification of the risk

In this section, for simplicity, we focus on binary classification where $\mathcal{Y} = \{-1, 1\}$ with the 0-1 loss, but many of the concepts extend to the more general structured prediction set-up (see Chapter 15).

As our goal is to estimate a binary-valued function, the first idea that comes into mind is to minimize the empirical risk over a hypothesis space of binary-valued functions f (or equivalently, the subsets of \mathcal{X} by considering the set $\{x \in \mathcal{X}, f(x) = 1\}$). However, this approach leads to a combinatorial problem that can be computationally intractable. Moreover, how to control the capacity (i.e., how to regularize) for these types of hypothesis spaces needs to be clarified. Learning a real-valued function instead through the framework of convex surrogates simplifies and overcomes this problem as it convexifies the problem. Classical penalty-based regularization techniques can then be used for theoretical analysis (this chapter) and algorithms (Chapter 5).

This choice of treating classification problems through real-valued prediction functions allows us to avoid introducing Vapnik-Chervonenkis dimensions (see [Vapnik and Chervonenkis, 2015](#)) to obtain general convergence results for empirical risk minimization in this chapter, where we will use the generic tool of Rademacher complexities in Section 4.5.

Instead of learning $f : \mathcal{X} \rightarrow \{-1, 1\}$, we will thus learn a function $g : \mathcal{X} \rightarrow \mathbb{R}$ and define $f(x) = \text{sign}(g(x))$ where

$$\text{sign}(a) = \begin{cases} 1 & \text{if } a > 0 \\ 0 & \text{if } a = 0 \\ -1 & \text{if } a < 0. \end{cases}$$

The convention $\text{sign}(0) = 0$ implies that the prediction can never be correct when $g(x) = 0$. Within our context, for maximally ambiguous observations, this corresponds to choosing none of the two labels (other conventions consider taking +1 or -1 uniformly at random).

The risk of the function $f = \text{sign} \circ g$, still denoted $\mathcal{R}(g)$ (! slight overloading $\mathcal{R}(g) = \mathcal{R}(\text{sign} \circ g)$), is then equal to:

$$\mathcal{R}(g) = \mathbb{P}(\text{sign}(g(x)) \neq y) = \mathbb{E}[1_{\text{sign}(g(x)) \neq y}] = \mathbb{E}[1_{yg(x) \leq 0}] = \mathbb{E}[\Phi_{0-1}(yg(x))],$$

where $\Phi_{0-1} : \mathbb{R} \rightarrow \mathbb{R}$, with $\Phi_{0-1}(u) = 1_{u \leq 0}$ is called the “margin-based” 0-1 loss function or simply the 0-1 loss function.

! Note the slightly overloaded notation above where the 0-1 loss function is defined on \mathbb{R} , compared to the 0-1 loss function from Chapter 2, which is defined on $\{-1, 1\} \times \{-1, 1\}$.

In practice, for empirical risk minimization, we then minimize with respect to $g : \mathcal{X} \rightarrow \mathbb{R}$ the corresponding empirical risk $\frac{1}{n} \sum_{i=1}^n \Phi_{0-1}(y_i g(x_i))$. The function Φ_{0-1} is not continuous (and thus also non-convex) and leads to difficult optimization problems.

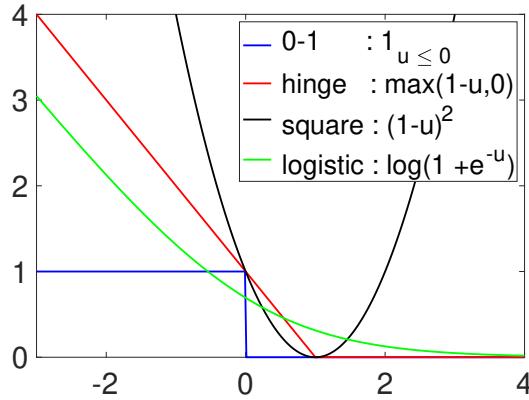


Figure 4.1: Classical convex surrogates for binary classification with the 0-1 loss.

4.1.1 Convex surrogates

A key concept in machine learning is the use of *convex surrogates*, where we replace Φ_{0-1} by another function Φ with better numerical properties (all will be convex). See classic examples below, plotted in Figure 4.1.

Instead of minimizing the classical risk $\mathcal{R}(g)$ or its empirical version, one then minimizes the Φ -risk (and its empirical version) defined as

$$\mathcal{R}_\Phi(g) = \mathbb{E}[\Phi(yg(x))].$$

In this context, the function g is sometimes called the *score function*.

The critical question we tackle in this section is: does it make sense to convexify the problem? In other words, does it lead to good predictions for the 0-1 loss?

Classical examples. We first review the primary examples used in practice:

- **Quadratic / square loss:** $\Phi(u) = (u - 1)^2$, leading to, since $y^2 = 1$: $\Phi(yg(x)) = (y - g(x))^2 = (g(x) - y)^2$. We get back least-squares, ignore that the labels have to belong to $\{-1, 1\}$, and take the sign of $g(x)$ for the prediction. Note the overpenalization for a large positive value of $yg(x)$ that will not be present for the other losses below (which are non-increasing).
- **Logistic loss:** $\Phi(u) = \log(1 + e^{-u})$, leading to

$$\Phi(yg(x)) = \log(1 + e^{-yg(x)}) = -\log\left(\frac{1}{1 + e^{-yg(x)}}\right) = -\log(\sigma(yg(x))),$$

where: $\sigma(v) = \frac{1}{1+e^{-v}}$ is the sigmoid function. Note the link with maximum likelihood estimation, where we define the model through

$$\mathbb{P}(y = 1|x) = \sigma(g(x)) \text{ and } \mathbb{P}(y = -1|x) = \sigma(-g(x)) = 1 - \sigma(g(x)).$$

The risk is then the negative conditional log-likelihood $\mathbb{E}[-\log p(y|x)]$. It is also often called the cross-entropy loss.¹ See more details about probabilistic methods in Chapter 14.

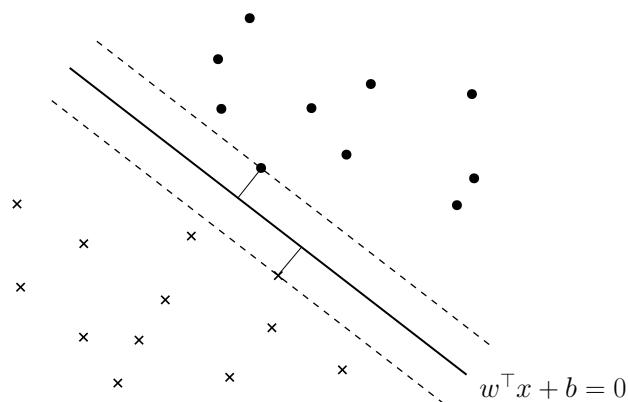
- **Hinge loss:** $\Phi(u) = \max(1 - u, 0)$. With linear predictors, this leads to the support vector machine, and $yf(x)$ is often called the “margin” in this context. This loss has a geometric interpretation (see Section 4.1.2 below).²
- **Squared hinge loss:** $\Phi(u) = \max(1 - u, 0)^2$. This is a smooth counterpart to the regular hinge loss.

In this section, we analyze precisely how replacing the 0-1 loss with convex surrogates still leads to optimal predictions. This allows us to only focus on *real-valued prediction functions* in the rest of this book. We will consider loss function $\ell(y, f(x))$ that will be the square loss $(y - f(x))^2$ for regression, and any of the ones above for binary classification, that is, $\Phi(yf(x))$. We will consider alternatives only in Chapter 15.

4.1.2 Geometric interpretation of the support vector machine (♦)

In this section, we provide a geometrical (and historical perspective) on the hinge loss to highlight why it leads to a learning architecture called the “support vector machine” (SVM). We consider n observations $(x_i, y_i) \in \mathbb{R}^d \times \{-1, 1\}$, for $i = 1, \dots, n$.

Separable data. We first assume that the data are separable by an affine hyperplane, that is, there exist $w \in \mathbb{R}^d$ and $b \in \mathbb{R}$ such that for all $i \in \{1, \dots, n\}$, $y_i(w^\top x_i + b) > 0$. Among the infinitely many separating hyperplanes, we aim to select the one for which the closest points from the dataset are the farthest.



¹See https://en.wikipedia.org/wiki/Logistic_regression for details.

²See also https://en.wikipedia.org/wiki/Support_vector_machine for details.

The distance from x_i to the hyperplane $\{x \in \mathbb{R}^d, w^\top x + b = 0\}$ is equal to $\frac{|w^\top x_i + b|}{\|w\|_2}$, and thus, this minimal distance is

$$\min_{i \in \{1, \dots, n\}} \frac{y_i(w^\top x_i + b)}{\|w\|_2},$$

and we thus aim at maximizing this quantity. Because of the invariance by rescaling (that is, we can multiply w and b by the same scalar constant without modifying the affine separator), this problem is equivalent to the following problem

$$\min_{w \in \mathbb{R}^d, b \in \mathbb{R}} \frac{1}{2} \|w\|_2^2 \text{ such that } \forall i \in \{1, \dots, n\}, y_i(w^\top x_i + b) \geq 1. \quad (4.1)$$

General data. When a hyperplane may not separate data, then we can introduce so-called “slack variables” $\xi_i \geq 0$, $i = 1, \dots, n$, allowing the constraint $y_i(w^\top x_i + b) \geq 1$ to be not satisfied, by introducing the constraint $y_i(w^\top x_i + b) \geq 1 - \xi_i$ instead. The overall amount of slack is then minimized, leading to the following problem (with $C > 0$):

$$\min_{w \in \mathbb{R}^d, b \in \mathbb{R}, \xi \in \mathbb{R}^n} \frac{1}{2} \|w\|_2^2 + C \sum_{i=1}^n \xi_i \text{ such that } \forall i \in \{1, \dots, n\}, y_i(w^\top x_i + b) \geq 1 - \xi_i \text{ and } \xi_i \geq 0. \quad (4.2)$$

With $\lambda = \frac{1}{nC}$, the problem above is equivalent to

$$\min_{w \in \mathbb{R}^d, b \in \mathbb{R}} \frac{1}{n} \sum_{i=1}^n (1 - y_i(w^\top x_i + b))_+ + \frac{\lambda}{2} \|w\|_2^2,$$

which is exactly an ℓ_2 -regularized empirical risk minimization with the hinge loss for the prediction function $f(x) = w^\top x + b$.

Lagrange dual and “support vectors” (\blacklozenge). The problem in Eq. (4.2) is a linearly constrained convex optimization problem and can be analyzed using Lagrangian duality (see, e.g., [Boyd and Vandenberghe, 2004](#)). We consider non-negative Lagrange multipliers α_i and β_i , $i \in \{1, \dots, n\}$, and the following Lagrangian:

$$\mathcal{L}(w, b, \xi, \alpha, \beta) = \frac{1}{2} \|w\|_2^2 + C \sum_{i=1}^n \xi_i - \sum_{i=1}^n \alpha_i (y_i(w^\top x_i + b) - 1 + \xi_i) - \sum_{i=1}^n \beta_i \xi_i.$$

Minimizing with respect to $\xi \in \mathbb{R}^n$ leads to the constraints $\forall i \in \{1, \dots, n\}$, $\alpha_i + \beta_i = C$, while minimizing with respect to b leads to the constraint $\sum_{i=1}^n y_i \alpha_i = 0$. Finally, minimizing with respect to w can be done in closed form as $w = \sum_{i=1}^n \alpha_i y_i x_i$. Overall, this leads to the dual optimization problem:

$$\max_{\alpha \in \mathbb{R}^n} \sum_{i=1}^n \alpha_i - \frac{1}{2} \sum_{i,j=1}^n \alpha_i \alpha_j y_i y_j x_i^\top x_j \text{ such that } \sum_{i=1}^n y_i \alpha_i = 0 \text{ and } \forall i \in \{1, \dots, n\}, \alpha_i \in [0, C]. \quad (4.3)$$

As we will show in Chapter 7 for all ℓ_2 -regularized learning problems with linear predictors, the optimization problem only depends on the dot-products $x_i^\top x_j$, $i, j = 1, \dots, n$, and the optimal predictor can be written as a linear combination of input data points x_i , $i = 1, \dots, n$. Moreover, for optimal primal and dual variables, the “complementary slackness” conditions for linear inequality constraints lead to $\alpha_i(y_i(w^\top x_i + b) - 1 + \xi_i) = 0$ and $(C - \alpha_i)\xi_i = 0$. This implies that $\alpha_i = 0$ as soon as $y_i(w^\top x_i + b) < 1$, and thus many of the α_i 's are equal to zero, and the optimal predictor is a linear combination of only a few of the data points x_i 's which are then called “support vectors”.

 The sparsity of the α_i 's does not directly justify the potential superiority of the hinge loss over other convex surrogates.

4.1.3 Conditional Φ -risk and classification calibration (♦)

Most of the convex surrogates are upper-bounds on the 0-1 loss, and all can be made so with rescaling. Using this as the sole justification for the good performance of a convex surrogate is a misleading justification, except for problems with almost surely zero loss for the Bayes (i.e., optimal) predictor (which is only possible when the Bayes risk is zero).

If we denote $\eta(x) = \mathbb{P}(y = 1|x) \in [0, 1]$, then we have, $\mathbb{E}[y|x] = 2\eta(x) - 1$, and, as seen in Chapter 2:

$$\mathcal{R}(g) = \mathbb{E}[\Phi_{0-1}(yg(x))] = \mathbb{E}[\mathbb{E}[1_{(g(x)) \neq y}|x]] \geq \mathbb{E}[\min(\eta(x), 1 - \eta(x))] = \mathcal{R}^*,$$

and one best classifier is $f^*(x) = \text{sign}(2\eta(x) - 1) = \text{sign}(\mathbb{E}[y|x])$. Note that there are **many** potential other functions $g(x)$ than $2\eta(x) - 1$ so that $f^*(x) = \text{sign}(g(x))$ is optimal. The first (minor) reason is the arbitrary choice of prediction for $\eta(x) = 1/2$. The other reason is that $g(x)$ has to have the same sign as $2\eta(x) - 1$, which leads to many possibilities beyond $2\eta(x) - 1$.

This section aims to ensure that the minimizers of the expected Φ -risk lead to optimal predictions.

Square loss. Before moving on to general functions Φ , the square loss leads to simple arguments. Indeed, as seen in Chapter 2, the function minimizing the expected Φ -risk is then $g(x) = \mathbb{E}(y|x) = 2\eta(x) - 1$, and taking its sign leads to the optimal prediction. Thus, using the square loss for binary classification leads to the optimal prediction in the population case.

General losses. To study the impact of using the Φ -risk, we first look at the conditional risk for a given x (as for the 0-1 loss, the function g that will minimize the Φ -risk can be determined by looking at each x separately).

Definition 4.1 (conditional Φ -risk) Let $g : \mathcal{X} \rightarrow \mathbb{R}$, we define the conditional Φ -risk as

$$\mathbb{E}[\Phi(yg(x))|x] = \eta(x)\Phi(g(x)) + (1 - \eta(x))\Phi(-g(x)) \text{ which we denote } C_{\eta(x)}(g(x)),$$

with $C_\eta(\alpha) = \eta\Phi(\alpha) + (1 - \eta)\Phi(-\alpha)$.

The least we can expect from a convex surrogate is that in the population case, where all x 's decouple, the optimal $g(x)$ obtained by minimizing the conditional Φ -risk exactly leads to the same prediction as the Bayes predictor (at least when this prediction is unique). In other words, since the prediction is $\text{sign}(g(x))$, we want that for any $\eta \in [0, 1]$:

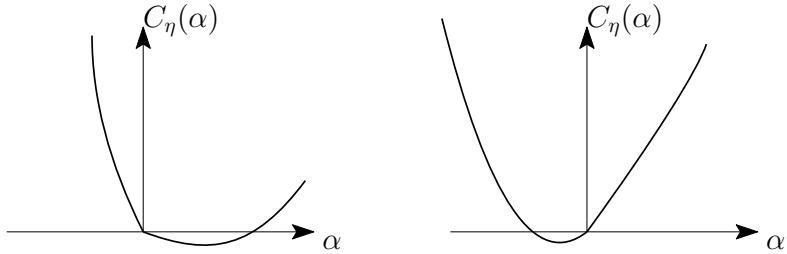
$$(\text{positive optimal prediction}) \quad \eta > 1/2 \Leftrightarrow \arg \min_{\alpha \in \mathbb{R}} C_\eta(\alpha) \subset \mathbb{R}_+^* \quad (4.4)$$

$$(\text{negative optimal prediction}) \quad \eta < 1/2 \Leftrightarrow \arg \min_{\alpha \in \mathbb{R}} C_\eta(\alpha) \subset \mathbb{R}_-^*. \quad (4.5)$$

A function Φ that satisfies these two statements is said *classification-calibrated*, or simply *calibrated*. It turns out that when Φ is convex, a simple sufficient and necessary condition is available:

Proposition 4.1 (Bartlett et al., 2006) let $\Phi : \mathbb{R} \rightarrow \mathbb{R}$ convex. The surrogate function Φ is classification-calibrated if and only if Φ is differentiable at 0 and $\Phi'(0) < 0$.

Proof Since Φ is convex, so is C_η for any $\eta \in [0, 1]$, and thus we simply consider left and right derivatives at zero to obtain conditions about the location of minimizers, with the two possibilities below (minimizer in \mathbb{R}_+^* if and only if the right derivative at zero is strictly negative, and minimizer in \mathbb{R}_-^* if and only if the left derivative at zero is strictly positive):



$$\arg \min_{\alpha \in \mathbb{R}} C_\eta(\alpha) \subset \mathbb{R}_+^* \Leftrightarrow (C_\eta)_+(0)' = \eta\Phi'_+(0) - (1 - \eta)\Phi'_-(0) < 0 \quad (4.6)$$

$$\arg \min_{\alpha \in \mathbb{R}} C_\eta(\alpha) \subset \mathbb{R}_-^* \Leftrightarrow (C_\eta)_-(0)' = \eta\Phi'_-(0) - (1 - \eta)\Phi'_+(0) > 0. \quad (4.7)$$

- (a) Assume Φ is calibrated. By letting η tend to $\frac{1}{2}+$ in Eq. (4.6), this leads to $(C_{1/2})_+(0)' = \frac{1}{2}[\Phi'_+(0) - \Phi'_-(0)] \leq 0$. Since Φ is convex, we always have $\Phi'_+(0) - \Phi'_-(0) \geq 0$. Thus the left and right derivatives are equal, which implies that Φ is differentiable at 0. Then $C'_\eta(0) = (2\eta - 1)\Phi'(0)$, and from Eq. (4.4) and Eq. (4.6), we need to have $\Phi'(0) < 0$.
- (b) Assume Φ is differentiable at 0 and $\Phi'(0) < 0$, then $C'_\eta(0) = (2\eta - 1)\Phi'(0)$; Eq. (4.4) and Eq. (4.5) are then direct consequences of Eq. (4.6) and Eq. (4.7).

■

Note that the proposition above excludes the convex surrogate $u \mapsto (-u)_+ = \max\{-u, 0\}$, which is not differentiable at zero, but that all examples from Section 4.1.1 are calibrated.

We now assume that Φ is classification-calibrated and convex, that is, Φ is convex, Φ differentiable at 0, and $\Phi'(0) < 0$.

4.1.4 Relationship between risk and Φ -risk (♦♦)

Now that we know that for any $x \in \mathcal{X}$, minimizing $C_{\eta(x)}(g(x))$ with respect to $g(x)$ leads to the optimal prediction through $\text{sign}(g(x))$, we would like to make sure that an explicit control of the excess Φ -risk (which we aim to do with empirical risk minimization using tools from later sections) leads to an explicit control of the original excess risk. In other words, we are looking for an increasing function $H : \mathbb{R}_+ \rightarrow \mathbb{R}_+$ such that $\mathcal{R}(g) - \mathcal{R}^* \leq H[\mathcal{R}_\Phi(g) - \mathcal{R}_\Phi^*]$, where \mathcal{R}_Φ^* is the minimum possible Φ -risk. The function H is often called the *calibration function*.

 As opposed to the least-squares regression case, where the loss function used for testing is directly the one used within empirical risk minimization, there are two notions here: the testing *error* $\mathcal{R}(g)$, which is obtained after thresholding at zero the function g , and the quantity $\mathcal{R}_\Phi(g)$, which is sometimes called the testing *loss*.

We first start with a simple lemma expressing the excess risk, as well as an upper bound (adapted from Theorem 2.2 from Devroye et al., 1996), that we will need for comparison inequalities below:

Lemma 4.1 *For any function $g : \mathcal{X} \rightarrow \mathbb{R}$, and for a Bayes predictor $g^* : \mathcal{X} \rightarrow \mathbb{R}$, we have:*

$$\mathcal{R}(g) - \mathcal{R}(g^*) = \mathbb{E}[1_{g(x)g^*(x)<0} \cdot |2\eta(x) - 1|].$$

Moreover, we have $\mathcal{R}(g) - \mathcal{R}(g^*) \leq \mathbb{E}[|2\eta(x) - 1 - g(x)|]$.

Proof We express the excess risk as:

$$\mathcal{R}(g) - \mathcal{R}(g^*) = \mathbb{E}[\mathbb{E}[1_{\text{sign}(g(x)) \neq y} - 1_{\text{sign}(g^*)(x) \neq y} | x]] \text{ by definition of the 0-1 loss.}$$

For any given $x \in \mathcal{X}$, we can look at the two possible cases for the signs of $\eta(x) - 1/2$ and $g(x)$ that lead to different predictions for g and g^* , namely (a) $\eta(x) > 1/2$ and $g(x) < 0$, and (b) $\eta(x) < 1/2$ and $g(x) > 0$ (equality cases are irrelevant). For the first case the expectation with respect to y is $\eta(x) - (1 - \eta(x)) = 2\eta(x) - 1$, while for the second case, we get $1 - 2\eta(x)$. By combining these two cases into the condition $g(x)g^*(x) < 0$ and the conditional expectation $|2\eta(x) - 1|$, we get the first result.

For the second result, we use the fact that if $g(x)g^*(x) < 0$, then, by splitting the cases in two (the first one being $\eta(x) > 1/2$ and $g(x) < 0$, the second one being $\eta(x) < 1/2$ and $g(x) > 0$), we get $|2\eta(x) - 1| \leq |2\eta(x) - 1 - g(x)|$, and thus the second result. ■

Note that for any function $b : \mathbb{R} \rightarrow \mathbb{R}$ that preserves the sign (that is $b(\mathbb{R}_+^*) \subset \mathbb{R}_+^*$ and $b(\mathbb{R}_-^*) \subset \mathbb{R}_-^*$), we have $\mathcal{R}(g) - \mathcal{R}(g^*) \leq \mathbb{E}[|2\eta(x) - 1 - b(g(x))|]$.

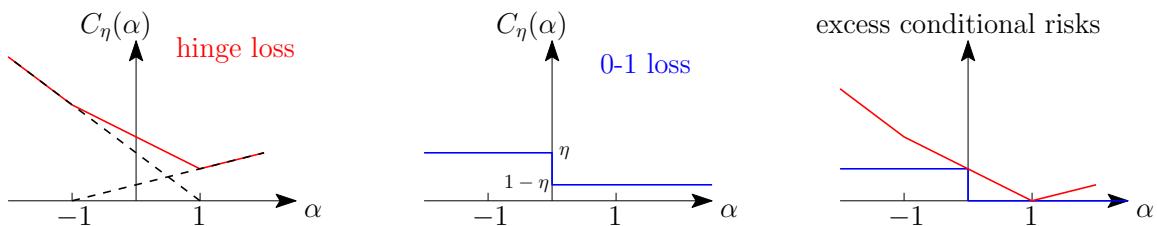
We see that the excess risk is the expectation of a quantity $|2\eta(x) - 1| \cdot 1_{g(x)g^*(x) < 0}$, which is equal to 0 if the classification through $g(x)$ is the same as the Bayes predictor and equal to $|2\eta(x) - 1|$ otherwise. The excess conditional Φ -risk is the quantity

$$\eta(x)\Phi(g(x)) + (1 - \eta(x))\Phi(-g(x)) - \inf_{\alpha} \{\eta(x)\Phi(\alpha) + (1 - \eta(x))\Phi(-\alpha)\},$$

which, as a function of $g(x)$, is the deviation between a convex function (of $g(x)$) and its minimum value. We simply need to relate it to the quantity $|2\eta(x) - 1| \cdot 1_{g(x)g^*(x) < 0}$ above for any $x \in \mathcal{X}$ and take expectations.

[Bartlett et al. \(2006\)](#) propose a general framework. We will only consider the hinge loss and smooth losses for simplicity (they already cover all cases from Section 4.1.1).

- For the hinge loss $\Phi(\alpha) = (1 - \alpha)_+ = \max\{1 - \alpha, 0\}$, we can easily compute the minimizer of the conditional Φ -risk (which leads to the minimizer of the Φ -risk). Indeed, we need to minimize $\eta(x)(1 - \alpha)_+ + (1 - \eta(x))(1 + \alpha)_+$, which is a piecewise affine function with kinks at -1 and 1 , with a minimizer attained at $u = 1$ for $\eta(x) > 1/2$ (see below), and symmetrically at $u = -1$ for $\eta(x) < 1/2$, with a minimum conditional Φ -risk equal to $2 \min\{1 - \eta(x), \eta(x)\}$. The two excess risks are plotted below for the hinge loss and the 0-1 loss, for $\eta(x) > 1/2$, showing pictorially that the conditional excess Φ -risk is greater than the excess risk.



This leads to the calibration function $H(\sigma) = \sigma$ for the hinge loss.

Note that when the Bayes risk is zero (but not in other cases), that is, $\eta(x) \in \{0, 1\}$ almost surely, then using the fact that the hinge loss is an upper-bound on the 0-1 loss is enough to show that the excess risk is less than the excess Φ -risk (indeed, the two optimal risks \mathcal{R}^* and \mathcal{R}_Φ^* are equal to zero).

- We consider smooth losses of the form (up to additive and multiplicative constants) $\Phi(v) = a(v) - v$, where $a(v) = \frac{1}{2}v^2$ for the quadratic loss, $a(v) = 2\log(e^{v/2} + e^{-v/2})$ for the logistic loss. We assume that a is even, $a(0) = 0$, a is β -smooth (that is, as defined in Chapter 5, $a''(v) \leq \beta$ for all $v \in \mathbb{R}$). This implies³ that for all $v \in \mathbb{R}$, $a(v) - \alpha v - \inf_{w \in \mathbb{R}} \{a(w) - \alpha w\} \geq \frac{1}{2\beta}|\alpha - a'(v)|^2$, leading to:

$$\begin{aligned}\mathcal{R}_\Phi(g) - \mathcal{R}_\Phi^* &= \mathbb{E}[a(g(x)) - (2\eta(x) - 1)g(x) - \inf_{w \in \mathbb{R}} \{a(w) - (2\eta(x) - 1)w\}] \\ &\geq \frac{1}{2\beta} \mathbb{E}[|2\eta(x) - 1 - a'(g(x))|^2] \text{ by the property above,} \\ &\geq \frac{1}{2\beta} (\mathbb{E}[|2\eta(x) - 1 - a'(g(x))|])^2 \text{ by Jensen's inequality,} \\ &\geq \frac{1}{2\beta} (\mathcal{R}(g) - \mathcal{R}^*)^2,\end{aligned}$$

using Lemma 4.1, and the fact that a' is sign-preserving (since $a'(0) = 0$). This leads to the calibration function $H(\sigma) = \sqrt{\sigma}$ for the square loss and $H(\sigma) = \sqrt{2\sigma}$ for the logistic loss.

Exercise 4.1 (♦) Show that the function a^* (the Fenchel conjugate of a) satisfies $a^*(\mathcal{R}(g) - \mathcal{R}^*) \leq \mathcal{R}_\Phi(g) - \mathcal{R}_\Phi^*$ for any function $g : \mathcal{X} \rightarrow \mathbb{R}$.

We can make the following observations:

- For the (non-smooth) hinge loss, the calibration function is identity, so if the excess Φ -risk goes to zero at a specific rate, the excess risk goes to zero at the same rate. In contrast, for smooth losses, the upper bound only ensures a (worse) rate with a square root. Therefore, when going from the excess Φ -risk to the excess risk, that is, after thresholding the function g at zero, the observed rates may be worse. However, as shown in Chapter 5, smooth losses can be easier to optimize. There is thus a trade-off between these two types of losses.

³Using the Fenchel conjugate $a^* : \mathbb{R} \rightarrow \mathbb{R}$ which is $1/(2\beta)$ -strongly convex (see Chapter 5), we have: $a(v) - \alpha v - \inf_{w \in \mathbb{R}} \{a(w) - \alpha w\} = a(v) - \alpha v + a^*(\alpha) = a^*(\alpha) - a^*(a'(v)) - (\alpha - a'(v))(a^*)'(a'(v)) \geq \frac{1}{2\beta}|\alpha - a'(v)|^2$, where a^* is the Fenchel conjugate of a (Boyd and Vandenberghe, 2004).

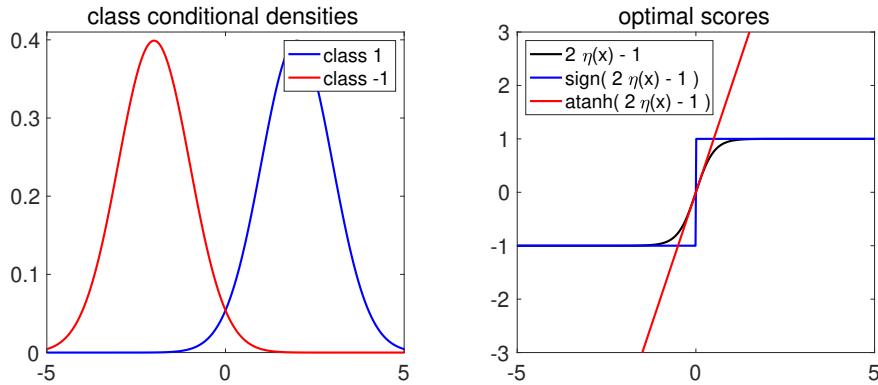


Figure 4.2: Optimal score functions for Gaussian class-conditional densities in one dimension. Left: conditional densities, right: optimal score functions for the square loss ($g^*(x) = 2\eta(x) - 1$), the hinge loss ($g^*(x) = \text{sign}(2\eta(x) - 1)$) and the logistic loss ($g^*(x) = \text{atanh}(2\eta(x) - 1)$).

- Note that the noiseless case where $\eta(x) \in \{0, 1\}$ (zero Bayes risk) leads to a stronger calibration function, as well as a series of intermediate “low-noise” conditions (see [Bartlett et al., 2006](#), for details, as well as the exercise below).

Exercise 4.2 (♦) Assume that $|2\eta(x) - 1| > \varepsilon$ almost surely, for some $\varepsilon \in (0, 1]$. Show that for any smooth convex classification calibrated function $\Phi : \mathbb{R} \rightarrow \mathbb{R}$ of the form $\Phi(v) = a(v) - v$ above, then we have for any function $g : \mathcal{X} \rightarrow \mathbb{R}$, $\mathcal{R}(g) - \mathcal{R}(g^*) \leq \frac{\varepsilon}{a^*(\varepsilon)} [\mathcal{R}_\Phi(g) - \mathcal{R}_\Phi^*]$.

Impact on approximation errors (♦). For the same classification problem, several convex surrogates can be used. While the Bayes classifier is always the same, that is, $f^*(x) = \text{sign}(2\eta(x) - 1)$, the minimizer of the testing Φ -risk will be different. For example, for the hinge loss, the minimizer $g(x)$ is exactly $\text{sign}(2\eta(x) - 1)$, while for losses of the form like above $\Phi(v) = a(v) - v$, we have $a'(g(x)) = 2\eta(x) - 1$, and thus for the square loss $g(x) = 2\eta(x) - 1$, while for the logistic loss, one can check that $g(x) = \text{atanh}(2\eta(x) - 1)$ (hyperbolic arc tangent). See examples in Figure 4.2, with $\mathcal{X} = \mathbb{R}$ and Gaussian class conditional densities.

The choice of surrogates will have an impact since to attain the minimal Φ -risk, different assumptions are needed on the class of functions used for empirical risk minimization, that is, $\text{sign}(2\eta(x) - 1)$ has to be in the class of functions we use (for the hinge loss), or $2\eta(x) - 1$ for the square loss, or $\text{atanh}(2\eta(x) - 1)$ for the logistic loss.

Exercise 4.3 For the logistic loss, show that for data generated with class-conditional densities of $x|y = 1$ and $x|y = -1$, which are Gaussians with the same covariance matrix, the function $g(x)$ minimizing the expected logistic loss is affine in x (this model is often referred to as linear discriminant analysis). Provides an extension to the multi-class setting.

4.2 Risk minimization decomposition

We consider a family \mathcal{F} of prediction functions $f : \mathcal{X} \rightarrow \mathcal{Y}$. Empirical risk minimization aims to find

$$\hat{f} \in \arg \min_{f \in \mathcal{F}} \widehat{\mathcal{R}}(f) = \frac{1}{n} \sum_{i=1}^n \ell(y_i, f(x_i)).$$

We can decompose the risk as follows into two terms:

$$\begin{aligned} \mathcal{R}(\hat{f}) - \mathcal{R}^* &= \left\{ \mathcal{R}(\hat{f}) - \inf_{f' \in \mathcal{F}} \mathcal{R}(f') \right\} + \left\{ \inf_{f' \in \mathcal{F}} \mathcal{R}(f') - \mathcal{R}^* \right\} \\ &= \text{estimation error} \quad + \text{approximation error}. \end{aligned}$$

A classic example is the situation where a subset of \mathbb{R}^d parameterizes the family of functions, that is, $\mathcal{F} = \{f_\theta, \theta \in \Theta\}$, for $\Theta \subset \mathbb{R}^d$. This includes neural networks (Chapter 9) and the simplest case of linear models of the form $f_\theta(x) = \theta^\top \varphi(x)$, for a particular feature vector $\varphi(x)$ (such as in Chapter 3). We will use linear models with Lipschitz-continuous loss functions as a motivating example, most often with constraints or penalties on the ℓ_2 -norm $\|\theta\|_2$, but other norms can be considered as well (such as the ℓ_1 -norm in Chapter 8).

We now turn separately to the approximation and estimation errors.

4.3 Approximation error

The approximation error $\inf_{f \in \mathcal{F}} \mathcal{R}(f) - \mathcal{R}^*$ is deterministic and depends on the underlying distribution, and the class \mathcal{F} of functions: the larger the class, the smaller the approximation error.

Bounding the approximation error requires assumptions on the Bayes predictor (sometimes also called the “target function”) f^* (and hence on the testing distribution) to achieve non-trivial learning rates.

In this section, we will focus on $\mathcal{F} = \{f_\theta, \theta \in \Theta\}$, for $\Theta \subset \mathbb{R}^d$ (we will consider infinite-dimensions in Chapter 7), and convex Lipschitz-continuous losses, assuming that θ_* is the minimizer of $\mathcal{R}(f_\theta)$ over $\theta \in \mathbb{R}^d$ (typically, θ_* does not belong to Θ). This implies that the approximation error decomposes into

$$\inf_{\theta \in \Theta} \mathcal{R}(f_\theta) - \mathcal{R}^* = \left(\inf_{\theta \in \Theta} \mathcal{R}(f_\theta) - \inf_{\theta \in \mathbb{R}^d} \mathcal{R}(f_\theta) \right) + \left(\inf_{\theta \in \mathbb{R}^d} \mathcal{R}(f_\theta) - \mathcal{R}^* \right).$$

- The second term $\inf_{\theta \in \mathbb{R}^d} \mathcal{R}(f_\theta) - \mathcal{R}^*$ is the incompressible approximation error coming from the chosen set of models f_θ .

- The function $\theta \mapsto \mathcal{R}(f_\theta) - \inf_{\theta \in \mathbb{R}^d} \mathcal{R}(f_\theta)$ is a positive function on \mathbb{R}^d , which can be typically upper bounded by a specific norm (or its square) $\Omega(\theta - \theta_*)$, and we can see the first term above $\inf_{\theta \in \Theta} \mathcal{R}(f_\theta) - \inf_{\theta \in \mathbb{R}^d} \mathcal{R}(f_\theta)$ as a “distance” between θ_* and Θ .

For example, if the loss which is considered is G -Lipschitz-continuous with respect to the second variable (which is possible for regression or when using a convex surrogate for binary classification as presented in Section 4.1), we have,

$$\mathcal{R}(f_\theta) - \mathcal{R}(f_{\theta'}) = \mathbb{E}[\ell(y, f_\theta(x)) - \ell(y, f_{\theta'}(x))] \leq G\mathbb{E}[|f_\theta(x) - f_{\theta'}(x)|],$$

and thus, this second part of the approximation error is upper bounded by G times the distance between f_{θ_*} and $\mathcal{F} = \{f_\theta, \theta \in \Theta\}$, for a particular pseudo-distance $d(\theta, \theta') = \mathbb{E}[|f_\theta(x) - f_{\theta'}(x)|]$.

A classical example will be $f_\theta(x) = \theta^\top \varphi(x)$, and $\Theta = \{\theta \in \mathbb{R}^d, \|\theta\|_2 \leq D\}$, leading to the upper bound

$$\inf_{\theta \in \Theta} \mathcal{R}(f_\theta) - \inf_{\theta \in \mathbb{R}^d} \mathcal{R}(f_\theta) \leq G \sup_{\|\theta\|_2 \leq D} \mathbb{E}[\|\varphi(x)\|_2] \cdot \|\theta - \theta_*\|_2 \leq G \mathbb{E}[\|\varphi(x)\|_2] (\|\theta_*\|_2 - D)_+,$$

which is equal to zero if $\|\theta_*\|_2 \leq D$ (well-specified model).

Exercise 4.4 Show that for $\Theta = \{\theta \in \mathbb{R}^d, \|\theta\|_1 \leq D\}$ (ℓ_1 -norm instead of the ℓ_2 -norm), we have

$$\inf_{\theta \in \Theta} \mathcal{R}(f_\theta) - \inf_{\theta \in \mathbb{R}^d} \mathcal{R}(f_\theta) \leq G \mathbb{E}[\|\varphi(x)\|_\infty] (\|\theta_*\|_1 - D)_+.$$

4.4 Estimation error

We will consider general techniques and apply them as illustrations to linear models with bounded ℓ_2 -norm by D and G -Lipschitz-losses. See further applications in Chapter 7 and Chapter 9.

The estimation error is often decomposed using $g_{\mathcal{F}} \in \arg \min_{g \in \mathcal{F}} \mathcal{R}(g)$ the minimizer of the expected risk for our class of models and $\hat{f} \in \arg \min_{f \in \mathcal{F}} \widehat{\mathcal{R}}(f)$ the minimizer of the empirical risk:

$$\begin{aligned} \mathcal{R}(\hat{f}) - \inf_{f \in \mathcal{F}} \mathcal{R}(f) &= \mathcal{R}(\hat{f}) - \mathcal{R}(g_{\mathcal{F}}) \\ &= \left\{ \mathcal{R}(\hat{f}) - \widehat{\mathcal{R}}(\hat{f}) \right\} + \left\{ \widehat{\mathcal{R}}(\hat{f}) - \widehat{\mathcal{R}}(g_{\mathcal{F}}) \right\} + \left\{ \widehat{\mathcal{R}}(g_{\mathcal{F}}) - \mathcal{R}(g_{\mathcal{F}}) \right\} \\ &\leq \sup_{f \in \mathcal{F}} \left\{ \mathcal{R}(f) - \widehat{\mathcal{R}}(f) \right\} + \left\{ \widehat{\mathcal{R}}(\hat{f}) - \widehat{\mathcal{R}}(g_{\mathcal{F}}) \right\} + \sup_{f \in \mathcal{F}} \left\{ \widehat{\mathcal{R}}(f) - \mathcal{R}(f) \right\} \\ &\leq \sup_{f \in \mathcal{F}} \left\{ \mathcal{R}(f) - \widehat{\mathcal{R}}(f) \right\} + 0 + \sup_{f \in \mathcal{F}} \left\{ \widehat{\mathcal{R}}(f) - \mathcal{R}(f) \right\} \text{ by definition of } \hat{f}. \quad (4.8) \end{aligned}$$

This is often further upper-bounded by $2 \sup_{f \in \mathcal{F}} |\widehat{\mathcal{R}}(f) - \mathcal{R}(f)|$. We can make the following observations:

- The key tool to remove the statistical dependence between $\widehat{\mathcal{R}}$ and \hat{f} is to take a uniform bound.
- When \hat{f} is not the global minimizer of $\widehat{\mathcal{R}}$ but satisfies $\widehat{\mathcal{R}}(\hat{f}) \leq \inf_{f \in \mathcal{F}} \widehat{\mathcal{R}}(f) + \varepsilon$, then the *optimization error* ε has to be added to the bound above (see more details in Chapter 5).
- The uniform deviation grows with the “size” of \mathcal{F} , is a random quantity (because of its dependence on data), and usually decays with n . See the examples below.
- A key issue is that we need a *uniform control* for all $f \in \mathcal{F}$: with a single f , we could apply any concentration inequality to the random variable $\ell(y, f(x))$ to obtain a bound in $O(1/\sqrt{n})$; however, when controlling the maximal deviations over many functions f , there is always a small chance that one of these deviations get large. We thus need explicit control of this phenomenon, which we now tackle by first showing that we can focus on the expectation alone.

4.4.1 Application of McDiarmid’s inequality

Let $H(z_1, \dots, z_n) = \sup_{f \in \mathcal{F}} \{ \mathcal{R}(f) - \widehat{\mathcal{R}}(f) \}$, where the random variables $z_i = (x_i, y_i)$ are independent and identically distributed, and $\widehat{\mathcal{R}}(f) = \frac{1}{n} \sum_{i=1}^n \ell(y_i, f(x_i))$. We let ℓ_∞ denote the maximal absolute value of the loss functions for all (x, y) in the support of the data generating distribution and $f \in \mathcal{F}$.

When changing a single $z_i \in \mathcal{X} \times \mathcal{Y}$ into $z'_i \in \mathcal{X} \times \mathcal{Y}$, the deviation in H is almost surely at most $\frac{2}{n} \ell_\infty$. Thus, applying McDiarmid’s inequality (see Section 1.2.2 in Chapter 1), with probability greater than $1 - \delta$, we have:

$$H(z_1, \dots, z_n) - \mathbb{E}[H(z_1, \dots, z_n)] \leq \frac{\ell_\infty \sqrt{2}}{\sqrt{n}} \sqrt{\log \frac{1}{\delta}}.$$

We thus only need to bound the expectation of $\sup_{f \in \mathcal{F}} \{ \mathcal{R}(f) - \widehat{\mathcal{R}}(f) \}$ and of $\sup_{f \in \mathcal{F}} \{ \widehat{\mathcal{R}}(f) - \mathcal{R}(f) \}$ (which will typically have the same bound), and add on top of it $\frac{\ell_\infty \sqrt{2}}{\sqrt{n}} \sqrt{\log \frac{2}{\delta}}$, to ensure a high-probability bound.

We now provide a series of bounds to bound these expectations, from simple to more refined, culminating in Rademacher complexities in Section 4.5.

4.4.2 Easy case I: quadratic functions

We will show what happens with a quadratic loss function and an ℓ_2 -ball constraint. We remember that in this case $\ell(y, \theta^\top \varphi(x)) = (y - \theta^\top \varphi(x))^2$. From that, we get

$$\begin{aligned}\widehat{\mathcal{R}}(f) - \mathcal{R}(f) &= \theta^\top \left(\frac{1}{n} \sum_{i=1}^n \varphi(x_i) \varphi(x_i)^\top - \mathbb{E}[\varphi(x) \varphi(x)^\top] \right) \theta \\ &\quad - 2\theta^\top \left(\frac{1}{n} \sum_{i=1}^n y_i \varphi(x_i) - \mathbb{E}[y \varphi(x)] \right) + \left(\frac{1}{n} \sum_{i=1}^n y_i^2 - \mathbb{E}[y^2] \right).\end{aligned}$$

Hence, the supremum can be upper-bounded in closed form as

$$\begin{aligned}\sup_{\|\theta\|_2 \leq D} |\mathcal{R}(f) - \widehat{\mathcal{R}}(f)| &\leq D^2 \left\| \frac{1}{n} \sum_{i=1}^n \varphi(x_i) \varphi(x_i)^\top - \mathbb{E}[\varphi(x) \varphi(x)^\top] \right\|_{\text{op}} \\ &\quad + 2D \left\| \frac{1}{n} \sum_{i=1}^n y_i \varphi(x_i) - \mathbb{E}[y \varphi(x)] \right\|_2 + \left| \frac{1}{n} \sum_{i=1}^n y_i^2 - \mathbb{E}[y^2] \right|,\end{aligned}$$

where $\|M\|_{\text{op}}$ is the operator norm of the matrix M defined as $\|M\|_{\text{op}} = \sup_{\|u\|_2=1} \|Mu\|_2$ (for which we have $|u^\top Mu| \leq \|M\|_{\text{op}} \|u\|_2^2$ for any vector u).

Thus, to get a uniform bound, we simply need to upper-bound the three *non-uniform* expectations of deviations, and therefore of order $O(1/\sqrt{n})$, and we get an overall uniform deviation bound. This case gives the impression that it should be possible to get such a rate in $O(1/\sqrt{n})$ for other types of losses than the quadratic loss. However, closed-form calculations are impossible, so we must introduce new tools.

Exercise 4.5 (♦) Provide an explicit bound on $\sup_{\|\theta\|_2 \leq D} |\mathcal{R}(f) - \widehat{\mathcal{R}}(f)|$ above, and compare it to the use of Rademacher complexities in Section 4.5. The concentration of averages of matrices from Section 1.2.6 can be used.



Note that from now on, in the sections below, unless otherwise stated, we do not require the loss to be convex.

4.4.3 Easy case II: Finite number of models

We assume in this section that the loss functions are bounded between 0 and ℓ_∞ , using the upper-bound $2 \sup_{f \in \mathcal{F}} |\widehat{\mathcal{R}}(f) - \mathcal{R}(f)|$ on the estimation error, and the union bound:

$$\mathbb{P}\left(\mathcal{R}(\hat{f}) - \inf_{f \in \mathcal{F}} \mathcal{R}(f) \geq t\right) \leq \mathbb{P}\left(2 \sup_{f \in \mathcal{F}} |\widehat{\mathcal{R}}(f) - \mathcal{R}(f)| \geq t\right) \leq \sum_{f \in \mathcal{F}} \mathbb{P}\left(2|\widehat{\mathcal{R}}(f) - \mathcal{R}(f)| \geq t\right).$$

We have, for $f \in \mathcal{F}$ fixed, $\widehat{\mathcal{R}}(f) = \frac{1}{n} \sum_{i=1}^n \ell(y_i, f(y_i))$, and we can apply Hoeffding's inequality from Section 1.2.1 to bound each $\mathbb{P}(2|\widehat{\mathcal{R}}(f) - \mathcal{R}(f)| \geq t)$, leading to

$$\mathbb{P}\left(\mathcal{R}(\hat{f}) - \inf_{f \in \mathcal{F}} \mathcal{R}(f) \geq t\right) \leq \sum_{f \in \mathcal{F}} 2 \exp(-2n(t/2)^2/\ell_\infty^2) = 2|\mathcal{F}| \exp(-nt^2/(2\ell_\infty^2)).$$

Thus, by setting $\delta = 2|\mathcal{F}| \exp(-nt^2/2\ell_\infty^2)$, and finding the corresponding t , with probability greater than $1 - \delta$, we get (using $\sqrt{a+b} \leq \sqrt{a} + \sqrt{b}$):

$$\begin{aligned} \mathcal{R}(\hat{f}) - \inf_{f \in \mathcal{F}} \mathcal{R}(f) &\leq t = \frac{\sqrt{2}\ell_\infty}{\sqrt{n}} \sqrt{\log \frac{2|\mathcal{F}|}{\delta}} = \frac{\sqrt{2}\ell_\infty}{\sqrt{n}} \sqrt{\log(|\mathcal{F}|) + \log \frac{2}{\delta}} \\ &\leq \sqrt{2}\ell_\infty \sqrt{\frac{\log(|\mathcal{F}|)}{n}} + \frac{\sqrt{2}\ell_\infty}{\sqrt{n}} \sqrt{\log \frac{2}{\delta}}. \end{aligned}$$

Exercise 4.6 (♦) In terms of expectation, show that (using the proof of the max of random variables from Section 1.2.4 in Chapter 2, which applies because bounded random variables are sub-Gaussian):

$$\mathbb{E}[\mathcal{R}(\hat{f}) - \inf_{f \in \mathcal{F}} \mathcal{R}(f)] \leq 2\mathbb{E}\left[\sup_{f \in \mathcal{F}} |\widehat{\mathcal{R}}(f) - \mathcal{R}(f)|\right] \leq \ell_\infty \sqrt{\frac{2 \log(|\mathcal{F}|)}{n}}.$$

Thus, according to the bound, learning is possible when the logarithm $\log(|\mathcal{F}|)$ of the number of models is small compared to n . This is the first generic control of uniform deviations.

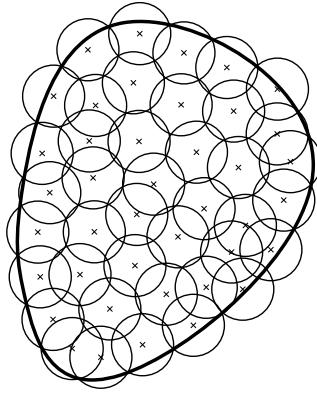
⚠ Note that this is only an upper bound, and learning is possible with infinitely many models (the most classical scenario). See below.

4.4.4 Beyond finite number models through covering numbers (♦)

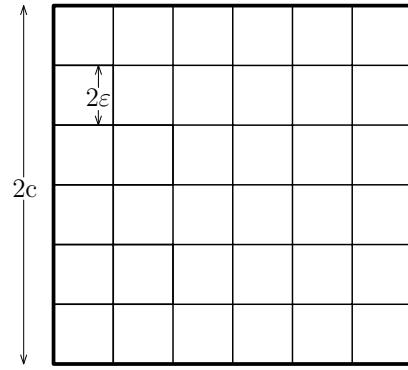
The simple idea behind covering numbers is to deal with function spaces with infinitely many elements by approximating them through a finite number of elements. This is often referred to as an “ ε -net argument.”

For simplicity, we assume that the loss functions are regular, for example, that they are G -Lipschitz-continuous with respect to their second argument.

Covering numbers. We assume there exists $m = m(\varepsilon)$ elements f_1, \dots, f_m such that for any $f \in \mathcal{F}$, $\exists i \in \{1, \dots, m\}$ such that $d(f, f_i) \leq \varepsilon$. The minimal possible number $m(\varepsilon)$ is the *covering number* of \mathcal{F} at precision ε . See an example below in two dimensions of a covering with Euclidean balls.



The covering number $m(\varepsilon)$ is a non-increasing function of ε . Typically, $m(\varepsilon)$ grows with ε as a power ε^{-d} when $\varepsilon \rightarrow 0$, where d is the underlying dimension. Indeed, for the ℓ_∞ -metric, if (in a certain parameterization) \mathcal{F} is included in a ball of radius c in the ℓ_∞ -ball of dimension d , it can be easily covered by $(c/\varepsilon)^d$ cubes of length 2ε . See below.



Given that all norms are equivalent in dimension d , we get the same dependence in ε^{-d} of $m(\varepsilon)$ for all bounded subsets of a finite-dimensional vector space, and thus $\log m(\varepsilon)$ grows as $d \log \frac{1}{\varepsilon}$, when ε tends to zero.

For some sets (e.g., all Lipschitz-continuous functions in d dimensions) $\log m(\varepsilon)$ grows faster, for example as ε^{-d} . See, e.g., [Wainwright \(2019\)](#).

ε -net argument. Given a cover of \mathcal{F} , for all $f \in \mathcal{F}$, and with $(f_i)_{i \in \{1, \dots, m(\varepsilon)\}}$ the associated cover elements,

$$\begin{aligned} |\widehat{\mathcal{R}}(f) - \mathcal{R}(f)| &\leqslant |\widehat{\mathcal{R}}(f) - \widehat{\mathcal{R}}(f_i)| + |\widehat{\mathcal{R}}(f_i) - \mathcal{R}(f_i)| + |\mathcal{R}(f_i) - \mathcal{R}(f)| \\ &\leqslant 2G\varepsilon + \sup_{i \in \{1, \dots, m(\varepsilon)\}} |\widehat{\mathcal{R}}(f_i) - \mathcal{R}(f_i)|. \end{aligned}$$

This implies that using bounds on the expectation of the maximum (Section 1.2.4), which apply because bounded random variables are sub-Gaussian (with the sub-Gaussianity pa-

parameter proportional to the almost sure bound):

$$\mathbb{E} \left[\sup_{f \in \mathcal{F}} |\widehat{\mathcal{R}}(f) - \mathcal{R}(f)| \right] \leq 2G\varepsilon + \mathbb{E} \left[\sup_{i \in \{1, \dots, m(\varepsilon)\}} |\widehat{\mathcal{R}}(f_i) - \mathcal{R}(f_i)| \right] \leq 2G\varepsilon + 2\ell_\infty \sqrt{\frac{2 \log(2m(\varepsilon))}{n}}.$$

Therefore, if $m(\varepsilon) \sim \varepsilon^{-d}$, ignoring constants, we need to balance $\varepsilon + \sqrt{d \log(1/\varepsilon)/n}$, which leads to, with a choice of ε proportional to $1/\sqrt{n}$, to a rate proportional to $\sqrt{(d/n) \log(n)}$, which shows that the dependence in n is also close to $1/\sqrt{n}$. Unfortunately, unless refined computations of covering numbers or more advanced tools (such as “chaining”) are used, this often leads to a non-optimal dependence on dimension and/or number of observations (see, e.g., [Wainwright, 2019](#), for examples of these refinements).

One powerful tool that allows sharp bounds at a reasonable cost is Rademacher complexities ([Boucheron et al., 2005](#)) or Gaussian complexities ([Bartlett and Mendelson, 2002](#)). In this chapter, we will focus on Rademacher complexity.

4.5 Rademacher complexity

We consider n independent and identically distributed random variables $z_1, \dots, z_n \in \mathcal{Z}$, and a class \mathcal{H} of functions from \mathcal{Z} to \mathbb{R} . In our context, the space of functions is related to the learning problem as: $z = (x, y)$, and $\mathcal{H} = \{(x, y) \mapsto \ell(y, f(x)), f \in \mathcal{F}\}$.

Our goal in this section is to provide an upper-bound on $\sup_{f \in \mathcal{F}} \{\mathcal{R}(f) - \widehat{\mathcal{R}}(f)\}$, which happens to be equal to

$$\sup_{h \in \mathcal{H}} \left\{ \mathbb{E}[h(z)] - \frac{1}{n} \sum_{i=1}^n h(z_i) \right\},$$

where $\mathbb{E}[h(z)]$ denotes the expectation with respect to a variable having the same distribution as all z_i 's.

We denote by $\mathcal{D} = \{z_1, \dots, z_n\}$ the data. We define the *Rademacher complexity* of the class of functions \mathcal{H} from \mathcal{Z} to \mathbb{R} :

$$R_n(\mathcal{H}) = \mathbb{E}_{\varepsilon, \mathcal{D}} \left(\sup_{h \in \mathcal{H}} \frac{1}{n} \sum_{i=1}^n \varepsilon_i h(z_i) \right), \quad (4.9)$$

where $\varepsilon \in \mathbb{R}^n$ is a vector of independent Rademacher random variable (that is, taking values -1 or 1 with equal probabilities), which is also independent of \mathcal{D} . It is a deterministic quantity that only depends on n and \mathcal{H} .

In words, the Rademacher complexity is equal to the expectation of the maximal dot-product between values of a function h at the observations z_i and random labels. It measures

the “capacity” of the set of functions \mathcal{H} . We will see later that it can be computed (or simply upper-bounded) in many interesting cases, leading to powerful bounds.

Exercise 4.7 Show the following properties of Rademacher complexities (see [Bartlett and Mendelson, 2002](#), for more details):

- (a) If $\mathcal{H} \subset \mathcal{H}'$, then $R_n(\mathcal{H}) \leq R_n(\mathcal{H}')$.
- (b) $R_n(\mathcal{H} + \mathcal{H}') \leq R_n(\mathcal{H}) + R_n(\mathcal{H}')$.
- (c) If $\alpha \in \mathbb{R}$, $R_n(\alpha\mathcal{H}) = |\alpha|R_n(\mathcal{H}')$.
- (d) $R_n(\mathcal{H}) = R_n(\text{convex hull}(\mathcal{H}))$.

4.5.1 Symmetrization

First, we relate the Rademacher complexity to the uniform deviation through a general “symmetrization” property, which shows that the Rademacher complexity directly controls the expected uniform deviation.

Proposition 4.2 (symmetrization) Given the Rademacher complexity of \mathcal{H} defined in Eq. (4.9), we have:

$$\mathbb{E}\left[\sup_{h \in \mathcal{H}} \left(\frac{1}{n} \sum_{i=1}^n h(z_i) - \mathbb{E}[h(z)] \right) \right] \leq 2R_n(\mathcal{H}) \quad \text{and} \quad \mathbb{E}\left[\sup_{h \in \mathcal{H}} \left(\mathbb{E}[h(z)] - \frac{1}{n} \sum_{i=1}^n h(z_i) \right) \right] \leq 2R_n(\mathcal{H}).$$

Proof (♦) Let $\mathcal{D}' = \{z'_1, \dots, z'_n\}$ be an independent copy of the data $\mathcal{D} = \{z_1, \dots, z_n\}$. Let $(\varepsilon_i)_{i \in \{1, \dots, n\}}$ be i.i.d. Rademacher random variables, which are also independent of \mathcal{D} and \mathcal{D}' . Using that for all i in $\{1, \dots, n\}$, $\mathbb{E}[h(z'_i)|\mathcal{D}] = \mathbb{E}[h(z_i)]$, we have:

$$\begin{aligned} \mathbb{E}\left[\sup_{h \in \mathcal{H}} \left(\mathbb{E}[h(z)] - \frac{1}{n} \sum_{i=1}^n h(z_i) \right) \right] &= \mathbb{E}\left[\sup_{h \in \mathcal{H}} \left(\frac{1}{n} \sum_{i=1}^n \mathbb{E}[h(z'_i)|\mathcal{D}] - \frac{1}{n} \sum_{i=1}^n h(z_i) \right) \right] \\ &= \mathbb{E}\left[\sup_{h \in \mathcal{H}} \left(\frac{1}{n} \sum_{i=1}^n \mathbb{E}[h(z'_i) - h(z_i)|\mathcal{D}] \right) \right] \end{aligned}$$

by definition of the independent copy \mathcal{D}' . Then

$$\mathbb{E}\left[\sup_{h \in \mathcal{H}} \left(\mathbb{E}[h(z)] - \frac{1}{n} \sum_{i=1}^n h(z_i) \right) \right] \leq \mathbb{E}\left[\mathbb{E}\left(\sup_{h \in \mathcal{H}} \left(\frac{1}{n} \sum_{i=1}^n [h(z'_i) - h(z_i)] \right) \middle| \mathcal{D} \right)\right],$$

using that the supremum of the expectation is less than the expectation of the supremum. Thus, by the tower law of expectation, we get

$$\mathbb{E} \left[\sup_{h \in \mathcal{H}} \left(\mathbb{E}[h(z)] - \frac{1}{n} \sum_{i=1}^n h(z_i) \right) \right] \leq \mathbb{E} \left[\sup_{h \in \mathcal{H}} \left(\frac{1}{n} \sum_{i=1}^n [h(z'_i) - h(z_i)] \right) \right].$$

We can now use the symmetry of the laws of ε_i and $h(z'_i) - h(z_i)$, to get:

$$\begin{aligned} & \mathbb{E} \left[\sup_{h \in \mathcal{H}} \left(\mathbb{E}[h(z)] - \frac{1}{n} \sum_{i=1}^n h(z_i) \right) \right] \\ & \leq \mathbb{E} \left[\sup_{h \in \mathcal{H}} \left(\frac{1}{n} \sum_{i=1}^n \varepsilon_i (h(z'_i) - h(z_i)) \right) \right] \\ & \leq \mathbb{E} \left[\sup_{h \in \mathcal{H}} \left(\frac{1}{n} \sum_{i=1}^n \varepsilon_i (h(z_i)) \right) \right] + \mathbb{E} \left[\sup_{h \in \mathcal{H}} \left(\frac{1}{n} \sum_{i=1}^n \varepsilon_i (-h(z_i)) \right) \right] \\ & = 2\mathbb{E} \left[\sup_{h \in \mathcal{H}} \left(\frac{1}{n} \sum_{i=1}^n \varepsilon_i h(z_i) \right) \right] = 2R_n(\mathcal{H}). \end{aligned}$$

The reasoning is essentially identical for $\mathbb{E} [\sup_{h \in \mathcal{H}} (\frac{1}{n} \sum_{i=1}^n h(z_i) - \mathbb{E}[h(z)])] \leq 2R_n(\mathcal{H})$. ■

Exercise 4.8 If \mathcal{H} is finite, and so that, for all $h \in \mathcal{H}$ and almost all z , $|h(z)| \leq \ell_\infty$, compute an upperbound on $R_n(\mathcal{H})$ and relate it to Section 4.4.3.

The lemma above only bounds the expectation of the deviation between the empirical average and the expectation by the Rademacher average. Together with concentration inequalities from Section 1.2, we can obtain high-probability bounds, as done in Section 4.4.1 with McDiarmid's inequality.

Exercise 4.9 (♦) The Gaussian complexity of a class of functions \mathcal{H} from \mathcal{Z} to \mathbb{R} is defined as $G_n(\mathcal{H}) = \mathbb{E}_{\varepsilon, \mathcal{D}} \left(\sup_{h \in \mathcal{H}} \frac{1}{n} \sum_{i=1}^n \varepsilon_i h(z_i) \right)$, where $\varepsilon \in \mathbb{R}^n$ is a vector of independent Gaussian variables with mean zero and variance one. Show that (a) $R_n(\mathcal{H}) \leq \sqrt{\frac{\pi}{2}} \cdot G_n(\mathcal{H})$ and (b) $G_n(\mathcal{H}) \leq 2\sqrt{\log n} \cdot R_n(\mathcal{H})$.

4.5.2 Lipschitz-continuous losses

A particularly appealing property in our context is the following property, sometimes called the “contraction principle,” using a simple proof from Meir and Zhang (2003, Lemma 5). See Prop. 4.4 below for a similar result for the Rademacher complexity defined with absolute values (and then with an extra factor of 2).

Proposition 4.3 (Contraction principle - Lipschitz-continuous functions) *Given any functions $b, a_i : \Theta \rightarrow \mathbb{R}$ (no assumption) and $\varphi_i : \mathbb{R} \rightarrow \mathbb{R}$ any 1-Lipschitz-functions, for $i = 1, \dots, n$, we have, for $\varepsilon \in \mathbb{R}^n$ a vector of independent Rademacher random variables:*

$$\mathbb{E}_\varepsilon \left[\sup_{\theta \in \Theta} \left\{ b(\theta) + \sum_{i=1}^n \varepsilon_i \varphi_i(a_i(\theta)) \right\} \right] \leq \mathbb{E}_\varepsilon \left[\sup_{\theta \in \Theta} \left\{ b(\theta) + \sum_{i=1}^n \varepsilon_i a_i(\theta) \right\} \right].$$

Proof (\blacklozenge) We consider a proof by induction on n . The case $n = 0$ is trivial, and we show how to go from $n \geq 0$ to $n + 1$. We thus consider $\mathbb{E}_{\varepsilon_1, \dots, \varepsilon_{n+1}} \left[\sup_{\theta \in \Theta} \left\{ b(\theta) + \sum_{i=1}^{n+1} \varepsilon_i \varphi_i(a_i(\theta)) \right\} \right]$ and compute the expectation with respect to ε_{n+1} explicitly, by considering the two potential values with probability 1/2:

$$\begin{aligned} & \mathbb{E}_{\varepsilon_1, \dots, \varepsilon_{n+1}} \left[\sup_{\theta \in \Theta} \left\{ b(\theta) + \sum_{i=1}^{n+1} \varepsilon_i \varphi_i(a_i(\theta)) \right\} \right] \\ &= \frac{1}{2} \mathbb{E}_{\varepsilon_1, \dots, \varepsilon_n} \left[\sup_{\theta \in \Theta} \left\{ b(\theta) + \sum_{i=1}^n \varepsilon_i \varphi_i(a_i(\theta)) + \varphi_{n+1}(a_{n+1}(\theta)) \right\} \right] \\ &\quad + \frac{1}{2} \mathbb{E}_{\varepsilon_1, \dots, \varepsilon_n} \left[\sup_{\theta \in \Theta} \left\{ b(\theta) + \sum_{i=1}^n \varepsilon_i \varphi_i(a_i(\theta)) - \varphi_{n+1}(a_{n+1}(\theta)) \right\} \right] \\ &= \mathbb{E}_{\varepsilon_1, \dots, \varepsilon_n} \left[\sup_{\theta, \theta' \in \Theta} \left\{ \frac{b(\theta) + b(\theta')}{2} + \sum_{i=1}^n \varepsilon_i \frac{\varphi_i(a_i(\theta)) + \varphi_i(a_i(\theta'))}{2} + \frac{\varphi_{n+1}(a_{n+1}(\theta)) - \varphi_{n+1}(a_{n+1}(\theta'))}{2} \right\} \right], \end{aligned}$$

by assembling the terms. By taking the supremum over (θ, θ') and (θ', θ) , we get

$$\begin{aligned} & \mathbb{E}_{\varepsilon_1, \dots, \varepsilon_n} \left[\sup_{\theta, \theta' \in \Theta} \left\{ \frac{b(\theta) + b(\theta')}{2} + \sum_{i=1}^n \varepsilon_i \frac{\varphi_i(a_i(\theta)) + \varphi_i(a_i(\theta'))}{2} + \frac{|\varphi_{n+1}(a_{n+1}(\theta)) - \varphi_{n+1}(a_{n+1}(\theta'))|}{2} \right\} \right] \\ &\leq \mathbb{E}_{\varepsilon_1, \dots, \varepsilon_n} \left[\sup_{\theta, \theta' \in \Theta} \left\{ \frac{b(\theta) + b(\theta')}{2} + \sum_{i=1}^n \varepsilon_i \frac{\varphi_i(a_i(\theta)) + \varphi_i(a_i(\theta'))}{2} + \frac{|a_{n+1}(\theta) - a_{n+1}(\theta')|}{2} \right\} \right], \end{aligned}$$

using Lipschitz-continuity. We can redo the same sequence of *equalities* with φ_{n+1} being the identity to obtain that the last expression above is equal to

$$\begin{aligned} & \mathbb{E}_{\varepsilon_1, \dots, \varepsilon_n} \mathbb{E}_{\varepsilon_{n+1}} \left[\sup_{\theta \in \Theta} \left\{ b(\theta) + \varepsilon_{n+1} a_{n+1}(\theta) + \sum_{i=1}^n \varepsilon_i \varphi_i(a_i(\theta)) \right\} \right] \\ &\leq \mathbb{E}_{\varepsilon_1, \dots, \varepsilon_n, \varepsilon_{n+1}} \left[\sup_{\theta \in \Theta} \left\{ b(\theta) + \varepsilon_{n+1} a_{n+1}(\theta) + \sum_{i=1}^n \varepsilon_i a_i(\theta) \right\} \right] \text{ by the induction hypothesis,} \end{aligned}$$

which leads to the desired result. ■

We can apply the contraction principle above to supervised learning situations where $u_i \mapsto \ell(y_i, u_i)$ is G -Lipschitz-continuous for all i almost surely (which is possible for regression or when using a convex surrogate for binary classification as presented in Section 4.1), leading to, by the contraction principle (applied conditioned on the data \mathcal{D}):

$$\mathbb{E}_\varepsilon \left(\sup_{f \in \mathcal{F}} \frac{1}{n} \sum_{i=1}^n \varepsilon_i \ell(y_i, f(x_i)) \mid \mathcal{D} \right) \leq G \cdot \mathbb{E}_\varepsilon \left(\sup_{f \in \mathcal{F}} \frac{1}{n} \sum_{i=1}^n \varepsilon_i f(x_i) \mid \mathcal{D} \right),$$

which leads to

$$R_n(\mathcal{H}) \leq G \cdot R_n(\mathcal{F}). \quad (4.10)$$

Thus the Rademacher complexity of the class of prediction functions controls the uniform deviations of the empirical risk. We consider below simple examples but give before without proof a contraction result that we will need in Section 9.2.3 (See proof by [Ledoux and Talagrand, 1991](#), Theorem 4.12).

Proposition 4.4 (Contraction principle - absolute values) *Given any functions $a_i : \Theta \rightarrow \mathbb{R}$ (no assumption) and $\varphi_i : \mathbb{R} \rightarrow \mathbb{R}$ any 1-Lipschitz-functions such that $\varphi_i(0) = 0$, for $i = 1, \dots, n$, we have, for $\varepsilon \in \mathbb{R}^n$ a vector of independent Rademacher random variables:*

$$\mathbb{E}_\varepsilon \left[\sup_{\theta \in \Theta} \left| \sum_{i=1}^n \varepsilon_i \varphi_i(a_i(\theta)) \right| \right] \leq 2 \mathbb{E}_\varepsilon \left[\sup_{\theta \in \Theta} \left| \sum_{i=1}^n \varepsilon_i a_i(\theta) \right| \right].$$

4.5.3 Ball-constrained linear predictions

We now assume that $\mathcal{F} = \{f_\theta(x) = \theta^\top \varphi(x), \Omega(\theta) \leq D\}$ where Ω is a norm on \mathbb{R}^d . We denote the design matrix by $\Phi \in \mathbb{R}^{n \times d}$. We have (with expectations both with respect to ε and the data):

$$\begin{aligned} R_n(\mathcal{F}) &= \mathbb{E} \left[\sup_{\Omega(\theta) \leq D} \left\{ \frac{1}{n} \sum_{i=1}^n \varepsilon_i \theta^\top \varphi(x_i) \right\} \right] = \mathbb{E} \left[\sup_{\Omega(\theta) \leq D} \frac{1}{n} \varepsilon^\top \Phi \theta \right] \\ &= \frac{D}{n} \mathbb{E} [\Omega^*(\Phi^\top \varepsilon)], \end{aligned}$$

where $\Omega^*(u) = \sup_{\Omega(\theta) \leq 1} u^\top \theta$ is the *dual norm* of Ω . For example, when Ω is the ℓ_p -norm, with $p \in [1, \infty]$, then Ω^* is the ℓ_q -norm, where q is such that $\frac{1}{p} + \frac{1}{q} = 1$, e.g., $\|\cdot\|_2^* = \|\cdot\|_2$, $\|\cdot\|_1^* = \|\cdot\|_\infty$, and $\|\cdot\|_\infty^* = \|\cdot\|_1$. For more details, see [Boyd and Vandenberghe \(2004\)](#).

Thus, computing Rademacher complexities is equivalent to computing expectations of norms. When $\Omega = \|\cdot\|_2$, we get:

$$\begin{aligned}
R_n(\mathcal{F}) &= \frac{D}{n} \mathbb{E} [\|\Phi^\top \varepsilon\|_2] \leq \frac{D}{n} \sqrt{\mathbb{E} [\|\Phi^\top \varepsilon\|_2^2]} \text{ by Jensen's inequality,} \\
&= \frac{D}{n} \sqrt{\mathbb{E} [\text{tr}[\Phi^\top \varepsilon \varepsilon^\top \Phi]]} = \frac{D}{n} \sqrt{\mathbb{E} [\text{tr}[\Phi^\top \Phi]]} \text{ using that } \mathbb{E}[\varepsilon \varepsilon^\top] = I, \\
&= \frac{D}{n} \sqrt{\sum_{i=1}^n \mathbb{E}(\Phi^\top \Phi)_i} = \frac{D}{n} \sqrt{\sum_{i=1}^n \mathbb{E}\|\varphi(x_i)\|_2^2} = \frac{D}{\sqrt{n}} \sqrt{\mathbb{E}\|\varphi(x)\|_2^2}. \tag{4.11}
\end{aligned}$$

We thus obtain a *dimension-independent* Rademacher complexity that we can use in the summary in Section 4.5.4 below.

Exercise 4.10 (ℓ_1 -norm) Assume that almost surely $\|\varphi(x)\|_\infty \leq R$. Show that the Rademacher complexity $R_n(\mathcal{F})$ for $\mathcal{F} = \{f_\theta(x) = \theta^\top \varphi(x), \Omega(\theta) \leq D\}$ with $\Omega = \|\cdot\|_1$ is upper-bounded by $RD\sqrt{\frac{2\log(2d)}{n}}$.

Exercise 4.11 (\spadesuit) Let $p > 1$, and q such that $1/p + 1/q = 1$. Assume that almost surely $\|\varphi(x)\|_q \leq R$. Show that the Rademacher complexity $R_n(\mathcal{F})$ for $\mathcal{F} = \{f_\theta(x) = \theta^\top \varphi(x), \Omega(\theta) \leq D\}$, with $\Omega = \|\cdot\|_p$, is upper-bounded by $\frac{RD}{\sqrt{n}} \frac{1}{\sqrt{p-1}}$ (hint: use Exercise 1.15). Recover the result of Exercise 4.10 by taking $p = 1 + \frac{1}{\log(2d)}$.

4.5.4 Putting things together (linear predictions)

With all the elements above, we can now propose the following general result (where no convexity of the loss function is assumed).

Proposition 4.5 (Estimation error) Assume a G -Lipschitz-continuous loss function, linear prediction functions with $\mathcal{F} = \{f_\theta(x) = \theta^\top \varphi(x), \|\theta\|_2 \leq D\}$, where $\mathbb{E}\|\varphi(x)\|_2^2 \leq R^2$. Let $\hat{f} = f_{\hat{\theta}} \in \mathcal{F}$ be the minimizer of the empirical risk, then:

$$\mathbb{E}[\mathcal{R}(f_{\hat{\theta}})] \leq \inf_{\|\theta\|_2 \leq D} \left\{ \mathcal{R}(f_\theta) + \frac{4GRD}{\sqrt{n}} \right\}.$$

Proof Using Prop. 4.2, Eq. (4.10) and Eq. (4.11), we get the desired result. Note that the factor of 4 comes from symmetrization (Prop. 4.2), and Eq. (4.8) in Section 4.4. ■

If we assume that there exists a minimizer θ_* of $\mathcal{R}(f_\theta)$ over \mathbb{R}^d , the approximation error

is upper-bounded by, following derivations from Section 4.3 (using Cauchy-Schwarz and Jensen's inequalities):

$$\begin{aligned}\inf_{\|\theta\|_2 \leq D} \mathcal{R}(f_\theta) - \mathcal{R}(f_{\theta_*}) &\leq G \inf_{\|\theta\|_2 \leq D} \mathbb{E}[|f_\theta(x) - f_{\theta_*}(x)|] \\ &= G \inf_{\|\theta\|_2 \leq D} \mathbb{E}[|\varphi(x)^\top (\theta - \theta_*)|] \\ &\leq G \inf_{\|\theta\|_2 \leq D} \|\theta - \theta_*\|_2 \mathbb{E}[\|\varphi(x)\|_2^2] \leq GR \inf_{\|\theta\|_2 \leq D} \|\theta - \theta_*\|_2.\end{aligned}$$

This leads to

$$\mathbb{E}[\mathcal{R}(f_\theta)] - \mathcal{R}(f_{\theta_*}) \leq GR \inf_{\|\theta\|_2 \leq D} \|\theta - \theta_*\|_2 + \frac{4GRD}{\sqrt{n}} = GR(\|\theta_*\|_2 - D)_+ + \frac{4GRD}{\sqrt{n}}.$$

We see that for $D = \|\theta_*\|_2$, we obtain the bound $\frac{4GR\|\theta_*\|_2}{\sqrt{n}}$, but this setting requires to know $\|\theta_*\|_2$ which is not possible in practice. If D is too large, the estimation error gets larger (overfitting). At the same time, if D is too small, the approximation error can quickly kick in (with a value that does not go to zero when n tends to infinity), leading to underfitting.

Exercise 4.12 We consider a learning problem with 1-Lipschitz-continuous loss (with respect to the second variable), with a function class $f_\theta(x) = \theta^\top \varphi(x)$, with $\|\theta\|_1 \leq D$, and $\varphi : \mathcal{X} \rightarrow \mathbb{R}^d$ with $\|\varphi(x)\|_\infty$ almost surely less than R . Given the expected risk $\mathcal{R}(f_\theta)$ and the empirical risk $\hat{\mathcal{R}}(f_\theta)$. Show that $\mathbb{E}[\mathcal{R}(f_{\hat{\theta}})] \leq \inf_{\|\theta\|_1 \leq D} \mathcal{R}(f_\theta) + 4RD\sqrt{\frac{2\log(2d)}{n}}$.

4.5.5 From constrained to regularized estimation (♦)

In practice, it is preferable to penalize by the norm $\Omega(\theta)$ instead of constraining. While the respective sets of solutions when letting the respective constraint and regularization parameters vary are the same, the main reason is that the hyperparameter is easier to find, and the optimization is typically easier. For simplicity, we only consider the ℓ_2 -norm in this section.

We now denote $\hat{\theta}_\lambda$ the minimizer of

$$\hat{\mathcal{R}}(f_\theta) + \frac{\lambda}{2} \|\theta\|_2^2. \tag{4.12}$$

If the loss is always positive, then $\frac{\lambda}{2} \|\hat{\theta}_\lambda\|_2^2 \leq \hat{\mathcal{R}}(f_{\hat{\theta}_\lambda}) + \frac{\lambda}{2} \|\hat{\theta}_\lambda\|_2^2 \leq \hat{\mathcal{R}}(f_0)$, leading to a bound $\|\hat{\theta}_\lambda\|_2 = O(1/\sqrt{\lambda})$. Thus, with $D = O(1/\sqrt{\lambda})$ in the bound above, this leads to a deviation of $O(1/\sqrt{\lambda n})$, which is not optimal.

We now give an interesting stronger result using the strong convexity of the squared ℓ_2 -norm (with now a convex loss), adapted from Sridharan et al. (2009); Bartlett et al. (2005).

Proposition 4.6 (Fast rates for regularized objectives) Assume a G -Lipschitz-continuous **convex** loss function, linear prediction functions with $\mathcal{F} = \{f_\theta(x) = \theta^\top \varphi(x), \theta \in \mathbb{R}^d\}$, where $\|\varphi(x)\|_2 \leq R$ almost surely. Let $\hat{\theta}_\lambda \in \mathbb{R}^d$ be the minimizer of the regularized empirical risk in Eq. (4.12), then:

$$\mathbb{E}[\mathcal{R}(f_{\hat{\theta}_\lambda})] \leq \inf_{\theta \in \mathbb{R}^d} \left\{ \mathcal{R}(f_\theta) + \frac{\lambda}{2} \|\theta\|_2^2 \right\} + \frac{32G^2R^2}{\lambda n}.$$

Proof (♦) Let $\mathcal{R}_\lambda(f_\theta) = \mathcal{R}(f_\theta) + \frac{\lambda}{2} \|\theta\|_2^2$, with minimum value \mathcal{R}_λ^* attained at θ_λ^* . We consider the convex set $\mathcal{C}_\varepsilon = \{\theta \in \mathbb{R}^d, \mathcal{R}_\lambda(f_\theta) - \mathcal{R}_\lambda^* \leq \varepsilon\}$ for an $\varepsilon > 0$ to be chosen later. If $\hat{\theta}_\lambda \notin \mathcal{C}_\varepsilon$, then, by convexity, there has to be an η in the segment $[\theta_\lambda^*, \hat{\theta}_\lambda]$ such that $\mathcal{R}_\lambda(f_\eta) - \mathcal{R}_\lambda^* = \mathcal{R}_\lambda(f_\eta) - \mathcal{R}_\lambda(f_{\theta_\lambda^*}) = \varepsilon$, and $\hat{\mathcal{R}}_\lambda(f_\eta) \leq \hat{\mathcal{R}}_\lambda(f_{\theta_\lambda^*})$.⁴ This implies that

$$\mathcal{R}_\lambda(f_\eta) - \hat{\mathcal{R}}_\lambda(f_\eta) + \hat{\mathcal{R}}_\lambda(f_{\theta_\lambda^*}) - \mathcal{R}_\lambda(f_{\theta_\lambda^*}) = \mathcal{R}_\lambda(f_\eta) - \mathcal{R}_\lambda(f_{\theta_\lambda^*}) + \hat{\mathcal{R}}_\lambda(f_{\theta_\lambda^*}) - \hat{\mathcal{R}}_\lambda(f_\eta) \geq \varepsilon. \quad (4.13)$$

By strong convexity, we have, $\mathcal{R}_\lambda(f_\theta) - \mathcal{R}_\lambda^* \geq \frac{\lambda}{2} \|\theta - \theta_\lambda^*\|_2^2$ for all θ , and thus \mathcal{C}_ε is included in the ℓ_2 -ball of center θ_λ^* and radius $\sqrt{2\varepsilon/\lambda}$. Thus, from Eq. (4.13), we get $\sup_{\|\eta - \theta_\lambda^*\|_2 \leq \sqrt{2\varepsilon/\lambda}} \left\{ \mathcal{R}_\lambda(f_\eta) - \mathcal{R}_\lambda(f_{\theta_\lambda^*}) - [\hat{\mathcal{R}}_\lambda(f_\eta) - \hat{\mathcal{R}}_\lambda(f_{\theta_\lambda^*})] \right\} \geq \varepsilon$. Using Section 4.5.3, we have

$$\begin{aligned} & \mathbb{E} \left[\sup_{\|\eta - \theta_\lambda^*\|_2 \leq \sqrt{2\varepsilon/\lambda}} \left\{ \mathcal{R}_\lambda(f_\eta) - \mathcal{R}_\lambda(f_{\theta_\lambda^*}) - [\hat{\mathcal{R}}_\lambda(f_\eta) - \hat{\mathcal{R}}_\lambda(f_{\theta_\lambda^*})] \right\} \right] \\ & \leq 2\mathbb{E} \left[\sup_{\|\eta - \theta_\lambda^*\|_2 \leq \sqrt{2\varepsilon/\lambda}} \left\{ \frac{1}{n} \sum_{i=1}^n \varepsilon_i [\ell(y_i, \varphi(x_i)^\top \eta) - \ell(y_i, \varphi(x_i)^\top \theta_\lambda^*)] \right\} \right] \leq 2GR\sqrt{2\varepsilon/\lambda}. \end{aligned}$$

Moreover, by McDiarmid's inequality,

$$\mathbb{P} \left(\mathcal{R}_\lambda(f_\eta) - \hat{\mathcal{R}}_\lambda(f_\eta) + \hat{\mathcal{R}}_\lambda(f_{\theta_\lambda^*}) - \mathcal{R}_\lambda(f_{\theta_\lambda^*}) \geq 2GR\sqrt{2\varepsilon/\lambda} + t \frac{2\frac{GR}{\sqrt{n}}\sqrt{2\varepsilon/\lambda}}{\sqrt{2n}} \right) \leq e^{-t^2}.$$

Thus, if $\varepsilon \geq 2\frac{GR}{\sqrt{n}}\sqrt{2\varepsilon/\lambda}(1 + \frac{t}{\sqrt{2}})$, that is, if $\varepsilon \geq 8\frac{G^2R^2}{\lambda n}(2 + t^2)$, we have the high probability bound $\mathbb{P}(\mathcal{R}_\lambda(f_{\hat{\theta}_\lambda}) - \mathcal{R}_\lambda^* > \varepsilon) \leq e^{-t^2}$. This leads to, by integration, $\mathbb{E}[\mathcal{R}_\lambda(f_{\hat{\theta}_\lambda}) - \mathcal{R}_\lambda^*] \leq \frac{32G^2R^2}{\lambda n}$.

■

Note that we obtain a “fast rate” in $O(R^2/(\lambda n))$, which has a better dependence in n but depends on λ , which can be very small in practice. One classical choice of λ that we have seen in Chapter 3 also applies here, as $\lambda \propto \frac{GR}{\sqrt{n}\|\theta_*\|}$, leading to the slow rate

$$\mathbb{E}[\mathcal{R}(f_{\hat{\theta}_\lambda})] \leq \mathcal{R}(f_{\theta_*}) + O\left(\frac{GR}{\sqrt{n}}\|\theta_*\|_2\right).$$

⁴This can be shown by taking η at the intersection of the segment $[\theta_\lambda^*, \hat{\theta}_\lambda]$ and the set $\partial\mathcal{C}_\varepsilon$ (the boundary of \mathcal{C}_ε).

This is a result similar to the one obtained in Chapter 3 for ridge (least-squares) regression, but now for all Lipschitz-continuous losses. Note that the amount of regularization to get the result above still depends on the unknown quantity $\|\theta_*\|_2$. Below, we consider the general case of penalization by a norm, where we will obtain similar results but with a hyperparameter that does not depend on the unknown norm of $\|\theta_*\|_2$.

Exercise 4.13 (♦♦) Extend the result in Prop. 4.6 to features that are almost surely bounded in ℓ_p -norm by R , and a regularizer ψ which is strongly-convex with respect to the ℓ_p -norm, that is, such that for all $\theta, \eta \in \mathbb{R}^d$, $\psi(\theta) \geq \psi(\eta) + \psi'(\eta)^\top(\theta - \eta) + \frac{\mu}{2}\|\theta - \eta\|_p^2$, where $\psi'(\eta)$ is a subgradient of ψ at η .

Norm-penalized estimation. (♦♦) We now focus on the following objective function:

$$\hat{\mathcal{R}}_\lambda(\theta) = \frac{1}{n} \sum_{i=1}^n \ell(y_i, \theta^\top \varphi(x_i)) + \lambda \Omega(\theta),$$

where we assume that $\mathcal{R}_0(\theta) = \mathbb{E}_{p(x,y)}[\ell(y, \theta^\top \varphi(x))]$ is minimized at some $\theta_* \in \mathbb{R}^d$, and that the function $\theta \mapsto \ell(y, \theta^\top \varphi(x))$ is GR -Lipschitz continuous in θ for $\Omega(\theta) \leq 2\Omega(\theta_*)$, and $\Omega^*(\varphi(x)) \leq R$ almost surely. We consider θ_λ^* a minimizer of the population regularized risk $\mathcal{R}_\lambda(\theta) = \mathcal{R}(\theta) + \lambda \Omega(\theta)$. It satisfies $\Omega(\theta_\lambda^*) \leq \Omega(\theta_*)$.

We denote by $\rho_\Omega = \sup_{\Omega^*(z_1), \dots, \Omega^*(z_n) \leq 1} \mathbb{E}_\varepsilon \Omega^*\left(\frac{1}{\sqrt{n}} \sum_{i=1}^n \varepsilon_i z_i\right)$, so that the Rademacher complexity of the set of linear predictors such that $\Omega(\theta) \leq D$ for $D \leq 2\Omega(\theta_*)$, is less than $\frac{\rho_\Omega GRD}{\sqrt{n}}$ (see Section 4.5.3).

For example, for the ℓ_2 -norm, we have $\rho_\Omega = 1$, while for the ℓ_1 -norm, we have $\rho_\Omega = \sqrt{2 \log(2d)}$. In terms of losses, for the logistic loss, we have $G = 1$, while for the square loss (with a factor of $1/2$) with a model $y = \varphi(x)^\top \theta^* + \varepsilon$ with $|\varepsilon| \leq \sigma$ almost surely, we get $G = \sigma + 3R\Omega(\theta^*)$.

Using McDiarmid's inequality like in Section 4.4.1, by fixing any θ_0 such that $\Omega(\theta_0) \leq D$, with probability greater than $1 - e^{-t^2}$, for all θ such that $\Omega(\theta) \leq 2\Omega(\theta_*)$, $\mathcal{R}(\theta) - \mathcal{R}(\theta_0) \leq \hat{\mathcal{R}}(\theta) - \hat{\mathcal{R}}(\theta_0) + \frac{\rho_\Omega GRD}{\sqrt{n}} + t \frac{2GRD\sqrt{2}}{\sqrt{n}}$.

We consider the set $\mathcal{C}_{\nu, \varepsilon} = \{\theta \in \mathbb{R}^d, \Omega(\theta) \leq 2\Omega(\theta_\lambda^*), \mathcal{R}_\lambda(\theta) - \mathcal{R}_\lambda(\theta_\lambda^*) \leq \varepsilon\}$. This is a convex set, with boundary $\partial \mathcal{C}_{\nu, \varepsilon} = \{\theta \in \mathbb{R}^d, \Omega(\theta) \leq 2\Omega(\theta_\lambda^*), \mathcal{R}_\lambda(\theta) - \mathcal{R}_\lambda(\theta_\lambda^*) = \varepsilon\}$ for a well-chosen ε (that is, the saturated constraint has to be one on the expected risk). Indeed, if

$\Omega(\theta) = 2\Omega(\theta_\lambda^*)$, then, using that the optimality conditions for θ_λ^* implies that $\Omega^*(\mathcal{R}'(\theta_\lambda^*)) \leq \lambda$:

$$\begin{aligned}
\mathcal{R}_\lambda(\theta) - \mathcal{R}_\lambda(\theta_\lambda^*) &= \mathcal{R}(\theta) - \mathcal{R}(\theta_\lambda^*) + \lambda\Omega(\theta) - \lambda\Omega(\theta_\lambda^*) \text{ by definition,} \\
&\geq \mathcal{R}'(\theta_\lambda^*)^\top(\theta - \theta_\lambda^*) + \lambda\Omega(\theta) - \lambda\Omega(\theta_\lambda^*) \text{ by convexity,} \\
&\geq -\Omega^*(\mathcal{R}'(\theta_\lambda^*)) \cdot \Omega(\theta - \theta_\lambda^*) + \lambda\Omega(\theta) - \lambda\Omega(\theta_\lambda^*) \text{ by definition of the dual norm,} \\
&\geq -\lambda\Omega(\theta - \theta_\lambda^*) + \lambda\Omega(\theta) - \lambda\Omega(\theta_\lambda^*) \text{ by optimality of } \theta_\lambda^*, \\
&\geq 2\lambda\Omega(\theta) - 2\lambda\Omega(\theta_\lambda^*) \text{ by the triangular inequality,} \\
&= 2\lambda\Omega(\theta_\lambda^*) \text{ since we have assumed } \Omega(\theta) = 2\Omega(\theta_\lambda^*).
\end{aligned}$$

We thus need to impose that $\varepsilon \leq 2\Omega(\theta_\lambda^*)$.

We now show that with high probability, we must have $\hat{\theta}_\lambda \in \mathcal{C}_{\nu, \varepsilon}$. If $\hat{\theta}_\lambda \notin \mathcal{C}_{\nu, \varepsilon}$, since $\theta_\lambda^* \in \mathcal{C}_{\nu, \varepsilon}$, there has to be an element θ in the segment $[\theta_\lambda^*, \hat{\theta}_\lambda]$ which is in $\partial\mathcal{C}_{\nu, \varepsilon}$. Since our risks are convex, we have $\hat{\mathcal{R}}_\lambda(\theta) \leq \max\{\hat{\mathcal{R}}_\lambda(\theta_\lambda^*), \hat{\mathcal{R}}_\lambda(\hat{\theta}_\lambda)\} = \hat{\mathcal{R}}_\lambda(\theta_\lambda^*)$. Thus

$$\hat{\mathcal{R}}(\theta_\lambda^*) - \hat{\mathcal{R}}(\theta) - \mathcal{R}(\theta_\lambda^*) + \mathcal{R}(\theta) = \hat{\mathcal{R}}_\lambda(\theta_\lambda^*) - \hat{\mathcal{R}}_\lambda(\theta) - \mathcal{R}_\lambda(\theta_\lambda^*) + \mathcal{R}_\lambda(\theta) \geq -\mathcal{R}_\lambda(\theta_\lambda^*) + \mathcal{R}_\lambda(\theta) = \varepsilon.$$

Thus if we take, $\varepsilon \geq \frac{\rho_\Omega GRD}{\sqrt{n}} + t\frac{2GRD\sqrt{2}}{\sqrt{n}}$, with $D = 2\Omega(\theta_\lambda^*)$, this can only happen with probability less than $\exp(-t^2)$. This leads to the constraint $\varepsilon \geq \frac{2GR\Omega(\theta_\lambda^*)}{\sqrt{n}}(\rho_\Omega + 4t\sqrt{2})$. Thus, we can take $\lambda = \frac{GR}{\sqrt{n}}(\rho_\Omega + 4t\sqrt{2})$. and with probability greater than $1 - e^{-t^2}$ we have

$$\mathcal{R}_\lambda(\hat{\theta}_\lambda) - \mathcal{R}_\lambda(\theta_\lambda^*) \leq 2\lambda\Omega(\theta_\lambda^*) \leq 2\lambda\Omega(\theta^*).$$

Overall, denoting $\delta = e^{-t^2}$, we get that with probability greater than $1 - \delta$

$$\mathcal{R}(\hat{\theta}_\lambda) \leq \mathcal{R}(\theta_*) + \Omega(\theta_*) \frac{3GR}{\sqrt{n}} \left(\rho_\Omega + 4\sqrt{2 \log \frac{1}{\delta}} \right).$$

for $\lambda = \frac{GR}{\sqrt{n}}(\rho_\Omega + 4\sqrt{2 \log \frac{1}{\delta}})$. Note that we could get a result in expectation (left as an exercise). The key here is that the value of λ does not depend on $\Omega(\theta^*)$.

4.5.6 Extensions and improvements

In this chapter, we have focused on the simplest situations for empirical risk minimization technique: regression or binary classification with i.i.d. data. Statistical learning theory investigates many more complex cases along several lines:

- **Slower rates than $1/\sqrt{n}$:** In this chapter, we primarily studied the estimation error that decays as $1/\sqrt{n}$. When balancing it with approximation error (by adapting norm constraints or regularization parameters), we will obtain slower rates, but with weaker assumptions, in Chapter 7 (kernel methods) and Chapter 9 (neural networks).

- **Faster rates with discrete outputs:** When dealing with binary classification, or more generally discrete outputs, further analysis can be carried through, with potentially different convergence rates for the convex surrogate and the original loss function (i.e., after thresholding, where sometimes exponential rates can be obtained). This is often done under so-called “low noise” conditions (see, e.g., [Koltchinskii and Beznosova, 2005](#); [Audibert and Tsybakov, 2007](#)), as briefly exposed in Section 4.1.4.
- **Other generic learning theory frameworks:** In this chapter, we have focused primarily on the tools of Rademacher averages to obtain generic learning bounds. Other frameworks lead to similar bounds but from different mathematical perspectives. For example, PAC-Bayesian analysis ([Catoni, 2007](#); [Zhang, 2006](#)) is described in Section 14.4, while stability-based arguments ([Bousquet and Elisseeff, 2002](#)) lead to similar results (see exercise below).

Exercise 4.14 (♦) We consider a learning algorithm and a distribution p on (x, y) such that for all $(x, y) \in \mathcal{X} \times \mathcal{Y}$, and two outputs $f, f' : \mathcal{X} \rightarrow \mathcal{Y}$ of the learning algorithm on datasets of n observations which differ by a single observation, $|\ell(y, f(x)) - \ell(y, f'(x))| \leq \beta_n$, an assumption referred to as “uniform stability”. Show that the expected deviation between the expected risk and the empirical risk of the algorithm’s output is bounded by β_n . With the same assumptions as in Prop. 4.6, show that we have $\beta_n = \frac{2G^2R^2}{\lambda n}$ (see [Bousquet and Elisseeff, 2002](#), for more details).

- **Beyond independent observations:** Much of statistical learning theory deals with the simplifying assumptions that observations are i.i.d. from the same distribution as the one used during the testing phase. This leads to the reasonably simple results presented in this chapter. Several lines of work deal with situations when data are not independent: among them, online learning presented in Chapter 13 shows that many classical algorithms are indeed robust to such dependence. Another avenue coming from statistics is to make some assumptions on the dependence between observations, the most classical one being that the sequence of observations $(x_i, y_i)_{i \geq 1}$ form a Markov chain, and thus satisfies “mixing conditions” (see, e.g., [Mohri and Rostamizadeh, 2010](#)).
- **Mismatch between training and testing distributions:** In many application scenarios, the testing distribution may deviate from the training distribution: the input distribution of x may be different while the conditional distribution of y given x remains the same, a situation commonly referred to as “covariate shift”, or the entire distribution of (x, y) may deviate (often referred to as the need for “domain adaptation”). If no assumption is made on the proximity of these two distributions, no guarantee can be obtained. Several ideas have been explored to derive algorithms and/or guarantees, such as importance reweighting ([Sugiyama et al., 2007](#)) or finding projections of the data with similar test and train distributions ([Ganin et al., 2016](#)).

- **Semi-supervised learning:** In many applications, many unlabelled observations are available (that is, only with the input x being available). To leverage the abundance of unlabelled data, some assumptions are typically made to show an improvement of learning algorithms, such as the “cluster assumption” (points in the same class tend to cluster together) or “low-density separation” (for classification, decision boundaries tend to be in regions with few input observations). Many algorithms exist, such as Laplacian regularization (see [Cabannes et al., 2021](#), and references therein) or discriminative clustering ([Xu et al., 2004](#); [Bach and Harchaoui, 2007](#)).

4.6 Relationship with asymptotic statistics (♦)

In this last section, we will relate the non-asymptotic analysis presented in this chapter to results from asymptotic statistics (see the comprehensive book by [Van der Vaart \(2000\)](#), which presents this large literature).

To make this concrete, we will assume that we have a set of models $\mathcal{F} = \{f_\theta : \mathcal{X} \rightarrow \mathbb{R}, \theta \in \mathbb{R}^d\}$ parameterized by a vector $\theta \in \mathbb{R}^d$. We consider the empirical risk and expected risks (with a slight overloading of notations):

$$\mathcal{R}(\theta) = \mathcal{R}(f_\theta) = \mathbb{E}[\ell(y, f_\theta(x))] \quad \text{and} \quad \widehat{\mathcal{R}}(\theta) = \widehat{\mathcal{R}}(f_\theta) = \frac{1}{n} \sum_{i=1}^n \ell(y_i, f_\theta(x_i)).$$

We assume that we have a loss function $\ell : \mathcal{Y} \times \mathbb{R} \rightarrow \mathbb{R}$ (such as for regression or any of the convex surrogates for classification), which is sufficiently differentiable with respect to the second variable, so that results from [Van der Vaart \(2000\)](#) apply (e.g., Theorems 5.21 or 5.41 on “M-estimation”, which cover empirical risk minimization). In this section, we will only report their final result and provide an intuitive justification.

We assume that $\theta_* \in \mathbb{R}^d$ is a minimizer of $\mathcal{R}(\theta)$ and that the Hessian $\mathcal{R}''(\theta_*)$ is positive-definite (it has to be positive semi-definite as θ_* is a minimizer, we assume invertibility on top of it).

We let $\hat{\theta}_n$ denote a minimizer of $\widehat{\mathcal{R}}$. Since $\mathcal{R}'(\theta_*) = 0$, and $\widehat{\mathcal{R}}'(\theta_*) = \frac{1}{n} \sum_{i=1}^n \frac{\partial \ell(y_i, f_\theta(x_i))}{\partial \theta}$, by the law of large numbers, $\widehat{\mathcal{R}}'(\theta_*)$ tends to $\mathcal{R}'(\theta_*) = 0$ (e.g., almost surely), and we should thus expect that $\hat{\theta}_n$ (which is defined through $\widehat{\mathcal{R}}'(\hat{\theta}_n) = 0$) tends to θ_* (all these statements can be made rigorous, see [Van der Vaart \(2000\)](#)).

Then, a Taylor expansion of $\widehat{\mathcal{R}}'$ around θ_* leads to

$$0 = \widehat{\mathcal{R}}'(\hat{\theta}_n) \approx \widehat{\mathcal{R}}'(\theta_*) + \widehat{\mathcal{R}}''(\theta_*)(\hat{\theta}_n - \theta_*).$$

By the law of large numbers, $\widehat{\mathcal{R}}''(\theta_*)$ tends to $H(\theta_*) = \mathcal{R}''(\theta_*)$ when n tends to infinity, and thus we obtain:

$$\hat{\theta}_n - \theta_* \approx \mathcal{R}''(\theta_*)^{-1} \widehat{\mathcal{R}}'(\theta_*) = H(\theta_*)^{-1} \widehat{\mathcal{R}}'(\theta_*).$$

Moreover, $\widehat{\mathcal{R}}'(\theta_*)$ is the average of n i.i.d. random vectors, and by the central limit theorem, it is asymptotically Gaussian with mean zero and covariance matrix equal to $\frac{1}{n}G(\theta_*) = \frac{1}{n}\mathbb{E}\left[\left(\frac{\partial\ell(y, f_\theta(x))}{\partial\theta}\right)\left(\frac{\partial\ell(y, f_\theta(x))}{\partial\theta}\right)^\top\Big|_{\theta=\theta_*}\right]$. Therefore, we (intuitively) obtain that $\hat{\theta}_n$ is asymptotically Gaussian with mean θ_* and covariance matrix $\frac{1}{n}H(\theta_*)^{-1}G(\theta_*)H(\theta_*)^{-1}$.

This asymptotic result has the nice consequence that:

$$\begin{aligned}\mathbb{E}\left[\|\hat{\theta}_n - \theta_*\|_2^2\right] &\sim \frac{1}{n} \text{tr} [H(\theta_*)^{-1}G(\theta_*)H(\theta_*)^{-1}] \\ \mathbb{E}[\mathcal{R}(\hat{\theta}_n) - \mathcal{R}(\theta_*)] &\sim \frac{1}{n} \text{tr} [H(\theta_*)^{-1}G(\theta_*)].\end{aligned}$$

For example, for well-specified linear regression (like analyzed in Chapter 3), it turns out that we have $G(\theta_*) = \sigma^2 H(\theta_*)$ (proof left as an exercise), and thus we recover the rate $\sigma^2 d/n$.

Benefits of the asymptotic analysis. As shown above, the asymptotic analysis gives a precise picture of the asymptotic behavior of empirical risk minimization. Much more than simply providing an upper-bound on $\mathbb{E}[\mathcal{R}(\hat{\theta}_n) - \mathcal{R}(\theta_*)]$, it gives also a limit Gaussian distribution for $\hat{\theta}_n$, and a *fast rate* as $O(1/n)$. Moreover, because we have limits, we can compare limits between various learning algorithms and claim (asymptotic) superiority or inferiority of one method over another, which comparing upper bounds cannot achieve.

Pitfalls of the asymptotic analysis. The main drawback of this analysis is that it is... asymptotic. That is, n tends to infinity, and it is impossible to tell without further analysis when the asymptotic behavior will kick in. Sometimes, this is for reasonably small n , sometimes for large n . Further asymptotic expansions can be carried out, but small sample effects are hard to characterize, particularly when the underlying dimension d gets large.

Bridging the gap. Studying the validity of the asymptotic expansion described above can be done in several ways. See, e.g., [Ostrovskii and Bach \(2021\)](#) (and references therein) for finite-dimensional models, and Chapter 7 for results similar to $\sigma^2 d/n$ when the dimension of the feature space gets infinite.

Chapter 5

Optimization for machine learning

Chapter summary

- Gradient descent: the workhorse first-order algorithm for optimization, which converges exponentially fast for well-conditioned convex problems.
- Stochastic gradient descent (SGD): the workhorse first-order algorithm for large-scale machine learning, which converges as $1/t$ or $1/\sqrt{t}$, where t is the number of iterations.
- Generalization bounds through stochastic gradient descent: with only a single pass on the data, there is no risk of overfitting, and we obtain generalization bounds for unseen data.
- Variance reduction: when minimizing strongly-convex finite sums, this class of algorithms is exponentially convergent while having a small iteration complexity.

In this chapter, we present optimization algorithms based on gradient descent and analyze their performance, mainly on convex objective functions. We will consider generic algorithms that have applications beyond machine learning and algorithms dedicated to machine learning (such as stochastic gradient methods). See [Nesterov \(2018\)](#); [Bubeck \(2015\)](#) for further details.

5.1 Optimization in machine learning

In supervised machine learning, we are given n i.i.d. samples (x_i, y_i) , $i = 1, \dots, n$ of a couple of random variables (x, y) on $\mathcal{X} \times \mathcal{Y}$ and the goal is to find a predictor $f : \mathcal{X} \rightarrow \mathbb{R}$ with a small risk on unseen data

$$\mathcal{R}(f) := \mathbb{E}[\ell(y, f(x))],$$

where $\ell : \mathcal{Y} \times \mathbb{R} \rightarrow \mathbb{R}$ is a loss function. This loss is typically convex in the second argument (see Chapter 4) and is often considered a weak assumption.

In the empirical risk minimization approach described in Chapter 4, we choose the predictor by minimizing the empirical risk over a parameterized set of predictors, potentially with regularization. For a parameterization $\{f_\theta\}_{\theta \in \mathbb{R}^d}$ and a regularizer $\Omega : \mathbb{R}^d \rightarrow \mathbb{R}$ (e.g., $\Omega(\theta) = \|\theta\|_2^2$ or $\Omega(\theta) = \|\theta\|_1$), this requires to minimize the function

$$F(\theta) := \frac{1}{n} \sum_{i=1}^n \ell(y_i, f_\theta(x_i)) + \Omega(\theta). \quad (5.1)$$

In optimization, the function $F : \mathbb{R}^d \rightarrow \mathbb{R}$ is called the *objective function*.

In general, the minimizer has no closed form. Even when it has one (e.g., linear predictor and square loss in Chapter 3), it could be expensive to compute for large problems. We thus resort to iterative algorithms.

Accuracy of iterative algorithms. Solving optimization problems with high accuracy is computationally expensive, and the goal is not to minimize the training objective but the error on unseen data.

Then, which accuracy is satisfying in machine learning? If the algorithm returns $\hat{\theta}$, and we define $\theta_* \in \arg \min_{\theta} \mathcal{R}(f_\theta)$, we have the risk decomposition from Section 2.3.2 (where the approximation error due to the use of a specific set of models f_θ , $\theta \in \Theta$ is ignored):

$$\mathcal{R}(f_{\hat{\theta}}) - \inf_{\theta \in \mathbb{R}^d} \mathcal{R}(f_\theta) = \underbrace{\left\{ \mathcal{R}(f_{\hat{\theta}}) - \hat{\mathcal{R}}(f_{\hat{\theta}}) \right\}}_{\text{estimation error}} + \underbrace{\left\{ \hat{\mathcal{R}}(f_{\hat{\theta}}) - \hat{\mathcal{R}}(f_{\theta_*}) \right\}}_{\text{optimization error}} + \underbrace{\left\{ \hat{\mathcal{R}}(f_{\theta_*}) - \mathcal{R}(f_{\theta_*}) \right\}}_{\text{estimation error}},$$

where we added the second term (the optimization error). It is thus sufficient to reach an optimization accuracy of the order of the estimation error (usually of the order $O(1/\sqrt{n})$ or $O(1/n)$, see Chapter 3 and Chapter 4). Note that for machine learning, the optimization error defined above corresponds to characterizing approximate solutions through function values. While this will be one major focal point in this chapter, we will consider other performance measures.

In this chapter, we will first look at the minimization without focusing on machine learning problems (Section 5.2), with both smooth and non-smooth objective functions. We will then look at stochastic gradient descent in Section 5.4, which can be used to obtain

bounds on both the training and testing risks. We then briefly present variance reduction in Section 5.4.2.

 θ_* may mean different things in optimization and machine learning: minimizer of the *regularized empirical risk*, or minimizer of the *expected risk*. For the sake of clarity, we will use the notation η_* for the minimizer of empirical (potentially regularized) risk, that is, when we look at optimization problems, and θ_* for the minimizer of the expected risk, that is, when we look at statistical problems.

 Sometimes, we mention solving a problem with *high* precision. This corresponds to a *low* optimization error.

5.2 Gradient descent

Suppose we want to solve, for a function $F : \mathbb{R}^d \rightarrow \mathbb{R}$, the optimization problem

$$\min_{\theta \in \mathbb{R}^d} F(\theta).$$

We assume that we are given access to certain “oracles”: the *k-th-order oracle* corresponds to the access to: $\theta \mapsto (F(\theta), F'(\theta), \dots, F^{(k)}(\theta))$, that is all partial derivatives up to order k . All algorithms will call these oracles; thus, their computational complexity will depend directly on the complexity of this oracle. For example, for least-squares with a design matrix in $\mathbb{R}^{n \times d}$, computing a single gradient of the empirical risk costs $O(nd)$.

In this section, for the algorithms and proofs, we do not assume that the function F is the regularized empirical risk, but this situation will be our motivating example throughout. We will study the following first-order algorithm.

Algorithm 5.1 (Gradient descent (GD)) Pick $\theta_0 \in \mathbb{R}^d$ and for $t \geq 1$, let

$$\theta_t = \theta_{t-1} - \gamma_t F'(\theta_{t-1}), \quad (5.2)$$

for a well (potentially adaptively) chosen step-size sequence $(\gamma_t)_{t \geq 1}$.

For machine learning problems where the empirical risk is minimized, computing the gradient $F'(\theta_{t-1})$ requires computing all gradients of $\theta \mapsto \ell(y_i, f_\theta(x_i))$, and averaging them.

There are many ways to choose the step-size γ_t , either constant, decaying, or through a line search.¹ In practice, using some form of line search is usually advantageous and is

¹See, e.g., https://en.wikipedia.org/wiki/Line_search

implemented in most applications. See [Armijo \(1966\)](#) and [Goldstein \(1962\)](#) for convergence guarantees with typical procedures. In this chapter, since we want to focus on the simplest algorithms and proofs, we will focus on step-sizes that depend explicitly on problem constants and sometimes on the iteration number. When gradients are not available, gradient estimates may be built from function values (see, e.g., [Nesterov and Spokoiny, 2017](#), and Chapter 13). Note that the differences between convergence rates with and without line searches are generally not significantly different (see Exercise 5.2 below for quadratic functions).

We first start with the simplest example, namely convex quadratic functions, where the most important concepts already appear.

5.2.1 Simplest analysis: ordinary least-squares

We start with a case where the analysis is explicit: ordinary least squares (see Chapter 3 for the statistical analysis). Let $\Phi \in \mathbb{R}^{n \times d}$ be the design matrix and $y \in \mathbb{R}^n$ the vector of responses. Least-squares estimation amounts to finding a minimizer η_* of

$$F(\theta) = \frac{1}{2n} \|\Phi\theta - y\|_2^2. \quad (5.3)$$

⚠ A factor of $\frac{1}{2}$ has been added compared to Chapter 3 to get nicer looking gradients.

The gradient of F is $F'(\theta) = \frac{1}{n}\Phi^\top(\Phi\theta - y) = \frac{1}{n}\Phi^\top\Phi\theta - \frac{1}{n}\Phi^\top y$. Thus, denoting $H = \frac{1}{n}\Phi^\top\Phi \in \mathbb{R}^{d \times d}$ the Hessian matrix (equal for all θ , denoted $\widehat{\Sigma}$ in Chapter 3), minimizers η_* are characterized by

$$H\eta_* = \frac{1}{n}\Phi^\top y.$$

Since $\frac{1}{n}\Phi^\top y \in \mathbb{R}^d$ is in the column space of H , there is always a minimizer, but unless H is invertible, the minimizer is not unique. But all minimizers η_* have the same function value $F(\eta_*)$, and we have, from a simple exact Taylor expansion (and using $F'(\eta_*) = 0$):

$$F(\theta) - F(\eta_*) = F'(\eta_*)^\top(\theta - \eta_*) + \frac{1}{2}(\theta - \eta_*)^\top H(\theta - \eta_*) = \frac{1}{2}(\theta - \eta_*)^\top H(\theta - \eta_*).$$

Two quantities will be important in the following developments, the largest eigenvalue L and the smallest eigenvalue μ of the Hessian matrix H . As a consequence of the convexity of the objective, we have $0 \leq \mu \leq L$. We denote by $\kappa = \frac{L}{\mu} \geq 1$ the *condition number*.

Note that for least-squares, μ is the lowest eigenvalue of the non-centered empirical covariance matrix and that it is zero as soon as $d > n$, and, in most practical cases, *very* small. When adding a regularizer $\frac{\lambda}{2}\|\theta\|_2^2$ (like in ridge regression), then $\mu \geq \lambda$ (but then λ typically decreases with n , often between $\frac{1}{\sqrt{n}}$ and $\frac{1}{n}$, see Chapter 7 for more details).

Closed-form expression. Gradient descent iterates with fixed step-size $\gamma_t = \gamma$ can be computed in closed form:

$$\theta_t = \theta_{t-1} - \gamma F'(\theta_{t-1}) = \theta_{t-1} - \gamma \left[\frac{1}{n} \Phi^\top (\Phi \theta_{t-1} - y) \right] = \theta_{t-1} - \gamma H(\theta_{t-1} - \eta_*),$$

leading to

$$\theta_t - \eta_* = \theta_{t-1} - \eta_* - \gamma H(\theta_{t-1} - \eta_*) = (I - \gamma H)(\theta_{t-1} - \eta_*),$$

that is, we have a linear recursion, and we can unroll the recursion and now write

$$\theta_t - \eta_* = (I - \gamma H)^t (\theta_0 - \eta_*).$$

We can now look at various measures of performance:

$$\begin{aligned} \|\theta_t - \eta_*\|_2^2 &= (\theta_0 - \eta_*)^\top (I - \gamma H)^{2t} (\theta_0 - \eta_*) \\ F(\theta_t) - F(\eta_*) &= \frac{1}{2} (\theta_0 - \eta_*)^\top (I - \gamma H)^{2t} H (\theta_0 - \eta_*). \end{aligned}$$

The two optimization performance measures differ by the presence of the Hessian matrix H in the measure based on function values.

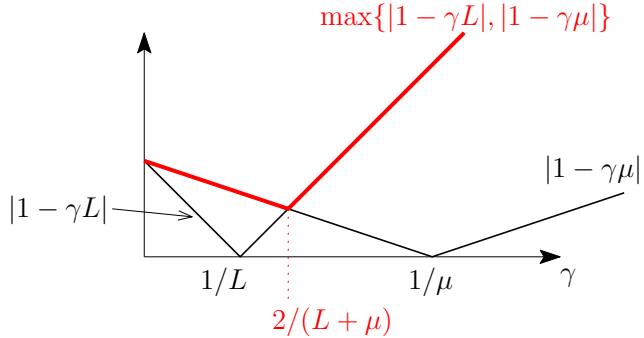
Convergence in distance to the minimizer. If we hope to have $\|\theta_t - \eta_*\|_2^2$ going to zero, we need to have a single minimizer η_* , and thus H has to be invertible, that is $\mu > 0$. Given the form of $\|\theta_t - \eta_*\|_2^2$, we simply need to bound the eigenvalues of $(I - \gamma H)^{2t}$ (since for a positive semi-definite matrix M , $u^\top M u \leq \lambda_{\max}(M) \|u\|_2^2$ for all vectors u).

The eigenvalues of $(I - \gamma H)^{2t}$ are exactly $(1 - \gamma \lambda)^{2t}$ for λ an eigenvalue of H (all of them are in the interval $[\mu, L]$). Thus all the eigenvalues of $(I - \gamma H)^{2t}$ have magnitude less than

$$\left(\max_{\lambda \in [\mu, L]} |1 - \gamma \lambda| \right)^{2t}.$$

We can then have several strategies for choosing the step-size γ :

- Optimal choice: one can check that minimizing $\max_{\lambda \in [\mu, L]} |1 - \gamma \lambda|$ is done by setting $\gamma = 2/(\mu + L)$, with an optimal value equal to $\frac{\kappa-1}{\kappa+1} = 1 - \frac{2}{\kappa+1} \in (0, 1)$. See geometric “proof” below.



- Choice independent of μ : with the simpler (slightly smaller) choice $\gamma = 1/L$, we get $\max_{\lambda \in [\mu, L]} |1 - \gamma \lambda| = (1 - \frac{\mu}{L}) = (1 - \frac{1}{\kappa})$, which is only slightly larger than the value for the optimal choice. Note that all step-sizes strictly less than $2/L$ will lead to exponential convergence.

For example, with the weaker choice $\gamma = 1/L$, we get:

$$\|\theta_t - \eta_*\|_2^2 \leq \left(1 - \frac{1}{\kappa}\right)^{2t} \|\theta_0 - \eta_*\|_2^2,$$

which is often referred to as exponential, geometric, or linear convergence.

⚠ The denomination “linear” is sometimes confusing and corresponds to a number of significant digits that grows linearly with the number of iterations.

We can further bound $(1 - \frac{1}{\kappa})^{2t} \leq \exp(-1/\kappa)^{2t} = \exp(-2t/\kappa)$, and thus the characteristic time of convergence is of order κ . We will often make the calculation $\varepsilon = \exp(-2t/\kappa) \Leftrightarrow t = \frac{\kappa}{2} \log \frac{1}{\varepsilon}$. Thus, for a relative reduction of squared distance to the optimum of ε , we need at most $t = \frac{\kappa}{2} \log \frac{1}{\varepsilon}$ iterations.

For $\kappa = +\infty$, the result remains true but simply says that for all minimizers $\|\theta_t - \eta_*\|_2^2 \leq \|\theta_0 - \eta_*\|_2^2$, which is a good sign (the algorithm does not move away from minimizers) but not indicative of any form of convergence. We will need to use a different criterion.

Convergence in function values. Using the same step-size $\gamma = 1/L$ as above, and using the upper-bound on eigenvalues of $(I - \gamma H)^{2t}$ (which are all less than $(1 - 1/\kappa)^{2t}$), we get

$$F(\theta_t) - F(\eta_*) \leq \left(1 - \frac{1}{\kappa}\right)^{2t} [F(\theta_0) - F(\eta_*)] \leq \exp(-2t/\kappa) [F(\theta_0) - F(\eta_*)]. \quad (5.4)$$

When $\kappa < \infty$ (that is, $\mu > 0$), then we also obtain linear convergence for this criterion, but when $\kappa = \infty$, this is non-informative.

To obtain a convergence rate, we will need to bound the eigenvalues of $(I - \gamma H)^{2t} \textcolor{blue}{H}$ instead of $(I - \gamma H)^{2t}$. The key difference is that for eigenvalues λ of H which are close to zero $(1 - \gamma \lambda)^{2t}$ does not have a strong contracting effect, but they count less as they are multiplied by λ in the bound.

We can make this trade-off precise, for $\gamma \leq 1/L$, as

$$\begin{aligned} |\lambda(1 - \gamma \lambda)^{2t}| &\leq \lambda \exp(-\gamma \lambda)^{2t} = \lambda \exp(-2t\gamma\lambda) \\ &= \frac{1}{2t\gamma} 2t\gamma \lambda \exp(-2t\gamma\lambda) \leq \frac{1}{2t\gamma} \sup_{\alpha \geq 0} \alpha \exp(-\alpha) = \frac{1}{2et\gamma} \leq \frac{1}{4t\gamma}, \end{aligned}$$

where we used that $\alpha e^{-\alpha}$ is maximized over \mathbb{R}_+ at $\alpha = 1$ (as the derivative is $e^{-\alpha}(1 - \alpha)$).

This leads to

$$F(\theta_t) - F(\eta_*) \leq \frac{1}{8t\gamma} \|\theta_0 - \eta_*\|_2^2. \quad (5.5)$$

We can make the following observations:

- ! The convergence results in $\exp(-2t/\kappa)$ in Eq. (5.4) for invertible Hessians or $1/t$ in general in Eq. (5.5) are only upper-bounds! It is good to understand the gap between the bounds and the actual performance, as this is possible for quadratic objective functions.

For the exponentially convergent case, the lowest eigenvalue μ dictates the rate for all eigenvalues. So if the eigenvalues are well-spread (or if only one eigenvalue is very small), there can be quite a strong discrepancy between the bound and the actual behavior.

For the rate in $1/t$, the bound in eigenvalues is tight when $t\gamma\lambda$ is of order 1, namely when λ is of order $1/(t\gamma)$. Thus, to see an $O(1/t)$ convergence rate in practice, we need to have sufficiently many small eigenvalues. As t grows, we often go to a local linear convergence phase where the smallest non-zero eigenvalue of H kicks in. See the simulations and the exercise below.

Exercise 5.1 Let μ_+ be the smallest non-zero eigenvalue of H . Show that gradient descent is linearly convergent with the contracting rate $(1 - \mu_+/L)$.

- From errors to numbers of iterations: as already mentioned, the bound in Eq. (5.4) says that after t steps, the reduction in suboptimality in function values is multiplied by $\varepsilon = \exp(-2t/\kappa)$. This can be reinterpreted as a need of $t = \frac{\kappa}{2} \log \frac{1}{\varepsilon}$ iterations to reach a relative error ε .
- Can an algorithm having the same access to oracles of F do better?

If we have access to matrix-vector products with the matrix Φ , then the conjugate gradient algorithm can be used with convergence rates in $\exp(-t/\sqrt{\kappa})$ and $1/t^2$ (see [Golub and Loan, 1996](#)). With only access to gradients of F (which is a bit weaker), Nesterov acceleration (see Section 5.2.5 below) will also lead to the same convergence rates, which are then optimal (for a sense to be defined later in this chapter and in more details in Chapter 12).

- Can we extend beyond least-squares? The convergence results above will generalize to convex functions (see Section 5.2.2) but with less direct proofs. Non-convex objectives are discussed in Section 5.2.6.

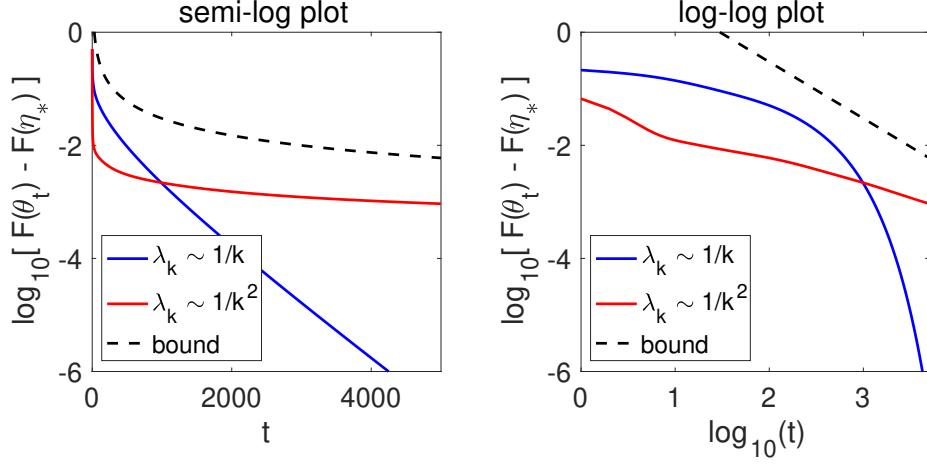


Figure 5.1: Gradient descent on two least-squares problems with step-size $\gamma = 1/L$, and two different sets of eigenvalues $(\lambda_k)_{k \in \{1, \dots, d\}}$ of the Hessian, together with the bound from Eq. (5.5). Left: semi-logarithmic scale. Right: joint logarithmic scale.

Experiments. We consider two quadratic optimization problems in dimension $d = 1000$, with two different decays of eigenvalues $(\lambda_k)_{k \in \{1, \dots, d\}}$ for the Hessian matrix H , one as $1/k$ (in blue below) and one in $1/k^2$ (in red below), and for which we plot in Figure 5.1 the performance for function values, both in semi-logarithm plots (left) and full-logarithm plots (right). For slow decays (blue), we see the linear convergence kicking in (line in the left “semi-log” plot), while for fast decays (red), we obtain a polynomial rate that is not exponential (line in the right “log-log” plot). Note that the bound in Eq. (5.5) is very pessimistic and does not lead to the correct power of t (which, as can be checked as an exercise, should be $1/\sqrt{t}$ for t small enough compared to d).

Exercise 5.2 (exact line search ♦) For the quadratic objective in Eq. (5.3), show that the optimal step-size γ_t in Eq. (5.2) is equal to $\gamma_t = \frac{\|F'(\theta_{t-1})\|_2^2}{F'(\theta_{t-1})^\top H F'(\theta_{t-1})}$. Show that when F is strongly-convex, $F(\theta_t) - F(\eta_*) \leq (\frac{\kappa-1}{\kappa+1})^2 [F(\theta_{t-1}) - F(\eta_*)]$, and compare the rate with constant step-size gradient descent.

Hint: prove and use the Kantorovich inequality $\sup_{\|z\|_2=1} z^\top H z z^\top H^{-1} z = \frac{(L+\mu)^2}{4\mu L}$.

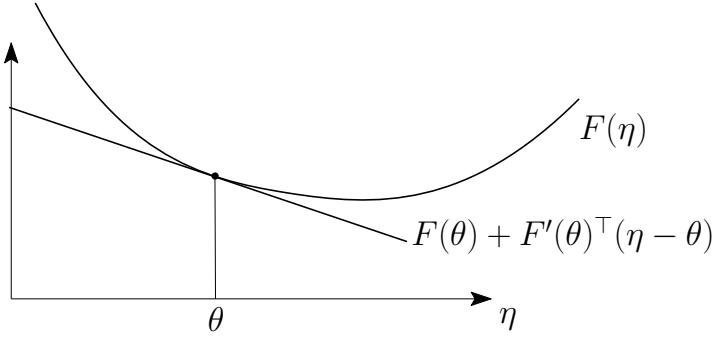
5.2.2 Convex functions and their properties

We now wish to analyze GD (and later its stochastic version SGD) in a broader setting. We will always assume convexity, although these algorithms are also used (and can sometimes also be analyzed) when this assumption does not hold (see Section 5.2.6). In other words, convexity is most often used for analysis rather than to define the algorithm.

Definition 5.1 (Convex function) A differentiable function $F : \mathbb{R}^d \rightarrow \mathbb{R}$ is said convex if and only if

$$F(\eta) \geq F(\theta) + F'(\theta)^\top (\eta - \theta), \quad \forall \eta, \theta \in \mathbb{R}^d. \quad (5.6)$$

This corresponds to the function F being above its tangent at θ , as illustrated below.



If f is twice-differentiable, this is equivalent to requiring $F''(x) \succcurlyeq 0, \forall x \in \mathbb{R}^d$; here \succcurlyeq denotes the semidefinite partial ordering—also called the Löwner order—characterized by $A \succcurlyeq B \Leftrightarrow A - B$ is positive semidefinite, see [Boyd and Vandenberghe \(2004\)](#); [Bhatia \(2009\)](#).

An important consequence that we will use a lot in this chapter is, for all $\theta \in \mathbb{R}^d$ (and using $\eta = \eta_*$)

$$F(\eta_*) \geq F(\theta) + F'(\theta)^\top (\eta_* - \theta) \Leftrightarrow F(\theta) - F(\eta_*) \leq F'(\theta)^\top (\theta - \eta_*), \quad (5.7)$$

that is, the distance to optimum in function values is upper bounded by a function of the gradient (note that it provides a proof that $F'(\theta) = 0$ implies that θ is a global minimizer of F).

A more general definition of convexity (without gradients) is that $\forall \theta, \eta \in \mathbb{R}^d$ and $\alpha \in [0, 1]$,

$$F(\alpha\eta + (1 - \alpha)\theta) \leq \alpha F(\eta) + (1 - \alpha)F(\theta),$$

which generalizes to the usual Jensen's inequality below.

Proposition 5.1 (Jensen's inequality) If $F : \mathbb{R}^d \rightarrow \mathbb{R}$ is convex and μ is a probability measure on \mathbb{R}^d , then

$$F\left(\int_{\mathbb{R}^d} \theta d\mu(\theta)\right) \leq \int_{\mathbb{R}^d} F(\theta) d\mu(\theta). \quad (5.8)$$

In words: “the image of the average is smaller than the average of the images”.

Exercise 5.3 Assume that the function $F : \mathbb{R}^d \rightarrow \mathbb{R}$ is strictly convex, that is, $\forall \theta, \eta \in \mathbb{R}^d$ such that $\theta \neq \eta$, and $\alpha \in (0, 1)$, $F(\alpha\eta + (1 - \alpha)\theta) < \alpha F(\eta) + (1 - \alpha)F(\theta)$. Show that there is equality in Jensen's inequality in Eq. (5.8) if and only if the random variable θ is almost surely constant.

The class of convex functions satisfies the following stability properties (proofs left as an exercise); for more properties on convex functions, see [Boyd and Vandenberghe \(2004\)](#):

- If $(F_j)_{j \in \{1, \dots, m\}}$ are convex and $(\alpha_j)_{j \in \{1, \dots, m\}}$ are nonnegative, then $\sum_{j=1}^m \alpha_j F_j$ is convex.
- If $F : \mathbb{R}^d \rightarrow \mathbb{R}$ is convex and $A : \mathbb{R}^{d'} \rightarrow \mathbb{R}^d$ is linear then $F \circ A : \mathbb{R}^{d'} \rightarrow \mathbb{R}$ is convex.

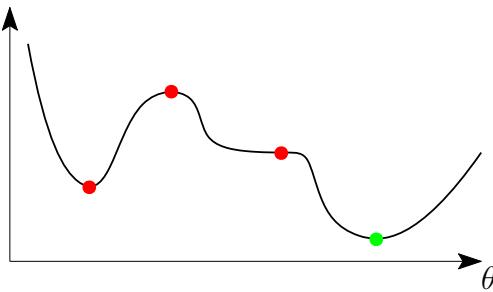
Classical machine learning example. Problems of the form in Eq. (5.1) are convex if the loss ℓ is convex in the second variable, $f_\theta(x)$ is linear in θ , and Ω is convex.

Global optimality from local information. It is also worth emphasizing the following property (immediate from the definition).

Proposition 5.2 *Assume that $F : \mathbb{R}^d \rightarrow \mathbb{R}$ is convex and differentiable. Then $\eta_* \in \mathbb{R}^d$ is a global minimizer of F if and only if*

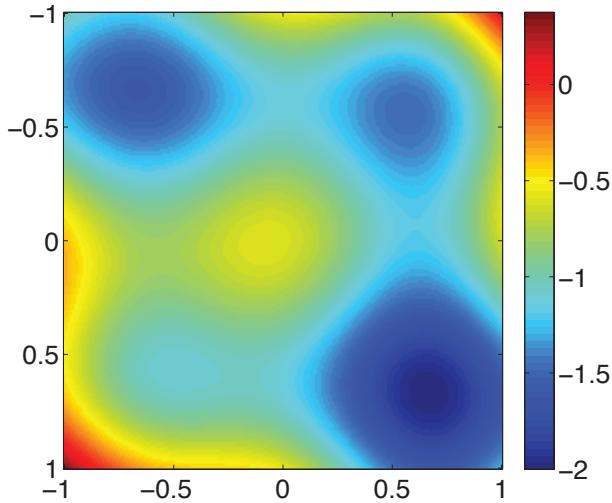
$$F'(\eta_*) = 0.$$

This implies that for convex functions, we only need to look for stationary points. This is *not* the case for potentially non-convex functions. For example, in one dimension below, all red points are stationary points that are not the global minimum (which is in green).



The situation is even more complex in higher dimensions. Note that without convexity assumptions, optimization of Lipschitz-continuous functions will need exponential time in dimension in the worst case (see Section 12.2.2).

Exercise 5.4 Identify all stationary points in the function in \mathbb{R}^2 depicted below.



5.2.3 Analysis of GD for strongly convex and smooth functions

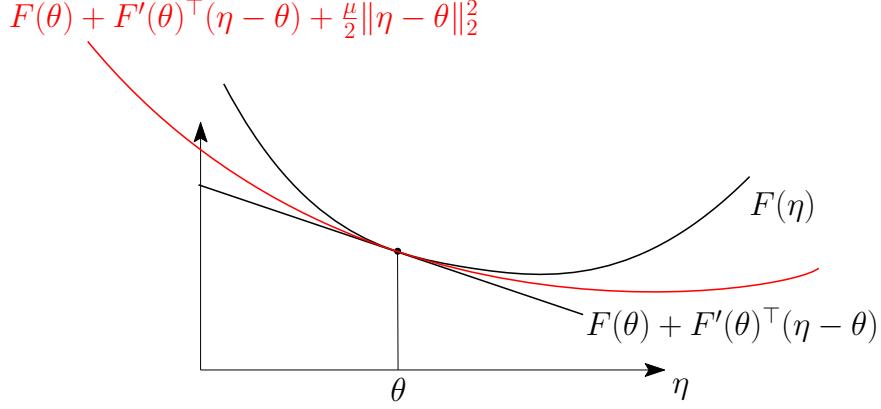
The analysis of optimization algorithms requires assumptions on the objective functions, like the ones introduced in this section. From these assumptions, additional properties are derived (typically inequalities), and then most convergence proofs look for a “Lyapunov function” (sometimes called a potential function) that goes down along the iterations. More precisely, if $V : \mathbb{R}^d \rightarrow \mathbb{R}_+$ is such that $V(\theta_t) \leq (1 - \alpha)V(\theta_{t-1})$, then $V(\theta_t) \leq (1 - \alpha)^t V(\theta_0)$ and we obtain linear convergence. The art is then to find the appropriate Lyapunov function.

We first consider an assumption allowing exponential convergence rates.

Definition 5.2 (Strong convexity) *A differentiable function F is said μ -strongly convex, with $\mu > 0$, if and only if*

$$F(\eta) \geq F(\theta) + F'(\theta)^\top (\eta - \theta) + \frac{\mu}{2} \|\eta - \theta\|_2^2, \quad \forall \eta, \theta \in \mathbb{R}^d. \quad (5.9)$$

The function F is strongly-convex if and only if the function F is strictly above its tangent and the difference is at least quadratic in the distance to the point where the two coincide. This notably allows us to define quadratic lower bounds on F . See below.



For twice differentiable functions, this is equivalent to $F''(\theta) \succcurlyeq \mu I$ for all θ , that is, all eigenvalues of $F''(\theta)$ are greater than or equal to μ (see Nesterov, 2018).

Exercise 5.5 Show that the differentiable function $F : \mathbb{R}^d \rightarrow \mathbb{R}$ is μ -strongly convex if and only if for all $\theta, \eta \in \mathbb{R}^d$, $\|F'(\theta) - F'(\eta)\|_2 \geq \mu\|\theta - \eta\|_2$.

Strong convexity through regularization. When an objective function F is convex, then $F + \frac{\mu}{2}\|\cdot\|_2^2$ is μ -strongly convex (proof left as an exercise). In practice, in machine learning problems with linear models, so that the empirical risk is convex, strong convexity most often comes from the regularizer (and thus μ decays with n), leading to condition numbers that grow with n (typically in \sqrt{n} or n).

Łojasiewicz inequality. Strong convexity implies that F admits a unique minimizer η_* , which is characterized by $F'(\eta_*) = 0$. Moreover, this guarantees that the gradient is large when a point is far from optimal (in function values):

Lemma 5.1 (Łojasiewicz inequality) If F is differentiable and μ -strongly convex with unique minimizer η_* , then we have:

$$\|F'(\theta)\|_2^2 \geq 2\mu(F(\theta) - F(\eta_*)), \quad \forall \theta \in \mathbb{R}^d.$$

Proof The right-hand side in Definition 5.2 is strongly convex in η and minimized with $\tilde{\eta} = \theta - \frac{1}{\mu}F'(\theta)$. Plugging this value into the bound and taking $\eta = \eta_*$ in the left-hand side, we get $F(\eta_*) \geq F(\theta) - \frac{1}{\mu}\|F'(\theta)\|_2^2 + \frac{1}{2\mu}\|F'(\theta)\|_2^2 = F(\theta) - \frac{1}{2\mu}\|F'(\theta)\|_2^2$. The conclusion follows by rearranging. ■

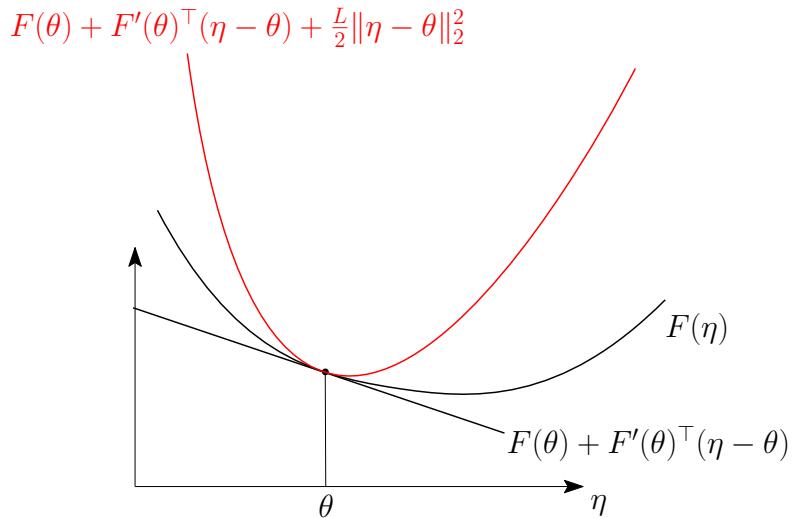
To obtain exponential convergence rates, strong-convexity is typically associated with smoothness, which we now define.

Definition 5.3 (Smoothness) A differentiable function F is said L -smooth if and only if

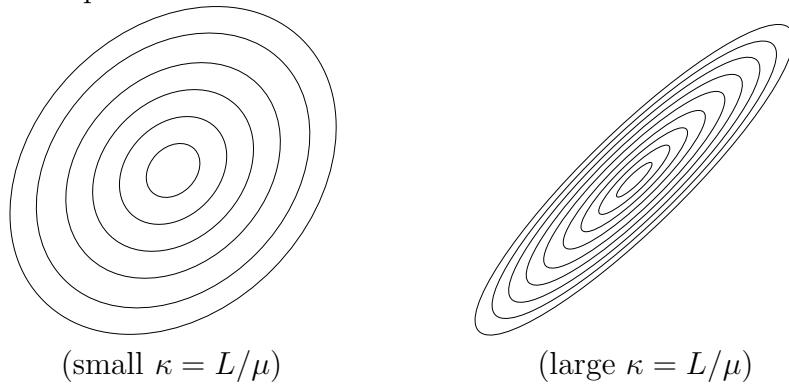
$$|F(\eta) - F(\theta) - F'(\theta)^\top(\eta - \theta)| \leq \frac{L}{2} \|\theta - \eta\|^2, \quad \forall \theta, \eta \in \mathbb{R}^d. \quad (5.10)$$

This is equivalent to F having a L -Lipschitz-continuous gradient, i.e., $\|F'(\theta) - F'(\eta)\|_2^2 \leq L^2\|\theta - \eta\|_2^2$, $\forall \theta, \eta \in \mathbb{R}^d$. For twice differentiable functions, this is equivalent to $-LI \preceq F''(\theta) \preceq LI$ (see [Nesterov, 2018](#)).

Note that when F is convex and L -smooth, we have a quadratic upper bound that is tight at any given point (strong convexity implies the corresponding lower bound with L replaced by μ). See below.



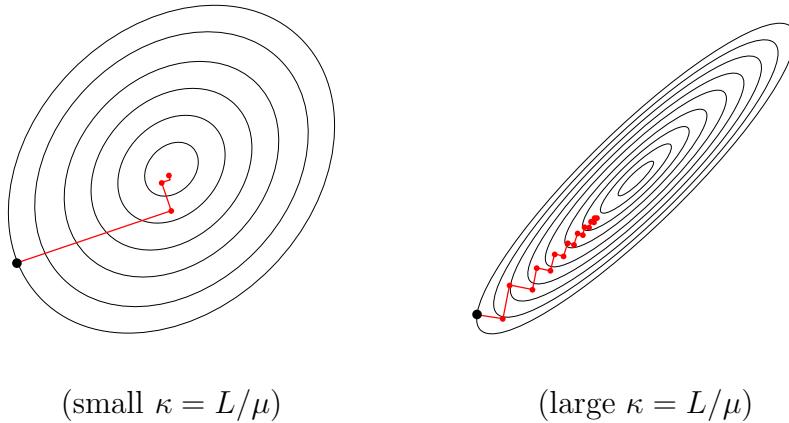
When a function is both smooth and strongly convex, we denote by $\kappa = L/\mu \geq 1$ its condition number (we recover the definition of Section 5.2.1 for quadratic functions). See examples below of level sets of functions with varying condition numbers: the condition number impacts the shapes of the level sets.



The performance of gradient descent will depend on this condition number (see steepest descent below, that is, gradient descent with exact line search): with a small condition

number (left), we get fast convergence, while for a large condition number (right), we get oscillations.

Exercise 5.6 (♦) We consider the angle α between the descent direction $-F'(\theta)$ and the deviation to optimum $\eta_* - \theta$, defined through $\cos \alpha = \frac{F'(\theta)^\top (\theta - \eta_*)}{\|F'(\theta)\| \cdot \|\theta - \eta_*\|_2}$. Show that for a μ -strongly-convex, L -smooth quadratic function, $\cos \alpha \geq \frac{2\sqrt{\mu L}}{L + \mu}$ (hint: prove and use the Kantorovich inequality $\sup_{\|z\|_2=1} z^\top H z z^\top H^{-1} z = \frac{(L+\mu)^2}{4\mu L}$). (♦♦) Show that the same result holds without the assumption that F is quadratic (hint: use the co-coercivity of the function $\theta \mapsto F(\theta) - \frac{\mu}{2} \|\theta\|_2^2$, from Prop. 5.3).



For machine learning problems, for linear predictions and smooth losses (square or logistic), we have smooth problems. If we use a squared ℓ_2 -regularizer $\frac{\mu}{2} \|\cdot\|_2^2$, we get a μ -strongly convex problem. Note that when using regularization, as explained in Chapters 3 and 4, the value of μ decays with n , typically between $1/n$ and $1/\sqrt{n}$, leading to condition numbers between \sqrt{n} and n .

In this context, gradient descent on the empirical risk is often called a “batch” technique because all the data points are accessed at every iteration.

In the next theorem, we show that gradient descent converges exponentially for such smooth and strongly-convex problems.

Theorem 5.1 (Convergence of GD for smooth strongly-convex functions) Assume that F is L -smooth and μ -strongly convex. Choosing $\gamma_t = 1/L$, the iterates $(\theta_t)_{t \geq 0}$ of GD on F satisfy

$$F(\theta_t) - F(\eta_*) \leq \left(1 - \frac{1}{\kappa}\right)^t (F(\theta_0) - F(\eta_*)) \leq \exp(-t/\kappa) (F(\theta_0) - F(\eta_*)).$$

Proof By the smoothness inequality in Eq. (5.10) applied to θ_{t-1} and $\theta_{t-1} - F'(\theta_{t-1})/L$, we have the following descent property, with $\gamma_t = 1/L$,

$$\begin{aligned} F(\theta_t) &= F\left(\theta_{t-1} - F'(\theta_{t-1})/L\right) \leq F(\theta_{t-1}) + F'(\theta_{t-1})^\top (-F'(\theta_{t-1})/L) + \frac{L}{2} \| -F'(\theta_{t-1})/L \|_2^2 \\ &= F(\theta_{t-1}) - \frac{1}{L} \| F'(\theta_{t-1}) \|_2^2 + \frac{1}{2L} \| F'(\theta_{t-1}) \|_2^2. \end{aligned}$$

Rearranging, we get

$$F(\theta_t) - F(\eta_*) \leq F(\theta_{t-1}) - F(\eta_*) - \frac{1}{2L} \| F'(\theta_{t-1}) \|_2^2.$$

Using Lemma 5.1, it follows

$$F(\theta_t) - F(\eta_*) \leq (1 - \mu/L)(F(\theta_{t-1}) - F(\eta_*)) \leq \exp(-\mu/L)(F(\theta_{t-1}) - F(\eta_*)).$$

We conclude by recursion and with the definition $\kappa = L/\mu$. ■

We can make the following observations:

- As mentioned before, we necessarily have $\mu \leq L$; the ratio $\kappa := L/\mu$ is called the *condition number*. It is a property of the objective function, which may be hard or easy to minimize. It is not invariant by linear changes of variables $\theta \rightarrow A\theta$, where A is an invertible linear map; finding a good A to reduce the condition number is the main principle behind “preconditioning” techniques (see, e.g., Nocedal and Wright, 1999 for more details).
- If we only assume that the function is smooth and convex (not strongly convex), then GD with constant step-size $\gamma = 1/L$ also converges when a minimizer exists, but at a slower rate in $O(1/t)$. See Section 5.2.4 below.
- Choosing the step-size only requires an upper bound L on the smoothness constant (in case it is over-estimated, the convergence rate only degrades slightly).
- Writing the update $(\theta_t - \theta_{t-1})/\gamma = -F'(\theta_{t-1})$, this algorithm can be seen, under the smoothness assumption, as the discretization of the gradient flow

$$\frac{d}{dt} \eta(t) = -F'(\eta),$$

where $\eta(t\gamma) \approx \theta_t$. This analogy can lead to several insights and proof ideas (see, e.g., Scieur et al., 2017).

- For this class of functions (convex and smooth), there exist first-order methods which achieve a faster rate, showing that gradient descent is not optimal. However, these improved algorithms also have drawbacks (lack of adaptivity, instability to noise,...). See below.

Exercise 5.7 Compute all constants for ℓ_2 -regularized logistic regression and for ridge regression.

Adaptivity. Note that gradient descent is adaptive to strong convexity: the exact same algorithm applies to both strongly convex and convex cases, and the two bounds apply. This adaptivity is important in practice, as often, locally around the global optimum, the strong convexity constant converges to the minimal eigenvalue of the Hessian at η_* , which can be significantly larger than μ (the global constant).

Fenchel conjugate (♦). Given some convex function $F : \mathbb{R}^d \rightarrow \mathbb{R}$, an important tool is the Fenchel-Legendre conjugate F^* defined as $F^*(\alpha) = \sup_{\theta \in \mathbb{R}^d} \alpha^\top \theta - F(\theta)$. In particular, when we allow extended-value functions (which may take the value $+\infty$), we can represent functions defined on a convex domain, and we have, under simple regularity conditions, that the conjugate of the conjugate of a convex function is the function itself. Thus, any convex function can be seen as a maximum of affine functions. Moreover, if the original function is not convex, the bi-conjugate is often referred to as the convex envelope and is the tightest convex lower-bound (this is often used when designing convex relaxations of non-convex problems). Moreover, the use of Fenchel conjugation is crucial when dealing with convex duality (which we will not cover in this chapter). See [Boyd and Vandenberghe \(2004\)](#) for details.

Exercise 5.8 Let F be an L -smooth convex function on \mathbb{R}^d . Show that its Fenchel conjugate is $(1/L)$ -strongly convex.

Exercise 5.9 Let F be an L -smooth convex function on \mathbb{R}^d , and F^* its Fenchel conjugate. Show that for any $\theta, z \in \mathbb{R}^d$, we have $F(\theta) + F^*(z) - z^\top \theta \geq 0$, if and only if $z = F'(\theta)$ (this is the Fenchel-Young inequality). (♦) Show in addition that $F(\theta) + F^*(z) - z^\top \theta \geq \frac{1}{2L} \|z - F'(\theta)\|_2^2$.

5.2.4 Analysis of GD for convex and smooth functions (♦)

To obtain the $1/t$ convergence rate without strong-convexity (like we got in Section 5.2.1 for quadratic functions), we will need an extra property of convex, smooth functions, sometimes called “co-coercivity”. This is an instance of inequalities we need to use to circumvent the lack of closed form for iterations.

Proposition 5.3 (co-coercivity) *If F is a convex L -smooth function on \mathbb{R}^d , then for all $\theta, \eta \in \mathbb{R}^d$, we have:*

$$\frac{1}{L} \|F'(\theta) - F'(\eta)\|_2^2 \leq [F'(\theta) - F'(\eta)]^\top (\theta - \eta).$$

Moreover, we have: $F(\theta) \geq F(\eta) + F'(\eta)^\top (\theta - \eta) + \frac{1}{2L} \|F'(\theta) - F'(\eta)\|^2$.

Proof We will show the second inequality, which implies the first one, by applying it twice with η and θ swapped, and summing them.

- Define $H(\theta) = F(\theta) - \theta^\top F'(\eta)$. The function $H : \mathbb{R}^d \rightarrow \mathbb{R}$ is convex with global minimum at η , since $H'(\theta) = F'(\theta) - F'(\eta)$, which is equal to zero for $\theta = \eta$. The function H is also L -smooth.
- From the definition of smoothness, we get $H(\theta - \frac{1}{L} H'(\theta)) \leq H(\theta) + H'(\theta)^\top (-\frac{1}{L} H'(\theta)) + \frac{L}{2} \|\theta - \frac{1}{L} H'(\theta)\|_2^2$, which is less than $H(\theta) - \frac{1}{2L} \|H'(\theta)\|_2^2$.
- This leads to $F(\eta) - \eta^\top F'(\eta) = H(\eta) \leq H(\theta - \frac{1}{L} H'(\theta)) \leq H(\theta) - \frac{1}{2L} \|H'(\theta)\|_2^2 = F(\theta) - \theta^\top F'(\eta) - \frac{1}{2L} \|F'(\theta) - F'(\eta)\|_2^2$, which leads to the desired inequality by shuffling terms.

■

We can now state the following convergence result for gradient descent with potentially no strong-convexity. Up to constants, we obtain the same rate as for quadratic functions in Eq. (5.5).

Theorem 5.2 (Convergence of GD for smooth convex functions) *Assume that F is L -smooth and convex, with a global minimizer η_* . Choosing $\gamma_t = 1/L$, the iterates $(\theta_t)_{t \geq 0}$ of GD on F satisfy*

$$F(\theta_t) - F(\eta_*) \leq \frac{L}{2t} \|\theta_0 - \eta_*\|_2^2.$$

Proof Following Bansal and Gupta (2019), the Lyapunov function that we will choose is

$$V_t(\theta_t) = t[F(\theta_t) - F(\eta_*)] + \frac{L}{2} \|\theta_t - \eta_*\|_2^2,$$

and our goal is to show that it decays along iterations. We can split the difference in Lyapunov functions in three terms (each with its own color):

$$V_t(\theta_t) - V_{t-1}(\theta_{t-1}) = t[F(\theta_t) - F(\theta_{t-1})] + F(\theta_{t-1}) - F(\eta_*) + \frac{L}{2} \|\theta_t - \eta_*\|_2^2 - \frac{L}{2} \|\theta_{t-1} - \eta_*\|_2^2.$$

To bound it:

- We use $F(\theta_t) - F(\theta_{t-1}) \leq -\frac{1}{2L} \|F'(\theta_{t-1})\|_2^2$ like in the proof of Theorem 5.1.
- We use $F(\theta_{t-1}) - F(\eta_*) \leq F'(\theta_{t-1})^\top (\theta_{t-1} - \eta_*)$, as a consequence of convexity (function above the tangent at θ_{t-1}), as in Eq. (5.7).
- We use $\frac{L}{2} \|\theta_t - \eta_*\|_2^2 - \frac{L}{2} \|\theta_{t-1} - \eta_*\|_2^2 = -L\gamma(\theta_{t-1} - \eta_*)^\top F'(\theta_{t-1}) + \frac{L\gamma^2}{2} \|F'(\theta_{t-1})\|_2^2$ by expanding the square.

This leads to, with the step-size $\gamma = 1/L$:

$$\begin{aligned} V_t(\theta_t) - V_{t-1}(\theta_{t-1}) &\leq t \left[-\frac{1}{2L} \|F'(\theta_{t-1})\|_2^2 \right] + F'(\theta_{t-1})^\top (\theta_{t-1} - \eta_*) \\ &\quad - L\gamma(\theta_{t-1} - \eta_*)^\top F'(\theta_{t-1}) + \frac{L\gamma^2}{2} \|F'(\theta_{t-1})\|_2^2 \\ &= -\frac{t-1}{2L} \|F'(\theta_{t-1})\|_2^2 \leq 0, \end{aligned}$$

which leads to

$$t[F(\theta_t) - F(\eta_*)] \leq V_t(\theta_t) \leq V_0(\theta_0) = \frac{L}{2} \|\theta_0 - \eta_*\|_2^2,$$

and thus $F(\theta_t) - F(\eta_*) \leq \frac{L}{2t} \|\theta_0 - \eta_*\|_2^2$. ■

The proof above is on purpose mysterious: the choice of Lyapunov function seems arbitrary at first, but all inequalities lead to nice cancellations. These proofs are sometimes hard to design. For an interesting line of work trying to automate these proofs, see <https://francisbach.com/computer-aided-analyses/>.

Exercise 5.10 (alternative convergence proof ♦) We consider an L -smooth convex function with a global minimizer η_* , and gradient descent with step-size $\gamma_t = 1/L$.

- Show that $\|\theta_t - \eta_*\|_2^2 \leq \|\theta_{t-1} - \eta_*\|_2^2$ for all $t \geq 1$.
- Show that $F(\theta_t) \leq F(\theta_{t-1}) - \frac{1}{2L} \|F'(\theta_{t-1})\|_2^2$.
- Denoting $\Delta_t = F(\theta_t) - F(\eta_*)$, show that $\Delta_t \leq \Delta_{t-1} - \frac{1}{2L\|\theta_0 - \eta_*\|^2} \Delta_{t-1}^2$ for all $t \geq 1$. Conclude that $\Delta_t \leq \frac{2L}{t+4} \|\theta_0 - \eta_*\|^2$.

5.2.5 Beyond gradient descent (♦)

While gradient descent is the simplest algorithm with a simple analysis, there are multiple extensions that we will only briefly mention (see more details by [Nesterov, 2004, 2007](#)):

Nesterov acceleration. For strongly-convex functions, a simple modification of gradient descent allows obtaining better convergence rates. The algorithm is as follows and is based on updating the following iterates:

$$\theta_t = \eta_{t-1} - \frac{1}{L} g'(\eta_{t-1}) \quad (5.11)$$

$$\eta_t = \theta_t + \frac{1 - \sqrt{\mu/L}}{1 + \sqrt{\mu/L}} (\theta_t - \theta_{t-1}), \quad (5.12)$$

and the convergence rate is then $F(\theta_t) - F(\eta_*) \leq L\|\theta_0 - \eta_*\|^2(1 - \sqrt{\mu/L})^t \leq L\|\theta_0 - \eta_*\|^2(1 - 1/\sqrt{\kappa})^t$, that is the characteristic time to convergence goes from κ to $\sqrt{\kappa}$. If κ is large (typically of order \sqrt{n} or n for machine learning), the gains are substantial. In practice, this leads to significant improvements. See a detailed description and many extensions by d'Aspremont et al. (2021).

For convex functions, we need the extrapolation step to depend on t as follows:

$$\theta_t = \eta_{t-1} - \frac{1}{L} F'(\eta_{t-1}) \quad (5.13)$$

$$\eta_t = \theta_t + \frac{t-1}{t+2} (\theta_t - \theta_{t-1}). \quad (5.14)$$

This simple modification dates back to Nesterov in 1983 and leads to the following convergence rate $F(\theta_t) - F(\eta_*) \leq \frac{2L\|\theta_0 - \eta_*\|^2}{(t+1)^2}$. See exercise below, and d'Aspremont et al. (2021) for more details.

Moreover, the last two rates are known to be optimal for the considered problems. For algorithms that access gradients and combine them linearly to select a new query point, it is impossible to have better dimension-independent rates. See Nesterov (2007) and Chapter 12 for more details.

Exercise 5.11 (♦♦) For the updates in Eq. (5.11) and Eq. (5.12), show that for $L(\theta, \eta) = f(\theta) - f(\eta_*) + \frac{\mu}{2} \left\| \eta - \eta_* + \frac{1 + \sqrt{\mu/L}}{\sqrt{\mu/L}} (\theta - \eta) \right\|_2^2$, then $L(\theta_t, \eta_t) \leq (1 - \sqrt{\mu/L}) L(\theta_{t-1}, \eta_{t-1})$. Show that this implies a convergence rate proportional to $(1 - \sqrt{\mu/L})^t$.

Exercise 5.12 (♦♦) For the updates in Eq. (5.13) and Eq. (5.14), show that for $L_t(\theta, \eta) = \left(\frac{t+1}{2}\right)^2 [f(\theta) - f(\eta_*) + \frac{L}{2} \left\| \eta - \eta_* + \frac{t}{2} (\eta - \theta) \right\|_2^2]$, then $L_t(\theta_t, \eta_t) \leq L_{t-1}(\theta_{t-1}, \eta_{t-1})$. Show that this implies a convergence rate proportional to $\frac{1}{t^2}$.

Newton method. Given θ_{t-1} , the Newton method minimizes the second-order Taylor expansion around θ_{t-1} (or, equivalently, finds a zero of F' by using a first-order Taylor

expansion of F' around θ_{t-1}):

$$F(\theta_{t-1}) + F'(\theta_{t-1})^\top(\theta - \theta_{t-1}) + \frac{1}{2}(\theta - \theta_{t-1})^\top F''(\theta_{t-1})^\top(\theta - \theta_{t-1}).$$

The gradient of this quadratic function is $\theta - \theta_{t-1} + F''(\theta_{t-1})^\top(\theta - \theta_{t-1})$, and setting it to zero leads to $\theta_t = \theta_{t-1} - F''(\theta_{t-1})^{-1}F'(\theta_{t-1})$, which is an expensive iteration, as the running-time complexity is $O(d^3)$ in general to solve the linear system. It leads to local quadratic convergence: If $\|\theta_{t-1} - \theta_*\|$ small enough, for some constant C , one can show $(C\|\theta_t - \theta_*\|) = (C\|\theta_{t-1} - \theta_*\|)^2$. See [Boyd and Vandenberghe \(2004\)](#) for more details and conditions for global convergence, in particular through the use of “self-concordance”, which is a property that relates third and second-order derivatives.

⚠ The denomination “quadratic” is sometimes confusing and corresponds to a number of significant digits that doubles at each iteration.

Note that for machine learning problems, quadratic convergence may be overkill compared to the computational complexity of each iteration since cost functions are averages of n terms and naturally have some uncertainty of order $O(1/\sqrt{n})$.

Exercise 5.13 (♦) Assume the function F is μ -strongly convex, twice differentiable, and such that the Hessian is Lipschitz-continuous, i.e., $\|f''(\theta) - f''(\eta)\|_{\text{op}} \leq M\|\theta - \eta\|_2$. Using the Taylor formula with integral remainder, show that for the iterates of Newton’s method, $\|\nabla F(\theta_t)\|_2 \leq \frac{M}{2\mu^2}\|\nabla F(\theta_{t-1})\|_2^2$. Show that this implies local quadratic convergence.

Proximal gradient descent (♦). Many optimization problems are said “composite”, that is, the objective function F is the sum of a smooth function G and a non-smooth function H (such as a norm). It turns out that a simple modification of gradient descent allows us to benefit from the fast convergence rates of smooth optimization (compared to the slower rates for non-smooth optimization that we would obtain from the subgradient method in the next section).

For this, we need to first see gradient descent as a *proximal method*. Indeed, one may see the iteration $\theta_t = \theta_{t-1} - \frac{1}{L}G'(\theta_{t-1})$, as

$$\theta_t = \arg \min_{\theta \in \mathbb{R}^d} G(\theta_{t-1}) + (\theta - \theta_{t-1})^\top G'(\theta_{t-1}) + \frac{L}{2}\|\theta - \theta_{t-1}\|_2^2,$$

where, for a L -smooth function G , the objective function above is an upper-bound of $G(\theta)$ which is tight at θ_{t-1} (see Eq. (5.10)).

While this reformulation does not bring much for gradient descent, we can extend this to the composite problem and consider the iteration

$$\theta_t = \arg \min_{\theta \in \mathbb{R}^d} G(\theta_{t-1}) + (\theta - \theta_{t-1})^\top G'(\theta_{t-1}) + \frac{L}{2}\|\theta - \theta_{t-1}\|_2^2 + H(\theta),$$

where H is left as is. It turns out that the convergence rates for $G + H$ are the same as smooth optimization, with potential acceleration (Nesterov, 2007; Beck and Teboulle, 2009).

The crux is to be able to compute the step above, that is, minimize with respect to θ functions of the form $\frac{L}{2}\|\theta - \eta\|_2^2 + H(\theta)$. When H is the indicator function of a convex set (which is equal to 0 inside the set, and $+\infty$ otherwise), we get projected gradient descent. When H is the ℓ_1 -norm, that is, $H = \lambda\|\cdot\|_1$, this can be shown to be a soft-thresholding step, as for each coordinate $\theta_i = (|\eta_i| - \lambda/L)_+ \frac{\eta_i}{|\eta_i|}$ (proof left as an exercise). See applications to model selection and sparsity-inducing norms in Chapter 8.

5.2.6 Non-convex objective functions (♦)

For smooth, potentially non-convex objective functions, the best one can hope for is to converge to a stationary point θ such that $F'(\theta) = 0$. The proof below provides the weaker result that at least one iterate has a small gradient. Indeed, using the same Taylor expansion as the convex case (which is still valid), we get, using the L -smoothness of F :

$$F(\theta_t) \leq F(\theta_{t-1}) - \frac{1}{2L}\|F'(\theta_{t-1})\|_2^2,$$

leading to, summing the inequalities above for all iterations between 1 and t :

$$\frac{1}{2Lt} \sum_{s=1}^t \|F'(\theta_{s-1})\|_2^2 \leq \frac{F(\theta_0) - F(\eta_*)}{t}.$$

Thus there has to be one s in $\{0, \dots, t-1\}$ for which $\|F'(\theta_s)\|_2^2 \leq O(1/t)$. Note that without further assumptions, this does not imply that any of the iterates is close to a stationary point.

5.3 Gradient methods on non-smooth problems

We now relax our assumptions and only require Lipschitz continuity in addition to convexity. The rates will be slower, but the extension to stochastic gradients will be easier.

Definition 5.4 (Lipschitz-continuous function) A function $F : \mathbb{R}^d \rightarrow \mathbb{R}$ is said B -Lipschitz-continuous if and only if

$$\|F(\eta) - F(\theta)\| \leq B\|\eta - \theta\|_2, \quad \forall \theta, \eta \in \mathbb{R}^d.$$

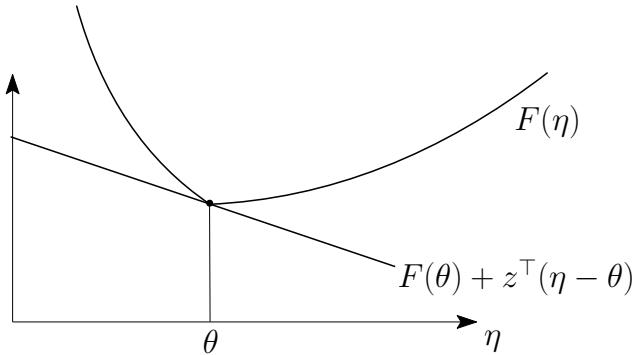
Without additional assumptions, this setting is usually referred to as *non-smooth* optimization.

Exercise 5.14 Show that if F is differentiable, this is equivalent to the assumption $\|F'(\theta)\|_2 \leq B, \forall \theta \in \mathbb{R}^d$.

From gradients to subgradients. We can apply non-smooth optimization to objective functions which are not differentiable (such as the hinge loss from Section 4.1.2). For convex Lipschitz-continuous objectives, one can show that the function is almost everywhere differentiable. In points where it is not, one can define the set of slopes of lower-bounding tangents as the *subdifferential* and any element of it as a *subgradient*. That is, we can define the subdifferential as (see illustration below):

$$\partial F(\theta) = \{z \in \mathbb{R}^d, \forall \eta \in \mathbb{R}^d, f(\eta) \geq f(\theta) + z^\top(\eta - \theta)\}.$$

See more details by [Rockafellar \(1997\)](#).



The gradient descent iteration is then meant as using any subgradient $z \in \partial F(\theta_{t-1})$ instead of $F'(\theta_{t-1})$. The method is then referred to as the subgradient method (it is not a descent method anymore, that is, the function values may go up once in a while).

Exercise 5.15 Compute the subdifferential of $\theta \mapsto |\theta|$ and $\theta \mapsto (1 - y\theta^\top x)_+$

Convergence rate of the subgradient method. We can prove convergence of the gradient descent algorithm, now with a decaying step-size and a slower rate than for smooth functions.

Theorem 5.3 (Convergence of the subgradient method) Assume that F is convex, B -Lipschitz-continuous, and admits a minimizer η_* that satisfies $\|\eta_* - \theta_0\|_2 \leq D$. By choosing $\gamma_t = \frac{D}{B\sqrt{t}}$ then the iterates $(\theta_t)_{t \geq 0}$ of GD on F satisfy

$$\min_{0 \leq s \leq t-1} F(\theta_s) - F(\eta_*) \leq DB \frac{2 + \log(t)}{2\sqrt{t}}. \quad (5.15)$$

Proof We look at how θ_t approaches η_* , that is, we try to use $\|\theta_t - \eta_*\|_2^2$ as a Lyapunov function. We have:

$$\begin{aligned}\|\theta_t - \eta_*\|_2^2 &= \|\theta_{t-1} - \gamma_t F'(\theta_{t-1}) - \eta_*\|_2^2 \\ &= \|\theta_{t-1} - \eta_*\|_2^2 - 2\gamma_t F'(\theta_{t-1})^\top (\theta_{t-1} - \eta_*) + \gamma_t^2 \|F'(\theta_{t-1})\|_2^2.\end{aligned}$$

Combining this with the convexity inequality $F(\theta_{t-1}) - F(\eta_*) \leq F'(\theta_{t-1})^\top (\theta_{t-1} - \eta_*)$ from Eq. (5.7), using the boundedness of the gradients (that is, $\|F'(\theta_{t-1})\|_2^2 \leq B^2$), it follows:

$$\|\theta_t - \eta_*\|_2^2 \leq \|\theta_{t-1} - \eta_*\|_2^2 - 2\gamma_t [F(\theta_{t-1}) - F(\eta_*)] + \gamma_t^2 B^2.$$

Thus, by isolating the distance to optimum in function values:

$$\gamma_t (F(\theta_{t-1}) - F(\eta_*)) \leq \frac{1}{2} \left(\|\theta_{t-1} - \eta_*\|_2^2 - \|\theta_t - \eta_*\|_2^2 \right) + \frac{1}{2} \gamma_t^2 B^2. \quad (5.16)$$

It is sufficient to sum these inequalities to get (in fact, for any $\eta_* \in \mathbb{R}^d$ and not only the minimizer),

$$\frac{1}{\sum_{s=1}^t \gamma_s} \sum_{s=1}^t \gamma_s (F(\theta_{s-1}) - F(\eta_*)) \leq \frac{\|\theta_0 - \eta_*\|_2^2}{2 \sum_{s=1}^t \gamma_s} + B^2 \frac{\sum_{s=1}^t \gamma_s^2}{2 \sum_{s=1}^t \gamma_s}.$$

As a weighted average, the left-hand side is larger than $\min_{0 \leq s \leq t-1} (F(\theta_s) - F(\eta_*))$, and also larger than $F(\bar{\theta}_t) - F(\eta_*)$ where $\bar{\theta}_t = (\sum_{s=1}^t \gamma_s \theta_{s-1}) / (\sum_{s=1}^t \gamma_s)$ by Jensen's inequality.

The upper bound goes to 0 if $\sum_{s=1}^t \gamma_s$ goes to ∞ (to forget the initial condition, sometimes called the “bias”) and $\gamma_t \rightarrow 0$ (to decrease the “variance” term). Let us choose $\gamma_s = \tau / \sqrt{s}$ for some $\tau > 0$. By using the series-integral comparisons below, we get the bound

$$\min_{0 \leq s \leq t-1} (F(\theta_s) - F(\eta_*)) \leq \frac{1}{2\sqrt{t}} \left(\frac{D^2}{\tau} + \tau B^2 (1 + \log(t)) \right).$$

We choose $\tau = D/B$ (which is suggested by optimizing the previous bound when $\log(t) = 0$), which leads to the result. In the proof, we used the following series-integral comparisons for decreasing functions:

$$\sum_{s=1}^t \frac{1}{\sqrt{s}} \geq \sum_{s=1}^t \frac{1}{\sqrt{t}} = \sqrt{t}$$

$$\text{and } \sum_{s=1}^t \frac{1}{s} \leq 1 + \sum_{s=2}^t \frac{1}{s} \leq 1 + \int_1^t \frac{ds}{s} = 1 + \log(t). \quad \blacksquare$$

The proof scheme above is very flexible. It can be extended in the following directions:

- There is no need to know in advance an upper-bound D on the distance to optimum; we then get with the same step-size $\gamma_t = \frac{D}{B\sqrt{t}}$ a rate of the form $\frac{BD}{2\sqrt{t}} \left(\frac{\|\theta_0 - \eta_*\|_2^2}{D^2} + (1 + \log(t)) \right)$. Moreover, a slightly modified version of the subgradient method removes the need to know the Lipschitz constant. See the exercise below.

Exercise 5.16 We consider the iteration $\theta_t = \theta_{t-1} - \frac{\gamma'_t}{\|F'(\theta_{t-1})\|_2} F'(\theta_{t-1})$. Show that with the step-size $\gamma'_t = D/\sqrt{t}$, we get the guarantee $\min_{0 \leq s \leq t-1} F(\theta_s) - F(\eta_*) \leq DB \frac{2+\log(t)}{2\sqrt{t}}$.

- The algorithm applies to constrained minimization over a convex set by inserting a projection step at each iteration (the proof, which uses the contractivity of orthogonal projections, is essentially the same; see the exercise below).

Exercise 5.17 Let $K \subset \mathbb{R}^d$ be a convex closed set, and $\Pi_K(\theta) = \arg \min_{\eta \in K} \|\eta - \theta\|_2^2$ be the orthogonal projection of θ onto K . Show that the function Π_K is contractive, that is, for all $\theta, \eta \in \mathbb{R}^d$, $\|\Pi_K(\theta) - \Pi_K(\eta)\|_2 \leq \|\theta - \eta\|_2$. For the algorithm $\theta_t = \Pi_K(\theta_{t-1} - \gamma_t F'(\theta_{t-1}))$, and η_* a minimizer of F on K , show that the guarantee of Theorem 5.3 still holds.

- The algorithm applies to non-differentiable convex and Lipschitz objective functions (using sub-gradients, i.e., any vector satisfying Eq. (5.6) in place of $F'(\theta_t)$).
- The algorithm can be applied to “non-Euclidean geometries”, where we consider bounds on the iterates or the gradient with different quantities, such as Bregman divergences. This can be done using the “mirror descent” framework, and for instance, can be applied to obtain multiplicative updates (see, e.g., Juditsky and Nemirovski, 2011a,b; Bubeck, 2015).

Exercise 5.18 (♦) Let $F : \mathbb{R}^d \rightarrow \mathbb{R}$ be a differentiable function, and $\psi : \mathbb{R}^d \rightarrow \mathbb{R}$ a strictly convex function:

- Show that the minimizer of $F(\theta) + F'(\theta)^\top (\eta - \theta) + \frac{1}{2\gamma} \|\eta - \theta\|_2^2$ is equal to $\eta = \theta - \gamma F'(\theta)$.
- Show that the Bregman divergence $D_\psi(\eta, \theta)$ defined as $D_\psi(\eta, \theta) = \psi(\eta) - \psi(\theta) - \psi'(\theta)^\top (\eta - \theta)$ is non-negative, and equal to zero if and only if $\eta = \theta$.
- Show that the minimizer of $F(\theta) + F'(\theta)^\top (\eta - \theta) + \frac{1}{\gamma} D_\psi(\eta, \theta)$ satisfies $\psi'(\eta) = \psi'(\theta) - \gamma F'(\theta)$. Show that the same conclusion holds if ψ is only defined on an open convex set $K \subset \mathbb{R}^d$, and so that the gradient ψ' is a bijection from K to \mathbb{R}^d .
- Apply to $\psi(\theta) = \sum_{i=1}^d \theta_i \log \theta_i$.

- Often the uniformly averaged iterate is used, as $\frac{1}{t} \sum_{s=0}^{t-1} \theta_s$. Convergence rates (without the $\log t$ factor) can be obtained using the Abel summation formula (see also Section 13.1.1).

Exercise 5.19 (♦) We consider the same assumptions as Exercise 5.17 and the same algorithm with orthogonal projections. With D the diameter of K , show that for the average iterate $\bar{\theta}_t = \frac{1}{t} \sum_{s=0}^{t-1} \theta_s$, we have: $F(\bar{\theta}_t) - F(\theta_*) \leq \frac{3BD}{2\sqrt{t}}$.

- The algorithm with the decaying step-size γ_t is an “anytime” algorithm; that is, it can be stopped at any time t , and the bound in Eq. (5.15) then applies. Computations are often easier when considering a constant step-size γ that depends on the number of iterations T that the user wishes to perform, T being usually referred to as the “horizon”. Starting from Eq. (5.16), we get the bound:

$$\frac{1}{T} \sum_{t=1}^T F(\theta_{t-1}) - F(\theta_*) \leq \frac{D^2}{2\gamma T} + \frac{\gamma B^2}{2},$$

where the optimal γ can be obtained as $\gamma = \frac{D}{B\sqrt{T}}$ and an optimized rate of $\frac{DB}{\sqrt{T}}$. We gain on the logarithmic factor, but we no longer have an anytime algorithm (since the bound only applies at time T). This applies as well to SGD in Section 5.4.

- Stochastic gradients can be used, as presented below (one interpretation is that the subgradient method is so slow that it is robust to noisy gradients).

Exercise 5.20 Compute all constants for ℓ_2 -regularized logistic regression and the support vector machine.

5.4 Convergence rate of stochastic gradient descent (SGD)

For machine learning problems, where $F(\theta) = \frac{1}{n} \sum_{i=1}^n \ell(y_i, f_\theta(x_i)) + \Omega(\theta)$, at each iteration, the gradient descent algorithm requires computing a “full” gradient $F'(\theta_{t-1})$, which could be costly as it requires accessing the entire data set (all n pairs of observations). An alternative is to instead only compute *unbiased* stochastic estimations of the gradient $g_t(\theta_{t-1})$, i.e., such that

$$\mathbb{E}[g_t(\theta_{t-1})|\theta_{t-1}] = F'(\theta_{t-1}), \quad (5.17)$$

which could be much faster to compute, in particular by accessing fewer observations.

⚠ Note that we need to condition over θ_{t-1} because θ_{t-1} encapsulates all the randomness due to past iterations, and we only require “fresh” randomness at time t .

⚠ Somewhat surprisingly, this unbiasedness does *not* need to be coupled with a vanishing variance: while there are always errors in the gradient, the use of a decreasing step-size will ensure convergence. If the noise in the gradient is not unbiased, then we only get convergence

if the noise magnitudes go to zero (see, e.g., d'Aspremont, 2008; Schmidt et al., 2011 and references therein).

This leads to the following algorithm.

Algorithm 5.2 (Stochastic gradient descent (SGD)) Choose a step-size sequence $(\gamma_t)_{t \geq 0}$, pick $\theta_0 \in \mathbb{R}^d$ and for $t \geq 1$, let

$$\theta_t = \theta_{t-1} - \gamma_t g_t(\theta_{t-1}),$$

where $g_t(\theta_{t-1})$ satisfies Eq. (5.17).

SGD in machine learning. There are two ways to use SGD for supervised machine learning:

- (1) **Empirical risk minimization:** If $F(\theta) = \frac{1}{n} \sum_{i=1}^n \ell(y_i, f_\theta(x_i))$ then at iteration t we can choose uniformly at random $i(t) \in \{1, \dots, n\}$ and define g_t as the gradient of $\theta \mapsto \ell(y_{i(t)}, f_\theta(x_{i(t)}))$. Here the randomness comes from the random choice of indices.

There exist “mini-batch” variants where at each iteration, the gradient is averaged over a random subset of the indices (we then reduce the variance of the gradient estimate, but we use more gradients, and thus the running time increases, see Exercise 5.21). We then converge to a *minimizer* η_* of the empirical risk.

Note here that since we sample *with replacement*, a given function will be selected several times, even within n iterations. Sampling without replacement can also be studied but its analysis is more involved (see, e.g., Nagaraj et al., 2019, and references therein).

- (2) **Expected risk minimization:** If $F(\theta) = \mathbb{E}[\ell(y, f_\theta(x))]$ is the expected (non-observable) risk, then at iteration t we can take a fresh sample (x_t, y_t) and define g_t as the gradient of $\theta \mapsto \ell(y_t, f_\theta(x_t))$, for which, if we swap the orders of expectation and differentiation, we get the unbiasedness. Note here that to preserve the unbiasedness, only a single pass is allowed (otherwise, this would create dependencies that would break it) and that the randomness comes from the observations (x_t, y_t) themselves.

Here, we *directly minimize the (generalization) risk*. The counterpart is that if we only have n samples, then we can only run n SGD iterations, and when n grows, the iterates will converge to a *minimizer* θ_* of the expected risk.

Note that in practice, multiple passes over the data (that is, using each observation multiple times) lead to better performance. To avoid overfitting, either a regularization term is added to the empirical risk, or the SGD algorithm is stopped before its convergence (and typically when some validation risk stops decreasing), which is referred to as regularization by “early stopping”.

We can study the two situations above using the latter one by considering the empirical risk as the expectation with respect to the empirical distribution of the data (and we thus use the notation θ_* for the global minimizer).

 Stochastic gradient descent is not a descent method: the function values often go up, but they go down “on average”. See, for example, an illustration in Figure 5.2.

Under the same usual assumptions on the objective functions, we now study SGD with the following extra assumptions:

- (H1) unbiased gradient: $\mathbb{E}[g_t(\theta_{t-1})|\theta_{t-1}] = F'(\theta_{t-1})$, $\forall t \geq 1$,
- (H2) bounded gradient: $\|g_t(\theta_{t-1})\|_2^2 \leq B^2$, $\forall t$ almost surely

Assumption (H2) could be replaced by other regularity conditions (e.g., Lipschitz-continuous gradients). Assumption (H1) is crucial and is often obtained by considering independent gradient functions g_t , for which we have $\mathbb{E}[g_t(\cdot)] = F'(\cdot)$. See Exercise 5.22 for SGD for smooth functions.

Theorem 5.4 (Convergence of SGD) *Assume that F is convex, B -Lipschitz and admits a minimizer θ_* that satisfies $\|\theta_* - \theta_0\|_2 \leq D$. Assume that the stochastic gradients satisfy (H1-2). Then, choosing $\gamma_t = (D/B)/\sqrt{t}$, the iterates $(\theta_t)_{t \geq 0}$ of SGD on F satisfy*

$$\mathbb{E}[F(\bar{\theta}_t) - F(\theta_*)] \leq DB \frac{2 + \log(t)}{2\sqrt{t}}.$$

where $\bar{\theta}_t = (\sum_{s=1}^t \gamma_s \theta_{s-1}) / (\sum_{s=1}^t \gamma_s)$.

We state our bound in terms of the average iterates because the cost of finding the best iterate could be higher than that of evaluating a stochastic gradient (since we cannot compute F in general).

Proof We follow essentially the same proof as in the deterministic case, adding some expectations at well-chosen places. We have:

$$\begin{aligned} \mathbb{E}[\|\theta_t - \theta_*\|_2^2] &= \mathbb{E}[\|\theta_{t-1} - \gamma_t g_t(\theta_{t-1}) - \theta_*\|_2^2] \\ &= \mathbb{E}[\|\theta_{t-1} - \theta_*\|_2^2] - 2\gamma_t \mathbb{E}[g_t(\theta_{t-1})^\top (\theta_{t-1} - \theta_*)] + \gamma_t^2 \mathbb{E}[\|g_t(\theta_{t-1})\|_2^2]. \end{aligned}$$

We can then compute the expectation of the middle term as:

$$\begin{aligned} \mathbb{E}[g_t(\theta_{t-1})^\top (\theta_{t-1} - \theta_*)] &= \mathbb{E}[\mathbb{E}[g_t(\theta_{t-1})^\top (\theta_{t-1} - \theta_*)|\theta_{t-1}]] \\ &= \mathbb{E}[\mathbb{E}[g_t(\theta_{t-1})|\theta_{t-1}]^\top (\theta_{t-1} - \theta_*)] = \mathbb{E}[F'(\theta_{t-1})^\top (\theta_{t-1} - \theta_*)], \end{aligned}$$

where we have crucially used the unbiasedness assumption (H1). This leads to

$$\mathbb{E}[\|\theta_t - \theta_*\|_2^2] \leq \mathbb{E}[\|\theta_{t-1} - \theta_*\|_2^2] - 2\gamma_t \mathbb{E}[F'(\theta_{t-1})^\top (\theta_{t-1} - \theta_*)] + \gamma_t^2 B^2.$$

Thus, combining with the convexity inequality $F(\theta_{t-1}) - F(\theta_*) \leq F'(\theta_{t-1})^\top (\theta_{t-1} - \theta_*)$ from Eq. (5.7), we get

$$\gamma_t \mathbb{E}[F(\theta_{t-1}) - F(\theta_*)] \leq \frac{1}{2} \left(\mathbb{E}[\|\theta_{t-1} - \theta_*\|_2^2] - \mathbb{E}[\|\theta_t - \theta_*\|_2^2] \right) + \frac{1}{2} \gamma_t^2 B^2. \quad (5.18)$$

Except for the expectations, this is the same bound as Eq. (5.16), so we can conclude as in the proof of Theorem 5.3. ■

We can make the following observations:

- Averaging of iterates is often performed after a certain number of iterations (e.g., one pass over the data when doing multiple passes): having such a “burn-in” period speeds up the algorithms by forgetting initial conditions faster.
- Many authors consider the projected version of the algorithm where after the gradient step, we orthogonally project onto the ball of radius D and center θ_0 . The bound is then exactly the same.
- The result that we obtain, when applied to single pass SGD, is a generalization bound; that is, after the n iterations, we have an excess risk proportional to $1/\sqrt{n}$, corresponding to the excess risk compared to the best predictor f_θ .

This is to be compared to using results from Chapter 4 (uniform deviation bounds) and non-stochastic gradient descent. It turns out that the estimation error due to having n observations is exactly the same as the generalization bound obtained by SGD (see Section 4.5.4 in Chapter 4). Still, we need to add on top of the optimization error proportional to $1/\sqrt{t}$ (with the same constants). The bounds match if $t = n$, that is, we run n iterations of gradient descent on the empirical risk. This leads to a running time complexity of $O(tnd) = O(n^2d)$ instead of $O(nd)$ using SGD, hence the strong gains in using SGD.

⚠ We are still comparing upper bounds.

- The bound in $O(BD/\sqrt{t})$ is optimal for this class of problem. That is, as shown for example by Agarwal et al. (2009), among all algorithms that can query stochastic gradients, having a better convergence rate (up to some constants) is impossible. See Section 12.3.
- As opposed to the deterministic case, the use of smoothness does not lead to significantly better results (see Exercise 5.22).

SGD or gradient descent on the empirical risk? As seen above, the number of iterations to reach a given precision will be larger for stochastic gradient descent than for smooth deterministic gradient descent, but with a complexity that is typically n times faster. Thus, for high precision, that is, low values of $F(\theta) - F(\eta_*)$ (which is not needed for machine learning), the number of iterations of SGD may become prohibitively large, and deterministic full gradient descent could be preferred. However, for low precision and large n , SGD is the method of choice (see also recent improvements in Section 5.4.2).

Exercise 5.21 We consider the mini-batch version of SGD, where at every iteration, we replace $g_t(\theta_{t-1})$ by the average of m independent samples of stochastic gradients at θ_{t-1} . Extend the convergence result of Theorem 5.4.

Exercise 5.22 (♦) We consider independent and identically distributed convex L -smooth random functions $f_t : \mathbb{R}^d \rightarrow \mathbb{R}$, $t \geq 1$, with expectation $F : \mathbb{R}^d \rightarrow \mathbb{R}$, that has a minimizer $\theta_* \in \mathbb{R}^d$. We consider the SGD recursion $\theta_t = \theta_{t-1} - \gamma_t f'_t(\theta_{t-1})$, with γ_t a deterministic step-size sequence. Using co-coercivity (Prop. 5.3), show that

$$\mathbb{E}[\|\theta_t - \theta_*\|_2^2] \leq \mathbb{E}[\|\theta_{t-1} - \theta_*\|_2^2] - 2\gamma_t(1 - \gamma_t L)\mathbb{E}[F'(\theta_{t-1})^\top(\theta_{t-1} - \theta_*)] + 2\gamma_t^2\mathbb{E}[\|f'_t(\theta_*)\|_2^2].$$

Extend the proof of Theorem 5.4 to obtain an explicit rate in $O(1/\sqrt{t})$.

5.4.1 Strongly convex problems (♦)

We consider the regularized problem $G(\theta) = F(\theta) + \frac{\mu}{2}\|\theta\|_2^2$, with the same assumption as above, and started at $\theta_0 = 0$. The SGD iteration is then, with $g_t(\theta_{t-1})$ a stochastic (sub)gradient of F at θ_{t-1} :

$$\theta_t = \theta_{t-1} - \gamma_t[g_t(\theta_{t-1}) + \mu\theta_{t-1}]. \quad (5.19)$$

We then have an improved convergence rate in $O(1/t)$ with a different decay for the step-size.

Theorem 5.5 (Convergence of SGD for strongly-convex problems) Assume that F is convex, B -Lipschitz and that $F + \frac{\mu}{2}\|\cdot\|_2^2$ admits a (necessarily unique) minimizer θ_* . Assume that the stochastic gradient g satisfies (H1-2). Then, choosing $\gamma_t = 1/(\mu t)$, the iterates $(\theta_t)_{t \geq 0}$ of SGD from Eq. (5.19) satisfy

$$\mathbb{E}[G(\bar{\theta}_t) - G(\theta_*)] \leq \frac{2B^2(1 + \log t)}{\mu t},$$

where $\bar{\theta}_t = \frac{1}{t} \sum_{s=1}^t \theta_s$.

Proof The beginning of the proof is essentially the same as for convex problems, leading to (with the new terms in blue):

$$\begin{aligned}\mathbb{E}[\|\theta_t - \theta_*\|_2^2] &= \mathbb{E}[\|\theta_{t-1} - \gamma_t(g_t(\theta_{t-1}) + \mu\theta_{t-1}) - \theta_*\|_2^2] \\ &= \mathbb{E}[\|\theta_{t-1} - \theta_*\|_2^2] - 2\gamma_t \mathbb{E}[(g_t(\theta_{t-1}) + \mu\theta_{t-1})^\top (\theta_{t-1} - \theta_*)] + \gamma_t^2 \mathbb{E}[\|g_t(\theta_{t-1}) + \mu\theta_{t-1}\|_2^2].\end{aligned}$$

From the iterations in Eq. (5.19), we see that $\theta_t = (1 - \gamma_t\mu)\theta_{t-1} + \gamma_t\mu[-\frac{1}{\mu}g_t(\theta_{t-1})]$ is a convex combination of gradients divided by $-\mu$, and thus $\|g_t(\theta_{t-1}) + \mu\theta_{t-1}\|_2^2$ is always less than $4B^2$. Thus

$$\mathbb{E}[\|\theta_t - \theta_*\|_2^2] \leq \mathbb{E}[\|\theta_{t-1} - \theta_*\|_2^2] - 2\gamma_t \mathbb{E}[G'(\theta_{t-1})^\top (\theta_{t-1} - \theta_*)] + 4\gamma_t^2 B^2.$$

Therefore, combining with the strong convexity inequality $G(\theta_{t-1}) - G(\theta_*) + \frac{\mu}{2}\|\theta_{t-1} - \theta_*\|_2^2 \leq G'(\theta_{t-1})^\top (\theta_{t-1} - \theta_*)$ (see Eq. (5.9)), it follows

$$\gamma_t \mathbb{E}[G(\theta_{t-1}) - G(\theta_*)] \leq \frac{1}{2}((1 - \gamma_t\mu) \mathbb{E}\|\theta_{t-1} - \theta_*\|^2 - \mathbb{E}\|\theta_t - \theta_*\|^2) + 2\gamma_t^2 B^2,$$

and thus, now using the specific step-size choice $\gamma_t = 1/(\mu t)$:

$$\begin{aligned}\mathbb{E}[G(\theta_{t-1}) - G(\theta_*)] &\leq \frac{1}{2}((\gamma_t^{-1} - \mu) \mathbb{E}\|\theta_{t-1} - \theta_*\|^2 - \gamma_t^{-1} \mathbb{E}\|\theta_t - \theta_*\|^2) + 2\gamma_t B^2, \\ &= \frac{1}{2}(\mu(t-1) \mathbb{E}\|\theta_{t-1} - \theta_*\|^2 - \mu t \mathbb{E}\|\theta_t - \theta_*\|^2) + \frac{2B^2}{\mu t}.\end{aligned}$$

Thus, we get a telescoping sum: summing between all indices between 1 and t , and using the bound $\sum_{s=1}^t \frac{1}{s} \leq 1 + \log t$, we get the desired result. ■

We can make the following observations:

- For smooth problems, we can show a similar bound of the form $O(\kappa/t)$. For quadratic problems, constant step-sizes can be used with averaging, leading to improved convergence rates (Bach and Moulines, 2013). See the exercise below.

Exercise 5.23 (♦) We consider the minimization of $F(\theta) = \frac{1}{2}\theta^\top H\theta - c^\top \theta$, where $H \in \mathbb{R}^{d \times d}$ is positive definite (and thus invertible). We consider the recursion $\theta_t = \theta_{t-1} - \gamma[F'(\theta_{t-1}) + \varepsilon_t]$, where all ε_t 's are independent, with zero mean and covariance matrix equal to C . Compute explicitly $\mathbb{E}[F(\theta_t) - F(\theta_*)]$, and provide an upper-bound of $\mathbb{E}[F(\bar{\theta}_t) - F(\theta_*)]$, where $\bar{\theta}_t = \frac{1}{t} \sum_{s=0}^{t-1} \theta_s$.

- The bound in $O(B^2/\mu t)$ is optimal for this class of problems. That is, as shown for example by Agarwal et al. (2009), among all algorithms that can query stochastic gradients, having a better convergence rate (up to some constants) is impossible (see Section 12.3).

- We note that for the same regularized problem, we could use a step size proportional to DB/\sqrt{t} and obtain a bound proportional to DB/\sqrt{t} , which looks worse than $B^2/(\mu t)$, but can, in fact, be better when μ is very small.

Note also the loss of adaptivity: the step-size now depends on the problem's difficulty (this was different for deterministic gradient descent). See experiments below for illustrations.

Exercise 5.24 *With the same assumptions as Theorem 5.5, show that with the step-size $\gamma_t = \frac{2}{\mu(t+1)}$, and with $\bar{\theta}_t = \frac{2}{t(t+1)} \sum_{s=1}^t s\theta_{s-1}$, we have: $\mathbb{E}[G(\bar{\theta}_t) - G(\theta_*)] \leq \frac{8B^2}{\mu(t+1)}$.*

Experiments. We consider a simple binary classification problem with linear predictors in dimension $d = 40$ (inputs generated from a Gaussian distribution, with binary outputs obtained as the sign of a linear function with additive Gaussian noise), with $n = 400$ observations, and observed features with ℓ_2 -norm bounded by R . We consider the hinge loss with a squared ℓ_2 -regularizer $\frac{\mu}{2}\|\cdot\|_2^2$ (that is, the support vector machine presented in Section 4.1.2). We measure the excess training objective. We consider two values of μ , and compare the two step-sizes $\gamma_t = 1/(R^2\sqrt{t})$ and $\gamma_t = 1/(\mu t)$ in Figure 5.2. We see that for large enough μ , the strongly-convex step-size is better. This is not the case for small μ .

The experiments above highlight the danger of a step-size equal to $1/(\mu t)$. In practice, it is often preferable to use $\gamma_t = \frac{1}{B^2\sqrt{t}+\mu t}$, as shown in the exercise below.

Exercise 5.25 (♦♦) *With the same assumptions as in Theorem 5.5, with $\gamma_t = \frac{1}{B^2\sqrt{t}+\mu t}$, provide a convergence rate for the averaged iterate.*

5.4.2 Variance reduction (♦)

We consider a finite sum $F(\theta) = \frac{1}{n} \sum_{i=1}^n f_i(\theta)$, where each f_i is R^2 -smooth (for example, logistic regression with features bounded by R in ℓ_2 -norm), and which is such that F is μ -strongly convex (for example by adding $\frac{\mu}{2}\|\theta\|_2^2$ to each f_i , or by benefitting from the strong convexity of the sum). We denote by $\kappa = R^2/\mu$ the condition number of the problem (note that it is more significant than L/μ , where L is the smoothness constant of F).

Using SGD, the convergence rate has been shown to be $O(\kappa/t)$ in Section 5.4.1, with iterations of complexity $O(d)$, while for GD, the convergence rate is $O(\exp(-t/\kappa))$ (see Section 5.2.3), but each iteration has complexity $O(nd)$. We now present a result allowing exponential convergence with an iteration cost of $O(d)$.

The idea is to use a form of *variance reduction*, made possible by keeping in memory past gradients. We denote by $z_i^{(t)} \in \mathbb{R}^d$ the version of gradient i stored at time t .

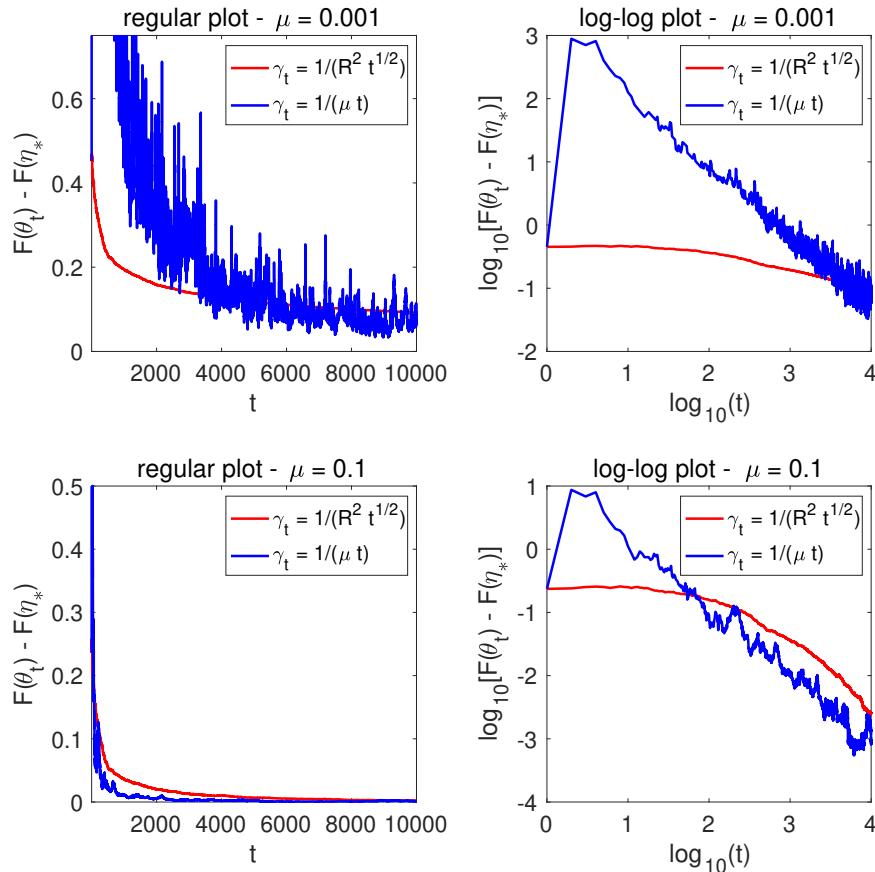


Figure 5.2: Comparison of step-sizes for SGD for the support vector machine, for two values of the regularization parameter μ (top: large μ , bottom: small μ). The performance is measured with a single run (hence the variability) on the excess training objective (left: regular plot, right: “log-log” plot).

The SAGA algorithm (Defazio et al., 2014), which combines the earlier algorithms SAG (Schmidt et al., 2017) and SVRG (Johnson and Zhang, 2013; Zhang et al., 2013), works as follows: at every iteration, an index $i(t)$ is selected uniformly at random in $\{1, \dots, n\}$, and we perform the iteration

$$\theta_t = \theta_{t-1} - \gamma \left[f'_{i(t)}(\theta_{t-1}) + \frac{1}{n} \sum_{i=1}^n z_i^{(t-1)} - z_{i(t)}^{(t-1)} \right],$$

with $z_{i(t)}^{(t)} = f'_{i(t)}(\theta_{t-1})$ and all others $z_i^{(t)}$ left unchanged (i.e., the same as $z_i^{(t-1)}$). In words, we add to the update with the stochastic gradient $f'_{i(t)}(\theta_{t-1})$ the term $\frac{1}{n} \sum_{i=1}^n z_i^{(t-1)} - z_{i(t)}^{(t-1)}$, which has zero expectation with respect to $i(t)$. Thus, since the expectation of $f'_{i(t)}(\theta_{t-1})$ with respect to $i(t)$ is equal to the full gradient $F'(\theta)$, the update is *unbiased* like for regular SGD. The goal is to reduce its variance.

The idea behind variance reduction is that if the random variable $z_{i(t)}^{(t-1)}$ (only considering the source of randomness coming from $i(t)$) is positively correlated with $f'_{i(t)}(\theta_{t-1})$, then the variance is reduced, and larger step-sizes can be used.

As the algorithm converges, then $z_i^{(t)}$ converges to $f'_i(\eta_*)$ (the individual gradient at optimum). We will show that *simultaneously* θ_t converges to η_* and $z_i^{(t)}$ converges to $f'_i(\eta_*)$ for all i , all at the same speed.

Theorem 5.6 (Convergence of SAGA) *If initializing with $z_i^{(0)} = f'_i(\theta_0)$ at the initial point $\theta_0 \in \mathbb{R}^d$, for all $i \in \{1, \dots, n\}$, we have, for the choice of step-size $\gamma = \frac{1}{4R^2}$:*

$$\mathbb{E}[\|\theta_t - \eta_*\|_2^2] \leq \left(1 - \min\left\{\frac{1}{3n}, \frac{3\mu}{16R^2}\right\}\right)^t \left(1 + \frac{n}{4}\right) \|\theta_0 - \eta_*\|_2^2. \quad (5.20)$$

Proof (♦♦) The proof consists in finding a Lyapunov function that decays along iterations.

Step 1. We first try our “usual” Lyapunov function, making the differences $\|z_i^{(t)} - f'_i(\eta_*)\|_2^2$ appear, with the update $\theta_t = \theta_{t-1} - \gamma \omega_t$, with $\omega_t = [f'_{i(t)}(\theta_{t-1}) + \frac{1}{n} \sum_{i=1}^n z_i^{(t-1)} - z_{i(t)}^{(t-1)}]$,

$$\begin{aligned} \|\theta_t - \eta_*\|_2^2 &= \|\theta_{t-1} - \eta_*\|_2^2 - 2\gamma(\theta_{t-1} - \eta_*)^\top \omega_t + \gamma^2 \|\omega_t\|_2^2 \text{ by expanding the square,} \\ \mathbb{E}_{i(t)} \|\theta_t - \eta_*\|_2^2 &= \|\theta_{t-1} - \eta_*\|_2^2 - 2\gamma(\theta_{t-1} - \eta_*)^\top F'(\theta_{t-1}) \\ &\quad + \gamma^2 \mathbb{E}_{i(t)} \left\| f'_{i(t)}(\theta_{t-1}) + \frac{1}{n} \sum_{i=1}^n z_i^{(t-1)} - z_{i(t)}^{(t-1)} \right\|_2^2 \\ &\quad \text{using the unbiasedness of the stochastic gradient,} \\ &\leq \|\theta_{t-1} - \eta_*\|_2^2 - 2\gamma(\theta_{t-1} - \eta_*)^\top F'(\theta_{t-1}) + 2\gamma^2 \mathbb{E}_{i(t)} \|f'_{i(t)}(\theta_{t-1}) - f'_{i(t)}(\eta_*)\|_2^2 \\ &\quad + 2\gamma^2 \mathbb{E}_{i(t)} \|f'_{i(t)}(\eta_*) - z_{i(t)}^{(t-1)} + \frac{1}{n} \sum_{i=1}^n z_i^{(t-1)}\|_2^2 \text{ using } \|a + b\|_2^2 \leq 2\|a\|_2^2 + 2\|b\|_2^2. \end{aligned}$$

In order to bound $\mathbb{E}_{i(t)} \|f'_{i(t)}(\theta_{t-1}) - f'_{i(t)}(\eta_*)\|_2^2$, we use co-coercivity of all functions f_i (see Prop. 5.3), to get:

$$\begin{aligned} \mathbb{E}_{i(t)} \|f'_{i(t)}(\theta_{t-1}) - f'_{i(t)}(\eta_*)\|_2^2 &= \frac{1}{n} \sum_{i=1}^n \|f'_i(\theta_{t-1}) - f'_i(\eta_*)\|_2^2 \\ &\leq \frac{1}{n} \sum_{i=1}^n R^2 [f'_i(\theta_{t-1}) - f'_i(\eta_*)]^\top (\theta_{t-1} - \theta_*) \\ &\leq R^2 F'(\theta_{t-1})^\top (\theta_{t-1} - \eta_*) \text{ since } \sum_{i=1}^n f'_i(\eta_*) = 0. \quad (5.21) \end{aligned}$$

In order to bound $\mathbb{E}_{i(t)} \|f'_{i(t)}(\eta_*) - z_i^{(t-1)} + \frac{1}{n} \sum_{i=1}^n z_i^{(t-1)}\|_2^2$, we can simply use the identity $\mathbb{E}_{i(t)} \|Z - \mathbb{E}_{i(t)} Z\|_2^2 \leq \mathbb{E}_{i(t)} \|Z\|_2^2$. We thus get

$$\begin{aligned} \mathbb{E}_{i(t)} \|\theta_t - \eta_*\|_2^2 &\leq \|\theta_{t-1} - \eta_*\|_2^2 - 2\gamma(\theta_{t-1} - \eta_*)^\top F'(\theta_{t-1}) + 2\gamma^2 R^2 (\theta_{t-1} - \eta_*)^\top F'(\theta_{t-1}) \\ &\quad + 2\gamma^2 \frac{1}{n} \sum_{i=1}^n \|f'_i(\eta_*) - z_i^{(t-1)}\|_2^2, \\ &\leq \|\theta_{t-1} - \eta_*\|_2^2 - 2\gamma(1 - \gamma R^2)(\theta_{t-1} - \eta_*)^\top F'(\theta_{t-1}) + 2\frac{\gamma^2}{n} \sum_{i=1}^n \|f'_i(\eta_*) - z_i^{(t-1)}\|_2^2. \end{aligned}$$

Step 2. We see the term $\sum_{i=1}^n \|f'_i(\eta_*) - z_i^{(t-1)}\|_2^2$ appearing, so we try to study how it varies across iterations. We have, by definition of the updates of the vectors $z_i^{(t)}$:

$$\sum_{i=1}^n \|f'_i(\eta_*) - z_i^{(t)}\|_2^2 = \sum_{i=1}^n \|f'_i(\eta_*) - z_i^{(t-1)}\|_2^2 - \|f'_{i(t)}(\eta_*) - z_{i(t)}^{(t-1)}\|_2^2 + \|f'_{i(t)}(\eta_*) - f'_{i(t)}(\theta_{t-1})\|_2^2.$$

Taking expectations with respect to $i(t)$, we get

$$\begin{aligned} \mathbb{E}_{i(t)} \left[\sum_{i=1}^n \|f'_i(\eta_*) - z_i^{(t)}\|_2^2 \right] &= \left(1 - \frac{1}{n}\right) \sum_{i=1}^n \|f'_i(\eta_*) - z_i^{(t-1)}\|_2^2 + \frac{1}{n} \sum_{i=1}^n \|f'_i(\eta_*) - f'_i(\theta_{t-1})\|_2^2 \\ &\leq \left(1 - \frac{1}{n}\right) \sum_{i=1}^n \|f'_i(\eta_*) - z_i^{(t-1)}\|_2^2 + R^2 (\theta_{t-1} - \eta_*)^\top F'(\theta_{t-1}), \end{aligned}$$

where we use the bound in Eq. (5.21). Thus, for a positive number Δ to be chosen later,

$$\begin{aligned} &\mathbb{E}_{i(t)} \left[\|\theta_t - \eta_*\|_2^2 + \Delta \sum_{i=1}^n \|f'_i(\eta_*) - z_i^{(t)}\|_2^2 \right] \\ &\leq \|\theta_{t-1} - \eta_*\|_2^2 - 2\gamma(1 - \gamma R^2 - \frac{R^2 \Delta}{2\gamma})(\theta_{t-1} - \eta_*)^\top F'(\theta_{t-1}) \\ &\quad + \left[2\frac{\gamma^2}{n\Delta} + (1 - 1/n) \right] \Delta \sum_{i=1}^n \|f'_i(\eta_*) - z_i^{(t-1)}\|_2^2. \end{aligned}$$

With $\Delta = 3\gamma^2$ and $\gamma = \frac{1}{4R^2}$, we get $1 - \gamma R^2 - \frac{R^2\Delta}{2\gamma} = \frac{3}{8}$ and $2\frac{\gamma^2}{n\Delta} = \frac{2}{3n}$. Moreover, using the identity $(\theta_{t-1} - \eta_*)^\top F'(\theta_{t-1}) \geq \mu\|\theta_{t-1} - \eta_*\|_2^2$ as a consequence of strong convexity, we then get:

$$\begin{aligned} \mathbb{E}_{i(t)} \left[\|\theta_t - \eta_*\|_2^2 + \Delta \sum_{i=1}^n \|f'_i(\eta_*) - z_i^{(t)}\|_2^2 \right] &\leq \left(1 - \min \left\{ \frac{1}{3n}, \frac{3\mu}{16R^2} \right\} \right) \left[\|\theta_{t-1} - \eta_*\|_2^2 \right. \\ &\quad \left. + \Delta \sum_{i=1}^n \|f'_i(\eta_*) - z_i^{(t-1)}\|_2^2 \right]. \end{aligned}$$

Thus

$$\mathbb{E}[\|\theta_t - \eta_*\|_2^2] \leq \left(1 - \min \left\{ \frac{1}{3n}, \frac{3\mu}{16R^2} \right\} \right)^t \left[\|\theta_0 - \eta_*\|_2^2 + \frac{3}{16R^4} \sum_{i=1}^n \|f'_i(\eta_*) - z_i^{(0)}\|_2^2 \right].$$

If initializing with $z_i^{(0)} = f'_i(\theta_0)$, we get the desired bound by using the Lipschitz-continuity of each f'_i , which leads to $(1 + \frac{3n}{16})\|\theta_0 - \eta_*\|_2^2 \leq (1 + \frac{n}{4})\|\theta_0 - \eta_*\|_2^2$. This leads to the final bound in Eq. (5.20). \blacksquare

We can make the following observations:

- The contraction rate after one iteration is $\left(1 - \min \left\{ \frac{1}{3n}, \frac{3\mu}{16R^2} \right\} \right)$, which is less than $\exp \left(- \min \left\{ \frac{1}{3n}, \frac{3\mu}{16R^2} \right\} \right)$. Thus, after an “effective pass” over the data, that is, n iterations, the contracting rate is $\exp \left(- \min \left\{ \frac{1}{3}, \frac{3\mu n}{16R^2} \right\} \right)$. It is only an effective pass because after we sample n indices with replacement, we will not see all functions (while some will be seen several times).

In order to have a contracting effect of ε , that is, having $\|\theta_t - \eta_*\|_2^2 \leq \varepsilon\|\theta_0 - \eta_*\|_2^2$, we need to have $\exp \left(- t \min \left\{ \frac{1}{3n}, \frac{3\mu}{16R^2} \right\} \right) 2n \leq \varepsilon$, which is equivalent to $t \geq \max \left\{ 3n, \frac{16R^2}{3\mu} \right\} \log \frac{2n}{\varepsilon}$. It just suffices to have $t \geq (3n + \frac{16R^2}{3\mu}) \log \frac{2n}{\varepsilon}$, and thus the running time complexity is equal to d times the minimal number, that is

$$d \left(3n + \frac{16R^2}{3\mu} \right) \log \frac{2n}{\varepsilon}.$$

This is to be contrasted with batch gradient descent with step-size $\gamma = 1/R^2$ (which is the simplest step-size that can be computed easily), whose complexity is

$$dn \frac{R^2}{\mu} \log \frac{1}{\varepsilon}.$$

We replace the product of n and condition number $\kappa = \frac{R^2}{\mu}$ by a sum, which is significant where κ is large.

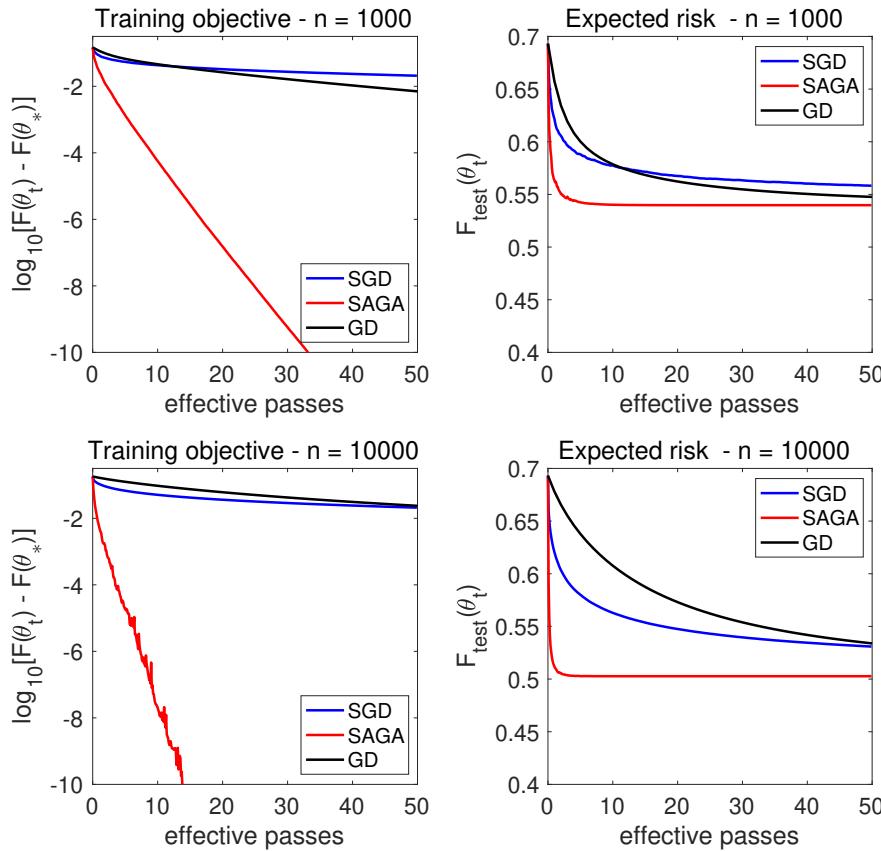


Figure 5.3: Comparison of stochastic gradient algorithms for logistic regression. Top: $n = 1000$, bottom: $n = 10000$. Left: training objective in semi-log plot, right: expected risk estimated with n test points.

- Multiple extensions of this result are available, such as a rate for non-strongly-convex functions, adaptivity to strong-convexity, proximal extensions, and acceleration. It is also worth mentioning that the need to store past gradients can be alleviated (see [Gower et al., 2020](#), for more details).
- Note that these fast algorithms allow very small optimization errors and that the best testing risks will typically be obtained after a few (10 to 100) passes.

Experiments. We consider ℓ_2 -regularized logistic regression, and we compare GD, SGD, and SAGA, all with their corresponding step-sizes coming from the theoretical analysis, with two values of n . We use a simple binary classification problem with linear predictors in dimension $d = 40$ (inputs generated from a Gaussian distribution, with binary outputs obtained as the sign of a linear function with additive Gaussian noise), with two different numbers of observations n , and regularization parameter $\mu = R^2/n$. See Figure 5.3 (top:

small n , left: large n). We see that for early iterations, SGD dominates GD, while for larger numbers of iterations, GD is faster. This last effect is not seen for large numbers of observations (right), where SGD always dominates GD. SAGA gets to machine precision after 50 effective passes over the data in the two cases. Note also the better performance on the testing data.

5.5 Conclusion

We can now provide a summary of convergence rates below, with the main rates we have seen in this chapter (and some that we have not seen). We separate between convex and strongly convex, and between smooth and non-smooth, as well as between deterministic and stochastic methods. Below, L is the smoothness constant, μ the strong convexity constant, B the Lipschitz constant, and D the distance to optimum at initialization.

| | convex | strongly convex |
|-----------|---|---|
| nonsmooth | deterministic: BD/\sqrt{t} stochastic: BD/\sqrt{t} | deterministic: $B^2/(t\mu)$ stochastic: $B^2/(t\mu)$ |
| smooth | deterministic: LD^2/t^2 stochastic: LD^2/\sqrt{t} finite sum: n/t | deterministic: $\exp(-t\sqrt{\mu/L})$ stochastic: $L/(t\mu)$ finite sum: $\exp(-\min\{1/n, \mu/L\}t)$ |

The convergence rates are often written as a number t of accesses to individual gradients to achieve excess function values of ε . This corresponds to inverting each formula for ε as a function of t to a formula for t as a function of ε . This leads to the following table:

| | convex | strongly convex |
|-----------|--|---|
| nonsmooth | deterministic: $(BD)^2/\varepsilon^2$ stochastic: $(BD)^2/\varepsilon^2$ | deterministic: $B^2/(\varepsilon\mu)$ stochastic: $B^2/(\varepsilon\mu)$ |
| smooth | deterministic: $\sqrt{LD}/\sqrt{\varepsilon}$ stochastic: $(LD^2)^2/\varepsilon^2$ finite sum: n/ε | deterministic: $\exp(-t\sqrt{\mu/L})$ stochastic: $L/(\varepsilon\mu)$ finite sum: $\max\{n, L/\mu\} \log(1/\varepsilon)$ |

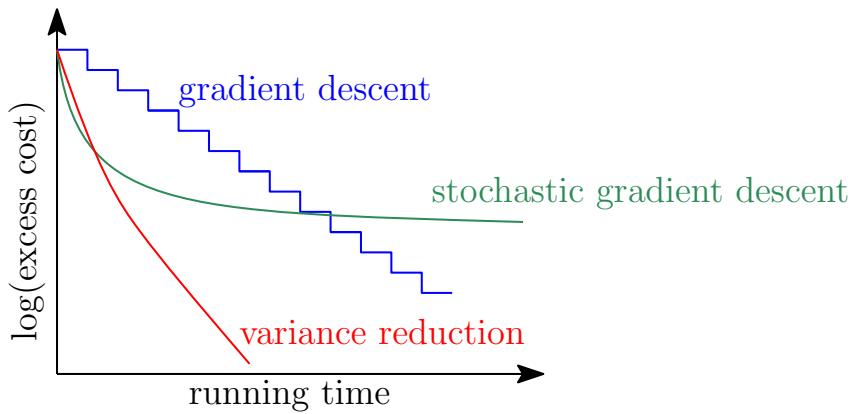


Like in the rest of the book, where we obtain explicit convergence rates, the homogeneity of all quantities can be checked (see exercise below). In the context optimization, this ensures that algorithms are invariant by change of variable $\theta \rightarrow \alpha\theta$ for $\alpha \neq 0$.

Exercise 5.26 Check the homogeneity of all quantities of this section (step-size and convergence rates).

Note that many important themes in optimization have been ignored, such as Frank-Wolfe methods (presented in Chapter 9), coordinate descent, or duality. See [Nesterov \(2018\)](#); [Bubeck \(2015\)](#) for further details. See also Chapter 7 and Chapter 9 for optimization methods for kernel methods and neural networks.

For strongly-convex smooth problems, the following toy figure also provides a good summary, with gradient descent being along a line in a semi-log plot (that is, exponential convergence) but with a staircase effect due to the lack of progress while computing the full gradient, SGD starting fast but having trouble reaching low optimization error, with variance reduction getting the best of both worlds, together with a faster rate of convergence than regular GD.



Chapter 6

Local averaging methods

Chapter summary

- “Linear” estimators: These are based on assigning weight functions to each observation so that each observation can vote for its label with the corresponding weight (typically non-linear in the input variables).
- Partitioning estimates: the input space is cut into non-overlapping cells, and the predictor is piecewise-constant.
- Nadaraya-Watson estimators (a.k.a. kernel regression): each observation assigns a weight proportional to its distance in input space.
- k -nearest-neighbors: each observation assigns an equal weight to its k nearest neighbors.
- Consistency: All of these methods can provably learn complex Lipschitz-continuous non-linear functions with a convergence rate of the form $O(n^{-2/(d+2)})$, where d is the underlying input dimension, leading to the curse of dimensionality.

6.1 Introduction

Like in most of this textbook, we are being given a training set: observations $(x_i, y_i) \in \mathcal{X} \times \mathcal{Y}$, $i = 1, \dots, n$, of inputs/outputs, features/variables are assumed independent and identically distributed (i.i.d.) random variables with common distribution p . We consider a loss function $\ell : \mathcal{Y} \times \mathcal{Y} \rightarrow \mathbb{R}$, where $\ell(y, z)$ is the loss of predicting z while the true label is y .

Our goal is to minimize the expected risk, that is, the generalization performance of a prediction function f from \mathcal{X} to \mathcal{Y} :

$$\mathcal{R}(f) = \mathbb{E}[\ell(y, f(x))],$$

where the expectation is taken with respect to the distribution p .

⚠ Like in the rest of the book, we assume that the testing distribution is the same as the training distribution.

⚠ Be careful with the randomness or lack thereof of f : The estimator \hat{f} we will use depends on the training data and not on the testing data, and thus $\mathcal{R}(\hat{f})$ is random because of the dependence on the training data.

As seen in Chapter 2, the two classical cases are:

- Binary classification: $\mathcal{Y} = \{0, 1\}$ (or often $\mathcal{Y} = \{-1, 1\}$), and $\ell(y, z) = 1_{y \neq z}$ (“0-1” loss). Then $\mathcal{R}(f) = \mathbb{P}(f(x) \neq y)$.
- Regression: $\mathcal{Y} = \mathbb{R}$ and $\ell(y, z) = (y - z)^2$ (square loss). Then $\mathcal{R}(f) = \mathbb{E}(y - f(x))^2$.

As seen in Chapter 2, minimizing the expected risk leads to an optimal “target function,” called the Bayes predictor $f^* \in \arg \min \mathcal{R}(f) = \mathbb{E}[\ell(y, f(x))]$. As shown in Section 2.2.3, the optimal predictor can be obtained from the conditional distribution of $y|x$ as

$$f^*(x) \in \arg \min_{z \in \mathcal{Y}} \mathbb{E}(\ell(y, z)|x).$$

Note that (a) the Bayes predictor is not unique but that all Bayes predictors lead to the same Bayes risk, and (b) that the Bayes risk is usually non-zero (unless the dependence between x and y is deterministic). The goal of supervised machine learning is thus to estimate f^* , knowing only the training data $\mathcal{D} = \{(x_1, y_1), \dots, (x_n, y_n)\}$ and the loss ℓ , with the goal of minimizing the risk or the excess risk $\mathcal{R}(f) - \mathcal{R}^*$. We have the following special cases:

- For binary classification: $\mathcal{Y} = \{0, 1\}$ and $\ell(y, z) = 1_{y \neq z}$, the Bayes predictor is equal to $f^*(x) \in \arg \max_{i \in \{0, 1\}} \mathbb{P}(y = i|x)$. This extends naturally to multi-category classification with the Bayes predictor $f^*(x) \in \arg \max_{i \in \{1, \dots, k\}} \mathbb{P}(y = i|x)$.
- For regression: $\mathcal{Y} = \mathbb{R}$ and $\ell(y, z) = (y - z)^2$, the Bayes predictor is $f^*(x) = \mathbb{E}(y|x)$. Moreover, we have $\mathcal{R}(f) - \mathcal{R}^* = \int_{\mathcal{X}} (f(x) - f^*(x))^2 dp(x) = \|f - f^*\|_{L_2(dp(x))}^2$.

In Chapter 3 and Chapter 4, we explored methods based on empirical risk minimization (and we will as well in Chapter 7 and Chapter 9). In this chapter, we focus on local averaging methods.

6.2 Local averaging methods

In local averaging methods, we aim at approximating the target function f^* directly *without any form of optimization*. This will be done by approximating the conditional distribution $p(y|x)$ of y given x , by some $\hat{p}(y|x)$. We then replace $f^*(x) \in \arg \min_{z \in \mathcal{Y}} \int_{\mathcal{Y}} \ell(y, z) dp(y|x)$ by $\hat{f}(x) \in \arg \min_{z \in \mathcal{Y}} \int_{\mathcal{Y}} \ell(y, z) d\hat{p}(y|x)$. These are often called “plug-in” estimators.

In the usual cases, this leads to the following predictions:

- For classification with the 0-1 loss: $\hat{f}(x) \in \arg \max_{j \in \{1, \dots, k\}} \hat{\mathbb{P}}(y = j|x)$.
- For regression with the square loss: $\hat{f}(x) = \int_{\mathcal{Y}} y d\hat{p}(y|x)$.

6.2.1 Linear estimators

In this chapter, we will consider “linear” estimators, where the conditional distribution is of the form

$$\hat{p}(y|x) = \sum_{i=1}^n \hat{w}_i(x) \delta_{y_i}(y),$$

where δ_{y_i} is the Dirac probability distribution at y_i (putting a unit mass at y_i), and the weight functions $\hat{w}_i : \mathcal{X} \rightarrow \mathbb{R}$, $i = 1, \dots, n$, depends on the input data only (for simplicity) and satisfy (almost surely in x):

$$\forall x \in \mathcal{X}, \quad \forall i \in \{1, \dots, n\}, \quad \hat{w}_i(x) \geq 0, \quad \text{and} \quad \sum_{i=1}^n \hat{w}_i(x) = 1.$$

These conditions ensure that for all $x \in \mathcal{X}$, $\hat{p}(y|x)$ is a probability distribution.

⚠ Some references allow for the weights not to sum to 1.

For our running examples, this leads to the following predictions:

- For classification: $\hat{f}(x) \in \arg \max_{j \in \{1, \dots, k\}} \sum_{i=1}^n \hat{w}_i(x) 1_{y_i=j}$, that is, each observation (x_i, y_i) votes for its label with weight $\hat{w}_i(x)$, a strategy often called “majority vote”.
- For regression: $\mathcal{Y} = \mathbb{R}$: $\hat{f}(x) = \sum_{i=1}^n \hat{w}_i(x) y_i$. This is why the terminology “linear estimators” is sometimes used, since, as a function of the response vector in \mathbb{R}^n , the

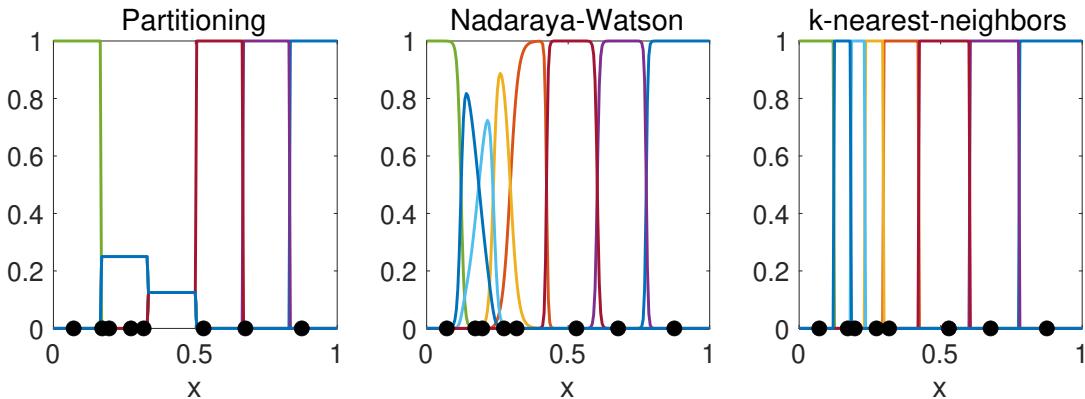


Figure 6.1: Weights of linear estimators in $d = 1$ dimension for the three types of local averaging estimators. The $n = 8$ weight functions $x \mapsto \hat{w}_i(x)$ are plotted with the observations in black.

estimator is linear (note that this is the case as well for kernel ridge regression in Chapter 7). If we only consider predictions $\hat{f}(x_i)$ at the observed inputs, the vector $\hat{y} \in \mathbb{R}^n$ of predictions $\hat{y}_i = \hat{f}(x_i)$, for $i \in \{1, \dots, n\}$ is of the form $\hat{y} = Hy$, where the matrix $H \in \mathbb{R}^{n \times n}$, often called the smoothing matrix or the “hat matrix”, is such that $H_{ij} = \hat{w}_j(x_i)$.

Note that on top of being a linear estimator, the estimator satisfies additional properties: if the same constant is added to all outputs, the exact same constant is added to the prediction function; moreover, given two vectors of outputs y and $y' \in \mathbb{R}^n$, with two prediction functions \hat{f} and \hat{f}' , if $y_i \leq y'_i$ for all $i \in \{1, \dots, n\}$, then $\hat{f}(x) \leq \hat{f}'(x)$ for all $x \in \mathcal{X}$.

Construction of weight functions. In most cases, for any i , the weight function $\hat{w}_i(x)$ is close to 1 for training points x_i which are close to x . We now show three classical ways of building them: (1) partition estimators, (2) Nearest-neighbors, and (3) Nadaraya-Watson estimator (a.k.a. kernel regression). See examples in Figure 6.1.

6.2.2 Partition estimators

If $\mathcal{X} = \bigcup_{j \in J} A_j$ is a partition (such that for all distinct $j, j' \in J$, $A_j \cap A_{j'} = \emptyset$) of \mathcal{X} with a countable index set J (which we will assume finite for simplicity, equal to $\{1, \dots, |J|\}$), then we can consider for any $x \in \mathcal{X}$ the corresponding element $A(x)$ of the partition (that is, $A(x)$ is the unique A_j , $j \in J$, such that $x \in A_j$), and define

$$\hat{w}_i(x) = \frac{1_{x_i \in A(x)}}{\sum_{i'=1}^n 1_{x_{i'} \in A(x)}}, \quad (6.1)$$

with the convention that if no training data point lies in $A(x)$, then $\hat{w}_i(x)$ is equal to $1/n$ for each $i \in \{1, \dots, n\}$. This implies that each w_i is piecewise constant with respect to the partition, that is, for any non-empty cell A_j (that is, for which at least one observation falls in A_j), for any $x \in A_j$, the vectors $(w_i(x))_{i \in \{1, \dots, n\}}$ has weights equal to $1/n_{A_j}$ for $i \in A_j$, where n_{A_j} is the number of training points in the set A_j , and 0 otherwise.

Equivalence with least-squares regression. When applied to regression where the estimator is $\hat{f}(x) = \sum_{i=1}^n \hat{w}_i(x)y_i$, then using a partition estimators can be seen as a least-squares estimator with feature vector $\begin{pmatrix} \varphi(x) \\ 1 \end{pmatrix} = \begin{pmatrix} 1_{x \in A_j} \\ 1 \end{pmatrix}_{j \in J} \in \mathbb{R}^{|J|+1}$, as we now show.

Indeed, we then aim to estimate $\begin{pmatrix} \theta \\ \eta \end{pmatrix} \in \mathbb{R}^{|J|+1}$ for the prediction function

$$\hat{f}(x) = \sum_{j \in J} \theta_j 1_{x \in A_j} + \eta.$$

From training data $(x_1, y_1), \dots, (x_n, y_n)$, as shown in Chapter 3, we can directly estimate the constant term as $\eta = \bar{y} = \frac{1}{n} \sum_{i=1}^n y_i$, while for the other components, we need to solve the normal equations

$$\sum_{i=1}^n \varphi(x_i) \varphi(x_i)^\top \theta = \sum_{i=1}^n (y_i - \bar{y}) \varphi(x_i).$$

It turns out that the matrix $n\widehat{\Sigma} = \sum_{i=1}^n \varphi(x_i) \varphi(x_i)^\top$ is diagonal where for each $j \in J$, $n\widehat{\Sigma}_{jj}$ is equal to n_{A_j} , the number of data points lying in cell A_j . This implies that for a non-empty cell A_j , θ_j is the average of all $y_i - \bar{y}$, for all i such that x_i lies in A_j . Thus, for all $x \in A_j$, the prediction is exactly $\theta_j + \bar{y}$, as obtained from weights in Eq. (6.1). For empty cells, θ_j is not determined by the normal equations above, and if we set it to zero, we recover our convention of predicting as the mean of all labels.

⚠ Other conventions exist (such as all zero weights when no data point lies in $A(x)$).

This equivalence with least-squares estimation with a diagonal (empirical or not) non-centered covariance matrix makes it attractive for theoretical purposes, as the inversion of the population and expected covariance matrices could be done in closed form.

Choice of partitions. There are two standard applications of partition estimators:

- Fixed partitions: for example, when $\mathcal{X} = [0, 1]^d$, we can consider cubes of length h , with $|J| = h^{-d}$ (see example below in $d = 2$ dimension with $|J| = 25$). Note here that the computation time for each $x \in \mathcal{X}$ is not necessarily proportional to $|J|$ but to n (by simply considering the bins where the data lie). This estimator is sometimes called a “regressogram”. We need then to choose the bandwidth h (see analysis in Section 6.3.1). See Figure 6.2 for an illustration in one dimension.

| | | | | |
|----------|----------|----------|----------|----------|
| A_1 | A_2 | A_3 | A_4 | A_5 |
| A_6 | A_7 | A_8 | A_9 | A_{10} |
| A_{11} | A_{12} | A_{13} | A_{14} | A_{15} |
| A_{16} | A_{17} | A_{18} | A_{19} | A_{20} |
| A_{21} | A_{22} | A_{23} | A_{24} | A_{25} |

- Decision trees: for data in a hypercube, we can recursively partition it by selecting a variable to split, leading to a maximum reduction in errors when defining the partitioning estimate.¹ Note here that the partition depends on the labels (so the analysis below does not apply unless the partitioning is learned on a different data than the one used for the estimation).

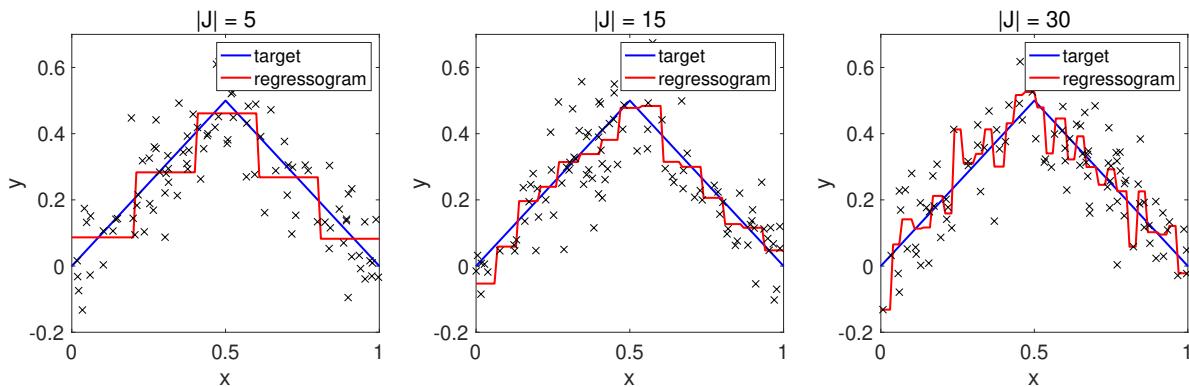


Figure 6.2: Regressograms in $d = 1$ dimension, with three values of $|J|$ (the number of sets in the partition). The $n = 100$ input data points are distributed uniformly on $[0, 1]$, and, for $i \in \{1, \dots, n\}$, the outputs y_i are equal to $\frac{1}{2} - |x_i - \frac{1}{2}| + \varepsilon_i$, where ε_i is a Gaussian with mean zero and variance $\sigma^2 = \frac{1}{100}$. We can observe both underfitting ($|J|$ too small) and overfitting ($|J|$ too large). Note that the target function f^* is piecewise affine and that on the affine parts, the estimator is far from linear; that is, the estimator cannot take advantage of extra-regularity (see Section 6.5 for more details).

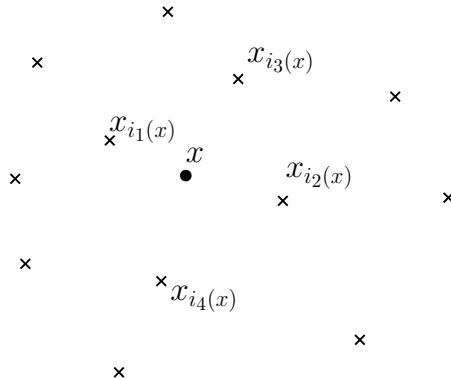
6.2.3 Nearest-neighbors

Given an integer $k \geq 1$, and a distance d on \mathcal{X} , for any $x \in \mathcal{X}$, we can order the n observations so that

$$d(x_{i_1(x)}, x) \leq d(x_{i_2(x)}, x) \leq \dots \leq d(x_{i_n(x)}, x),$$

¹See more details in https://en.wikipedia.org/wiki/Decision_tree_learning.

where $\{i_1(x), \dots, i_n(x)\} = \{1, \dots, n\}$, and ties are broken randomly² (that is, for all $x \in \mathcal{X}$, by sampling randomly once which indices should come first for each i). See the illustration below.



We then define

$$\hat{w}_i(x) = 1/k \text{ if } i \in \{i_1(x), \dots, i_k(x)\}, \text{ and } 0 \text{ otherwise.}$$

Given a new input $x \in \mathbb{R}^d$, the nearest neighbor predictor looks at the k nearest points x_i in the data set $\{(x_1, y_1), \dots, (x_n, y_n)\}$ and predicts a majority vote among them (for classification) or simply the averaged response (for regression). The number of nearest neighbors is the hyperparameter which needs to be estimated (typically by cross-validation); see Section 6.3.2 for an analysis. See a one-dimensional example in Figure 6.3.

Algorithms. Given a test point $x \in \mathcal{X}$, the naive algorithm looks at all training data points for computing the predicted response. Thus the complexity is $O(nd)$ per test point in \mathbb{R}^d . When n is large, this is costly in time and memory. Indexing techniques exist for (potentially approximate) nearest-neighbor search, such as “k-d-trees”, with typically a logarithmic complexity in n (but with some additional compiling time).³

²Other conventions share the weights among all ties.

³See https://en.wikipedia.org/wiki/K-d_tree.

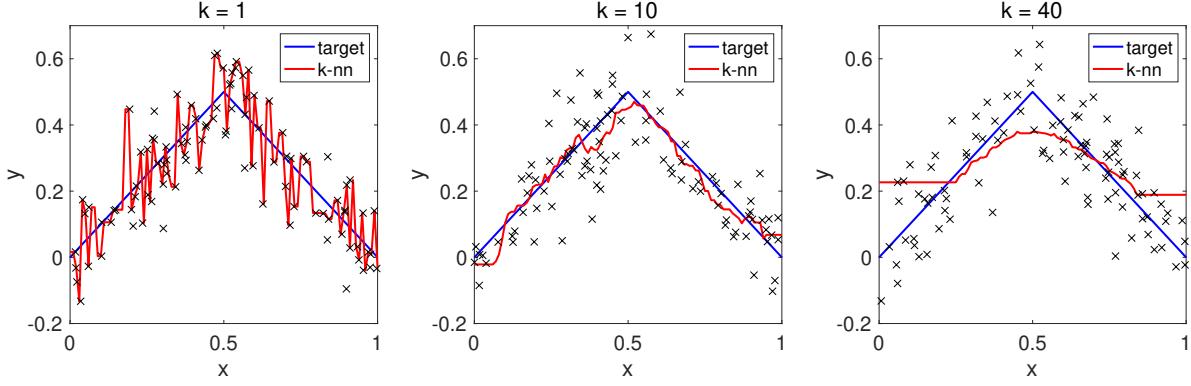


Figure 6.3: k -nearest neighbor regression in $d = 1$ dimension, with three values of k (the number of neighbors), with the same data as Figure 6.2. We can observe both underfitting (k too large) and overfitting (k too small).

Exercise 6.1 What is the pattern of non-zeros of the smoothing matrix $H \in \mathbb{R}^{n \times n}$?

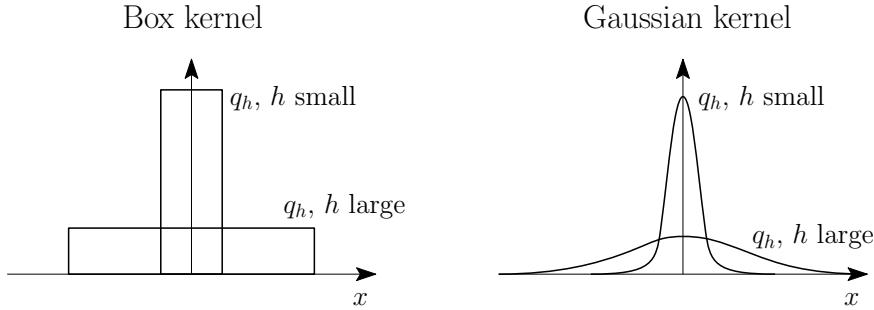
6.2.4 Nadaraya-Watson estimator a.k.a. kernel regression (♦)

Given a “kernel” function $k : \mathcal{X} \times \mathcal{X} \rightarrow \mathbb{R}_+$, which is pointwise non-negative, we define

$$\hat{w}_i(x) = \frac{k(x, x_i)}{\sum_{i'=1}^n k(x, x_{i'})},$$

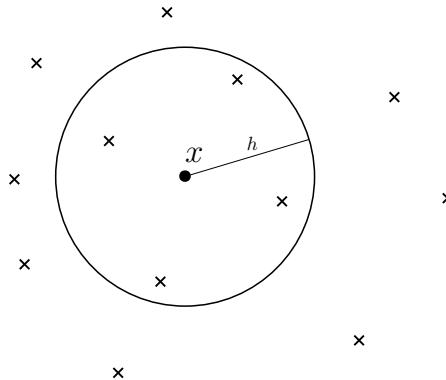
with the convention that if $k(x, x_i) = 0$ for all $i \in \{1, \dots, n\}$, then $\hat{w}_i(x)$ is equal to $1/n$ for each i (which is the same convention used for estimators based on partitions in Section 6.2.2).

In most cases where $\mathcal{X} \subset \mathbb{R}^d$, we take $k(x, x') = h^{-d}q(\frac{1}{h}(x - x'))$ for a certain function $q : \mathbb{R}^d \rightarrow \mathbb{R}_+$ that has large values around 0, and $h > 0$ a “bandwidth” parameter to be selected (see analysis in Section 6.3.3). If we assume that q is integrable with an integral equal to one, then $k(\cdot, x')$ is a probability density with mass around x' , which gets more concentrated as h goes to zero. See the illustration below for the two typical kernel functions (sometimes called “windows”).



Typical examples are:

- Box kernel: $q(x) \propto 1_{\|x\|_2 \leq 1}$, which leads to a weight functions \hat{w}_i with many zeros. See below for an illustration in $d = 2$ dimensions.



- Gaussian kernel $q(x) \propto e^{-\|x\|^2/2}$, where we use the fact it is non-negative *pointwise*, as opposed to positive-definiteness in Chapter 7.⁴ See a one-dimensional experiment in Figure 6.4.

In terms of algorithms, with a naive algorithm, for every test point, all the input data have to be considered, that is, a complexity proportional to n . The same techniques used for efficient k -nearest-neighbor search (e.g., k-d-trees) can also be applied here.

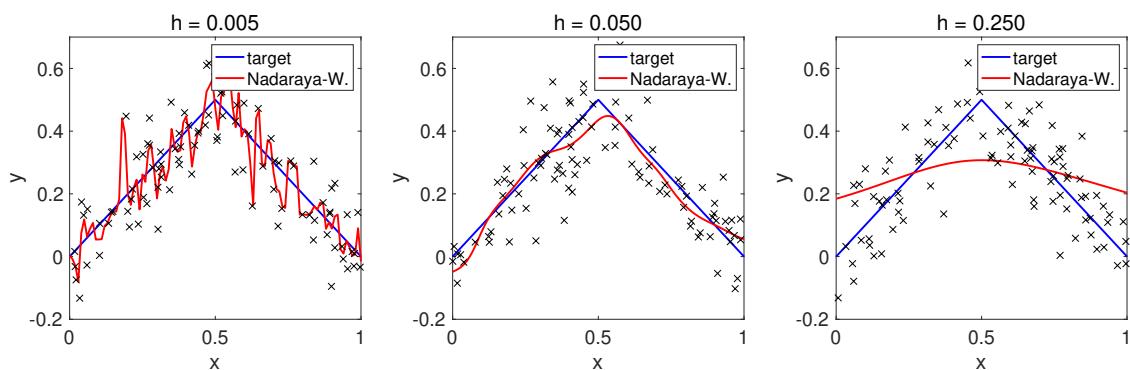


Figure 6.4: Nadaraya-Watson regression in $d = 1$ dimension, with three values of h (the bandwidth), for the Gaussian kernel, with the same data as Figure 6.2. We can observe both underfitting (h too large), or overfitting (h too small).

⁴See also <https://francisbach.com/cursed-kernels/>

6.3 Generic “simplest” consistency analysis

We consider for simplicity the regression case. For classification, convex surrogate techniques such as those used in Section 4.1 can be used, with, for example, the square loss or the logistic loss (with then a square root calibration function on top of the least-squares excess risk, see Exercise 6.2 below). Still, better rates can be obtained directly (see, e.g., [Chen and Shah, 2018](#); [Biau and Devroye, 2015](#); [Audibert and Tsybakov, 2007](#); [Chaudhuri and Dasgupta, 2014](#)).

We make the following generic simplifying assumptions (weaker ones could be considered with more involved proofs):

- (H-1) Bounded noise: There exists $\sigma \geq 0$ such that $|y - \mathbb{E}(y|x)|^2 \leq \sigma^2$ almost surely.
- (H-2) Regular target function: The target function $f^*(x) = \mathbb{E}(y|x)$ is B -Lipschitz-continuous with respect to a distance d . For weaker assumptions, see Section 6.4.

We have, with the target function $f^*(x) = \mathbb{E}(y|x)$, at a test point $x \in \mathcal{X}$ (and using that the weights $w_i(x)$ sum to one):

$$\begin{aligned}\hat{f}(x) - f^*(x) &= \sum_{i=1}^n y_i \hat{w}_i(x) - \mathbb{E}(y|x) \\ &= \sum_{i=1}^n \hat{w}_i(x) [y_i - \mathbb{E}(y_i|x_i)] + \sum_{i=1}^n \hat{w}_i(x) [\mathbb{E}(y_i|x_i) - \mathbb{E}(y|x)] \\ &= \sum_{i=1}^n \hat{w}_i(x) [y_i - \mathbb{E}(y_i|x_i)] + \sum_{i=1}^n \hat{w}_i(x) [f^*(x_i) - f^*(x)].\end{aligned}$$

Given x_1, \dots, x_n (and because we have assumed the weight functions do not depend on the labels), the left term has zero expectation, while the right term is deterministic. We thus have, using the independence of all (x_i, y_i) , $i = 1, \dots, n$, and for x fixed:

$$\begin{aligned}&\mathbb{E}[(\hat{f}(x) - f^*(x))^2 | x_1, \dots, x_n] \\ &= (\mathbb{E}(\hat{f}(x) | x_1, \dots, x_n) - f^*(x))^2 + \text{var}[\hat{f}(x) | x_1, \dots, x_n] \\ &= \left[\sum_{i=1}^n \hat{w}_i(x) [f^*(x_i) - f^*(x)] \right]^2 + \sum_{i=1}^n \hat{w}_i(x)^2 \mathbb{E}[(y_i - \mathbb{E}(y_i|x_i))^2 | x_i] \\ &= \text{bias} \quad + \quad \text{variance},\end{aligned}$$

with a “bias” term which is zero if f^* is constant,⁵ and a “variance” term which is zero, when y is a deterministic function of x (i.e., $\sigma = 0$). Note that at this point, we only had

⁵What we call bias in this book is sometimes referred to as the squared bias.

equalities in the argument; we can now upper-bound as:

$$\begin{aligned}
& \mathbb{E}[(\hat{f}(x) - f^*(x))^2 | x_1, \dots, x_n] \\
& \leq \left[\sum_{i=1}^n \hat{w}_i(x) |f^*(x_i) - f^*(x)| \right]^2 + \sigma^2 \sum_{i=1}^n \hat{w}_i(x)^2 \text{ using (H-1),} \\
& \leq \left[\sum_{i=1}^n \hat{w}_i(x) Bd(x_i, x) \right]^2 + \sigma^2 \sum_{i=1}^n \hat{w}_i(x)^2 \text{ using (H-2),} \\
& \leq B^2 \sum_{i=1}^n \hat{w}_i(x) d(x_i, x)^2 + \sigma^2 \sum_{i=1}^n \hat{w}_i(x)^2 \text{ using Jensen's inequality.}
\end{aligned} \tag{6.2}$$

We then have for the expected excess risk this generic bound we will use for all three cases (partitions, k -nn, and Nadaraya-Watson):

$$\int_{\mathcal{X}} \mathbb{E}[(\hat{f}(x) - f^*(x))^2] dp(x) \leq B^2 \int_{\mathcal{X}} \mathbb{E}\left[\sum_{i=1}^n \hat{w}_i(x) d(x_i, x)^2\right] dp(x) + \sigma^2 \sum_{i=1}^n \int_{\mathcal{X}} \mathbb{E}[\hat{w}_i(x)^2] dp(x). \tag{6.3}$$

! The expectation is with respect to the training data. The expectation with respect to the testing point x is kept as an integral to avoid confusion.

This upper bound can be divided into two terms:

- A variance term $\sigma^2 \sum_{i=1}^n \int_{\mathcal{X}} \mathbb{E}[\hat{w}_i(x)^2] dp(x)$, that depends on the noise on top of the optimal predictions. Since the weights sum to one, we can write $\sum_{i=1}^n \mathbb{E}[\hat{w}_i(x)^2] = \sum_{i=1}^n \mathbb{E}[(\hat{w}_i(x) - 1/n)^2] + 2/n - 1/n^2$, that is, up to vanishing constant, the variance term measures the deviation to uniform weights.
- A bias term $B^2 \int_{\mathcal{X}} \mathbb{E}\left[\sum_{i=1}^n \hat{w}_i(x) d(x_i, x)^2\right] dp(x)$, which depends on the regularity of the target function.

This leads to two conditions: both variance and bias have to go to zero when n grows, and this corresponds to two simple expressions that depend on the weights. For the variance, the worst case scenario is that $\hat{w}_i(x)^2 \approx \hat{w}_i(x)$, that is, weights are putting all the mass into a single label (usually different for different testing point), thus leading to overfitting. For the bias, the worst-case scenario is that weights are uniform (leading to underfitting).

In the following, we will specialize it for \mathcal{X} a subset of \mathbb{R}^d , with a distribution with a density with some minor regularity properties (all will have compact support, that is, \mathcal{X} compact), where we show that a proper setting of the hyperparameters leads to “good” predictions. This will be done for all three cases of local averaging methods.

We look at universal consistency in Section 6.4, where we will list assumption (H-2).

Exercise 6.2 For the binary classification problem, with $\mathcal{Y} = \{-1, 1\}$, assume that $f^*(x) = \mathbb{E}[y|x]$ is B -Lipschitz-continuous. Show that the excess risk is upper-bounded by

$$\sqrt{B^2 \int_{\mathcal{X}} \mathbb{E} \left[\sum_{i=1}^n \hat{w}_i(x) d(x_i, x)^2 \right] dp(x) + \sigma^2 \sum_{i=1}^n \int_{\mathcal{X}} \mathbb{E}[\hat{w}_i(x)^2] dp(x)}.$$

6.3.1 Fixed partition

For the partitioning estimate defined in Section 6.2.2, we can prove the following convergence rate.

Proposition 6.1 (Convergence rate for partition estimates) Assume bounded noise (H-1) and a Lipschitz-continuous target function (H-2), and a partition of the bounded support \mathcal{X} of p , as $\mathcal{X} = \bigcup_{j \in J} A_j$; then for the partitioning estimate \hat{f} , we have:

$$\int_{\mathcal{X}} \mathbb{E}[(\hat{f}(x) - f^*(x))^2] dp(x) \leq \left(8\sigma^2 + \frac{B^2}{2} \text{diam}(\mathcal{X})^2\right) \frac{|J|}{n} + B^2 \max_{j \in J} \text{diam}(A_j)^2. \quad (6.4)$$

Optimal trade-off between bias and variance. Before we look at the proof (which is based on Eq. (6.3)), we can look at the consequence of the bound in Eq. (6.4). We need to balance the terms (up to constants) $\max_{j \in J} \text{diam}(A_j)^2$ and $\frac{|J|}{n}$. In the simplest situation of the unit-cube $[0, 1]^d$, with $|J| = h^{-d}$ cubes of length h , we get $\frac{|J|}{n} = \frac{1}{nh^d}$ and $\max_{j \in J} \text{diam}(A_j)^2 = h^2$, which, with $h = n^{-1/(2+d)}$ to make them equal, leads to a rate proportional to $n^{-2/(2+d)}$. As shown by Györfi et al. (2006), this rate is optimal for the estimation of Lipschitz-continuous functions (see Chapter 12).

While optimal, this is a very slow rate and a typical example of the curse of dimensionality. For this rate to be small, n has to be exponentially large in dimension. This is unavoidable with so little regularity (only bounded first-order derivatives). In Chapter 7 (and also in Section 6.5), we show how to leverage the smoothness of the target function to get significantly improved bounds (local averaging cannot take strong advantage of such smoothness). In Chapter 8, we will leverage dependence on a small number of variables.

Experiments. For the problem shown in Section 6.2, we plot in Figure 6.5 (left plot) training and testing errors averaged over 32 replications (with error bars showing the standard deviations), where we clearly see the trade-off in the choice of $|J|$.

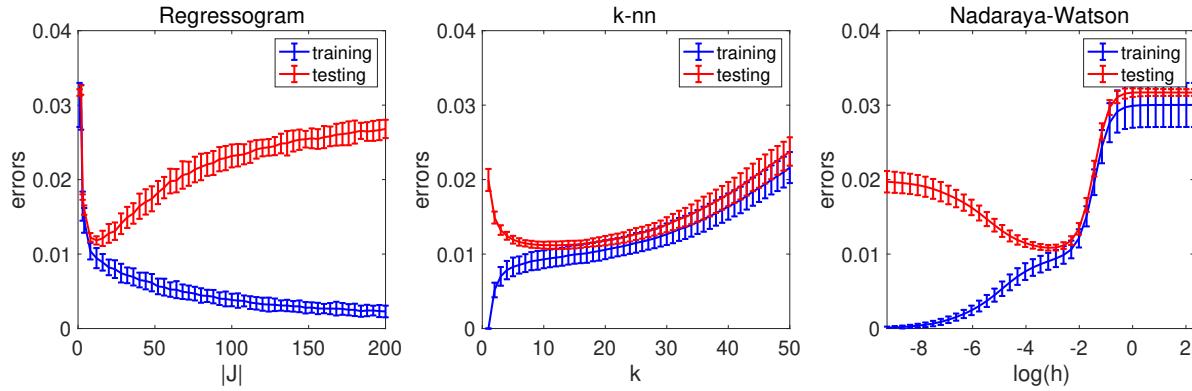


Figure 6.5: Learning curves for all three local averaging methods as a function of the corresponding hyperparameter. Left: regressogram (hyperparameter = number $|J|$ of sets in the partition), middle: k -nearest-neighbors (hyperparameter = number of neighbors k), right: Nadaraya-Watson (hyperparameter = bandwidth h). In all three cases, we see a trade-off between under-fitting and over-fitting.

Proof of Proposition 6.1 (♦) We consider an element A_j of the partition with at least one observation in it (a non-empty cell). Then for $x \in A_j$, and i among the indices of the points lying in A_j , $\hat{w}_i(x) = 1/n_{A_j}$ where $n_{A_j} \in \{1, \dots, n\}$ is the number of data points lying in A_j .

Variance. From Eq. (6.3), the variance term is bounded from above by σ^2 times

$$\sum_{i=1}^n \hat{w}_i(x)^2 = n_{A_j} \frac{1}{n_{A_j}^2} = \frac{1}{n_{A_j}}.$$

If A_j contains no input observations, then all weights are equal to $1/n$, and this sum is equal to $n \times \frac{1}{n^2} = 1/n$ for all $x \in A_j$. Thus, we get

$$\begin{aligned} \int_{\mathcal{X}} \mathbb{E} \left[\sum_{i=1}^n \hat{w}_i(x)^2 \right] dp(x) &= \int_{\mathcal{X}} \sum_{j \in J} 1_{x \in A_j} \mathbb{E} \left[\frac{1}{n_{A_j}} 1_{n_{A_j} > 0} + \frac{1}{n} 1_{n_{A_j} = 0} \right] dp(x) \\ &= \sum_{j \in J} \mathbb{P}(A_j) \cdot \mathbb{E} \left[\frac{1}{n_{A_j}} 1_{n_{A_j} > 0} + \frac{1}{n} 1_{n_{A_j} = 0} \right]. \end{aligned}$$

Intuitively, by the law of large numbers, n_{A_j}/n tends to $\mathbb{P}(A_j)$, so the variance term is expected to be of the order $\sigma^2 \sum_{j \in J} \mathbb{P}(A_j) \frac{1}{n \mathbb{P}(A_j)} = \sigma^2 \frac{|J|}{n}$, which is to be expected as this is essentially equivalent to least-squares regression with $|J|$ features $(1_{x \in A_j})_{j \in J}$.

More formally, we have $\mathbb{P}(n_{A_j} = 0) = (1 - \mathbb{P}(A_j))^n$, and, using Bernstein’s inequality (see Section 1.2.3) for the random variables $1_{x_i \in A_j}$, which have mean and variance upper

bounded by $\mathbb{P}(A_j)$, we have: $\mathbb{P}\left(\frac{n_{A_j}}{n} \leq \frac{1}{2}\mathbb{P}(A_j)\right) = \mathbb{P}\left(\frac{n_{A_j}}{n} \leq \mathbb{P}(A_j) - \frac{1}{2}\mathbb{P}(A_j)\right) \leq \exp\left(-\frac{n\mathbb{P}(A_j)^2/4}{2\mathbb{P}(A_j)+2(\mathbb{P}(A_j)/2)/3}\right) \leq \exp(-n\mathbb{P}(A_j)/10) \leq \frac{5}{n\mathbb{P}(A_j)}$, where we have used $\alpha e^{-\alpha} \leq 1/2$ for any $\alpha \geq 0$. This leads to the bound

$$\begin{aligned} \sum_{j \in J} \mathbb{P}(A_j) \mathbb{E}\left[\frac{1_{n_{A_j}>0}}{n_{A_j}} + \frac{1_{n_{A_j}=0}}{n}\right] &\leq \sum_{j \in J} \mathbb{P}(A_j) \mathbb{E}\left[\frac{1_{1 \leq n_{A_j} \leq \frac{n}{2}\mathbb{P}(A_j)}}{n_{A_j}} + \frac{1_{n_{A_j} > \frac{n}{2}\mathbb{P}(A_j)}}{n_{A_j}} + \frac{1_{n_{A_j}=0}}{n}\right] \\ &\leq \sum_{j \in J} \mathbb{P}(A_j) \left[\mathbb{P}\left(\frac{n_{A_j}}{n} \leq \frac{\mathbb{P}(A_j)}{2}\right) + \frac{2}{n\mathbb{P}(A_j)} + \frac{1}{n}\mathbb{P}(n_{A_j}=0) \right] \\ &\leq \sum_{j \in J} \mathbb{P}(A_j) \mathbb{E}\left[\frac{5}{n\mathbb{P}(A_j)} + \frac{2}{n\mathbb{P}(A_j)} + \frac{1}{n\mathbb{P}(A_j)}\right] \leq \frac{8|J|}{n}. \end{aligned}$$

Bias. We have, for $x \in A_j$ and a non-empty cell,

$$\sum_{i=1}^n \hat{w}_i(x) d(x, x_i)^2 \leq \text{diam}(A_j)^2,$$

with $\sum_{i=1}^n \hat{w}_i(x) d(x, x_i)^2 = \frac{1}{n} \sum_{i=1}^n d(x, x_i)^2 \leq \text{diam}(\mathcal{X})^2$ for empty-cells. Thus, separating the cases $n_{A_j} = 0$ and $n_{A_j} > 0$:

$$\begin{aligned} \int_{\mathcal{X}} \mathbb{E}\left[\sum_{i=1}^n \hat{w}_i(x) d(x, x_i)^2\right] dp(x) &\leq \sum_{j \in J} \mathbb{P}(A_j) \mathbb{E}\left[\text{diam}(A_j)^2 1_{n_{A_j}>0} + 1_{n_{A_j}=0} \text{diam}(\mathcal{X})^2\right] \\ &\leq \sum_{j \in J} \mathbb{P}(A_j) \left[\text{diam}(A_j)^2 + (1 - \mathbb{P}(A_j))^n \text{diam}(\mathcal{X})^2 \right] \\ &= \sum_{j \in J} \mathbb{P}(A_j) \text{diam}(A_j)^2 + \sum_{j \in J} \mathbb{P}(A_j) (1 - \mathbb{P}(A_j))^n \times \text{diam}(\mathcal{X})^2 \\ &\leq \sum_{j \in J} \mathbb{P}(A_j) \text{diam}(A_j)^2 + \sum_{j \in J} \mathbb{P}(A_j) \frac{1}{2n\mathbb{P}(A_j)} \times \text{diam}(\mathcal{X})^2 \\ &= \sum_{j \in J} \mathbb{P}(A_j) \text{diam}(A_j)^2 + \frac{1}{2} \frac{|J|}{n} \times \text{diam}(\mathcal{X})^2, \end{aligned}$$

which leads to the desired term. ■

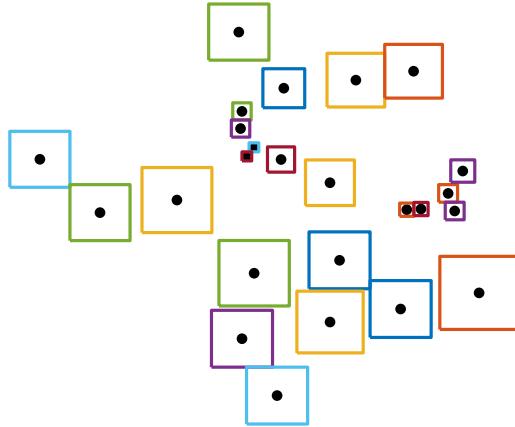
6.3.2 k -nearest neighbor

Here, since all weights are equal to zero except k of them, which are equal to $\frac{1}{k}$, we have $\sum_{i=1}^n \hat{w}_i(x)^2 = \frac{1}{k}$, so the variance term will go down as soon as k tends to infinity. For the

bias term, the needed term $\sum_{i=1}^n \hat{w}_i(x) d(x_i, x)^2$ is equal to the average of the squared distances between x and its k -nearest neighbors within $\{x_1, \dots, x_n\}$, and this is less than the expected distance to the k -th nearest neighbor $x_{i_k(x)}$, for which the two following lemmas, taken from Biau and Devroye (2015, Theorem 2.4), give an estimate for the ℓ_∞ -distance, and thus for all distances by equivalence of norms on \mathbb{R}^d .

Lemma 6.1 (distance to nearest neighbor) *Consider a probability distribution with compact support in $\mathcal{X} \subset \mathbb{R}^d$. Consider $n + 1$ points x_1, \dots, x_n, x_{n+1} sampled i.i.d. from \mathcal{X} . Then the expected squared ℓ_∞ -distance between x_{n+1} and its first-nearest-neighbor is less than $4 \frac{\text{diam}(\mathcal{X})^2}{n^{2/d}}$ for $d \geq 2$, and less than $\frac{2}{n} \text{diam}(\mathcal{X})^2$ for $d = 1$.*

Proof We denote by $x_{(i)}$ a nearest neighbor of x_i among the other n points. Since all $n + 1$ points are i.i.d., we can permute the indices without changing the distributions, and all $\|x_i - x_{(i)}\|_\infty^2$ have the same distribution as $\|x_{n+1} - x_{(n+1)}\|_\infty^2$; thus, we can instead compute $\frac{1}{n+1} \sum_{i=1}^{n+1} \mathbb{E}[\|x_i - x_{(i)}\|_\infty^2]$. We denote by $R_i = \|x_i - x_{(i)}\|_\infty$, and assume for simplicity $R_i > 0$ for all i (the general case is left as an exercise). Then the sets $B_i = \{x \in \mathbb{R}^d, \|x - x_i\|_\infty < \frac{R_i}{2}\}$ are disjoint since for $i \neq j$, $\|x_i - x_j\|_\infty \geq \max\{R_i, R_j\}$. See the illustration below in two dimensions, with squares representing the sets B_i centered as x_i (represented as dots).



Moreover, their union has diameter less than $\text{diam}(X) + \text{diam}(X) = 2\text{diam}(X)$. Thus, the volume of the union of all sets B_i , which is equal to the sum of their volumes, is less than $(2\text{diam}(X))^d$. Thus, we have: $\sum_{i=1}^{n+1} R_i^d \leq (2\text{diam}(X))^d$. Therefore, by Jensen’s inequality, for $d \geq 2$,

$$\left(\frac{1}{n+1} \sum_{i=1}^{n+1} R_i^2 \right)^{d/2} \leq \frac{1}{n+1} \sum_{i=1}^{n+1} (R_i)^d \leq \frac{2^d \text{diam}(\mathcal{X})^d}{n+1},$$

leading to the desired result. For $d = 1$, we have $\left(\frac{1}{n+1} \sum_{i=1}^{n+1} R_i^2\right) \leq \text{diam}(\mathcal{X}) \left(\frac{1}{n+1} \sum_{i=1}^{n+1} R_i\right) \leq \frac{2}{n+1} \text{diam}(\mathcal{X})^2$. \blacksquare

Lemma 6.2 (distance to k -nearest-neighbor) *Let $k \geq 1$. Consider a probability distribution with compact support in $\mathcal{X} \subset \mathbb{R}^d$. Consider $n+1$ points x_1, \dots, x_n, x_{n+1} sampled i.i.d. from \mathcal{X} . Then the expected squared ℓ_∞ -distance between x_{n+1} and its k -nearest-neighbor is less than $8\text{diam}(\mathcal{X})^2 \left(\frac{2k}{n}\right)^{2/d}$ for $d \geq 2$, and less than $\frac{8k}{n} \text{diam}(\mathcal{X})^2$ for $d = 1$.*

Proof (\blacklozenge) Without loss of generality, we assume $2k \leq n$ (otherwise, the proposed bounds are trivial). We can then divide randomly (and independently) the n first points into $2k$ sets of size approximately $\frac{n}{2k}$. We denote $x_{(k)}^j$ a 1-nearest neighbor of x_{n+1} within the j -th set. The squared distance from x_{n+1} to the k -nearest neighbor among all first n points is less than the k -th smallest of the distances $\|x_{n+1} - x_{(k)}^j\|_\infty^2$, $j \in \{1, \dots, 2k\}$, because we take a k -nearest neighbor over a smaller set. This k -th smallest distance is less than $\frac{1}{k} \sum_{j=1}^{2k} \|x_{n+1} - x_{(k)}^j\|_\infty^2$ (this is a general fact that the k -smallest element among non-negative p elements, is less than their sum divided by $p - k$, applied here for $p = k$).

Thus, using the lemma above on the 1-nearest-neighbor from $\frac{n}{2k}$ points, we get that the desired averaged distance is less than, for $d \geq 2$:

$$\frac{1}{k} \sum_{j=1}^{2k} 4 \frac{\text{diam}(\mathcal{X})^2}{\left(\frac{n}{2k}\right)^{2/d}} = 8 \frac{\text{diam}(\mathcal{X})^2}{n^{2/d}} (2k)^{2/d}.$$

A similar argument can be extended to $d = 1$ (left as an exercise). \blacksquare

Putting things together, we get the following result for the consistency of k -nearest-neighbors.

Proposition 6.2 (Convergence rate for k -nearest-neighbors) *Assume bounded noise (H-1) and a Lipschitz-continuous target function (H-2), with an input distribution with bounded support \mathcal{X} . Then for the k -nearest-neighbor estimate \hat{f} with the ℓ_∞ -norm, we have, for $d \geq 2$:*

$$\int_{\mathcal{X}} \mathbb{E}[(\hat{f}(x) - f^*(x))^2] dp(x) \leq \frac{\sigma^2}{k} + 8B^2 \text{diam}(\mathcal{X})^2 \left(\frac{2k}{n}\right)^{2/d}. \quad (6.5)$$

Balancing the two terms above is obtained with $k \propto n^{2/(2+d)}$, and we get the same result as for the other local averaging schemes. See more details by [Chen and Shah \(2018\)](#) and [Biau and Devroye \(2015\)](#).

Exercise 6.3 *Show that if the Bayes rate is 0 (that is, $\sigma = 0$), then 1-nearest-neighbor is consistent.*

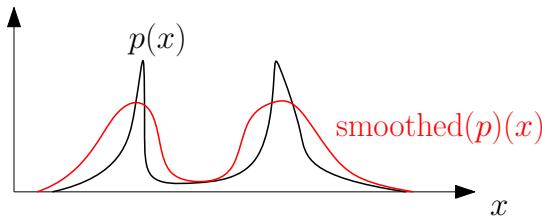
Experiments. For the problem shown in Section 6.2, we plot in Figure 6.5 (middle) training and testing errors averaged over 32 replications (with error bars showing the standard deviations), where we clearly see the trade-off in the choice of k .

6.3.3 Kernel regression (Nadaraya-Watson) (♦)

In this section, we assume that $\mathcal{X} = \mathbb{R}^d$, and for simplicity, we assume that the distribution of the inputs has a density (also denoted p) with respect to the Lebesgue measure. We also assume that the kernel is of the form $k(x, x') = q_h(x - x') = h^{-d}q(\frac{1}{h}(x - x'))$ for a probability density $q : \mathbb{R}^d \rightarrow \mathbb{R}_+$. The function q_h is also a density, which is the density of hz when z has density $q(z)$ (it thus gets more concentrated around 0 as h tends to zero). With these notations, the weights can be written:

$$\hat{w}_i(x) = \frac{q_h(x - x_i)}{\sum_{j=1}^n q_h(x - x_j)}.$$

Smoothing by convolution. When performing kernel regression, quantities of the form $\frac{1}{n} \sum_{i=1}^n q_h(x - x_i)g(x_i)$ naturally appear. When the number n of observations goes to infinity, and x is fixed, by the law of large numbers, it tends almost surely to $\int_{\mathbb{R}^d} q_h(x - z)g(z)p(z)dz$, which is exactly the convolution between the function q_h and the function $x \mapsto p(x)g(x)$, which we can denote $[(pg) * q_h](x)$. The function q_h is a probability density that puts most of its weights at a range of values of order h , e.g., for kernels like the Gaussian kernel or the box kernel. Thus convolution will smooth the function pg by averaging values at range h . Therefore, when h goes to zero, it converges to the function pg itself. See an example below for $g = 1$.



Note that for this limit to hold, we need to ensure the factors in n and h^d are present.

We can now look at the generalization bound from Eq. (6.3) and see how it applies to kernel regression. We now consider the ℓ_2 -distance for simplicity and consider the variance and bias terms separately, first with an asymptotic informal result where both h tends to zero and n tends to infinity, and then a formal result.

Variance term. We have, for a fixed $x \in \mathcal{X}$:

$$n \sum_{i=1}^n \hat{w}_i(x)^2 = \frac{\frac{1}{n} \sum_{i=1}^n q_h(x - x_i)^2}{\left(\frac{1}{n} \sum_{i=1}^n q_h(x - x_i)\right)^2}.$$

Using the law of large numbers and the smoothing reasoning above, this sum $n \sum_{i=1}^n \hat{w}_i(x)^2$ is converging almost surely to

$$\frac{\int_{\mathbb{R}^d} q_h(x - z)^2 p(z) dz}{\left(\int_{\mathbb{R}^d} q_h(x - z) p(z) dz\right)^2} = \frac{[q_h^2 * p](x)}{[q_h * p](x)^2}.$$

When h tends to zero, then the denominator above $[q_h * p](x)^2$ tends to $p(x)^2$ because the bandwidth of the smoothing goes to zero. The numerator above corresponds, up to a multiplicative constant, to the smoothing of p by the density $x \mapsto \frac{q_h(x)^2}{\int_{\mathbb{R}^d} q_h(u)^2 du}$, and is thus asymptotically equivalent to $p(x) \int_{\mathbb{R}^d} q_h(u)^2 du = p(x)h^{-d} \int_{\mathbb{R}^d} q(u)^2 du$.

Overall, when n tends to infinity, and h tends to zero, we get, asymptotically for x fixed when n tends to $+\infty$:

$$\sum_{i=1}^n \hat{w}_i(x)^2 \sim \frac{1}{nh^d} \frac{1}{p(x)} \int_{\mathbb{R}^d} q(u)^2 du,$$

and thus, still asymptotically,

$$\int_{\mathcal{X}} \left[\sum_{i=1}^n \hat{w}_i(x)^2 \right] p(x) dx \sim \frac{1}{nh^d} \text{vol}(\text{supp}(p)) \int_{\mathbb{R}^d} q(u)^2 du,$$

where $\text{vol}(\text{supp}(p))$ is the volume of the support of p in \mathbb{R}^d (the closure of all x for which $p(x) > 0$), which we assume bounded.

Bias. With the same intuitive reasoning, we get, when n tends to infinity:

$$\sum_{i=1}^n \hat{w}_i(x) d(x_i, x)^2 \rightarrow \frac{\int_{\mathbb{R}^d} q_h(x - z) \|x - z\|_2^2 p(z) dz}{\int_{\mathbb{R}^d} q_h(x - z) p(z) dz}.$$

The denominator has the same shape as for the variance term and tends to $p(x)$ when h tends to zero. With the change of variable $u = \frac{1}{h}(x - z)$, the numerator is equal to $\int_{\mathbb{R}^d} q_h(x - z) \|x - z\|_2^2 p(z) dz = h^2 \int_{\mathbb{R}^d} q(u) \|u\|_2^2 p(x - uh) du$, which is equivalent to $h^2 p(x) \int_{\mathbb{R}^d} q(u) \|u\|_2^2 du$ when h tends to zero. Overall, when n tends to infinity, and h tends to zero, we get:

$$\int_{\mathcal{X}} \left[\sum_{i=1}^n \hat{w}_i(x) d(x_i, x)^2 \right] p(x) dx \sim h^2 \int_{\mathbb{R}^d} q(u) \|u\|_2^2 du.$$

Therefore, overall we get an *asymptotic* bound proportional to (up to constants depending on q):

$$\frac{\sigma^2}{nh^d} + B^2 h^2,$$

leading to the same upper bound as for partitioning estimates by setting $h \propto n^{-1/(d+2)}$.

Formal reasoning (♦♦). We can make the informal reasoning above more formal using concentration inequalities, leading to non-asymptotic bounds of the same nature (simply more complicated) that make explicit the joint dependence on n and h . We will prove the following result:

Proposition 6.3 (Convergence rate for Nadaraya-Watson estimation) *We assume bounded noise (H-1) and a Lipschitz-continuous target function (H-2), and a function $q : \mathbb{R}^d \rightarrow \mathbb{R}$ such that $\int_{\mathbb{R}^d} q(z) dz = 1$, and $\|q\|_\infty = \sup_{z \in \mathbb{R}^d} q(z)$ is finite. We also assume that p has bounded support \mathcal{X} and density upper-bounded by $\|p\|_\infty$. Then for the Nadaraya-Watson estimate \hat{f} , we have:*

$$\int_{\mathcal{X}} \mathbb{E}[(\hat{f}(x) - f^*(x))^2] dp(x) \leq \left[\frac{8\|q\|_\infty}{nh^d} \left(1 + \frac{1}{2} \text{diam}(\mathcal{X})^2 \right) + 2Bh^2\|p\|_\infty c \right] \cdot C_h, \quad (6.6)$$

where $c = \int_{\mathbb{R}^d} q(u) \|u\|_2^2 du$ and $C_h = \int_{\mathcal{X}} \frac{p(x)}{[q_h * p](x)} dx$.

With additional assumptions, we can show that the constant C_h remains bounded when h tends to zero (see exercise below). Before giving the proof, we note that the optimal bandwidth parameter is indeed proportional to $h \propto n^{-1/(d+2)}$, with an overall excess risk proportional to $n^{-2/(d+2)}$, like the two other types of estimators.

Proof of Proposition 6.3 (♦) As for the proof for partitioning estimates, to deal with the denominator in the definition of the weights, we can first use Bernstein’s inequality (see Section 1.2.3), applied to the random variables $q_h(x - x_i)$ which is almost surely in $[0, h^{-d}\|q\|_\infty]$, to bound

$$\mathbb{P}\left(\frac{1}{n} \sum_{i=1}^n q_h(x - x_i) \leq \mathbb{E}[q_h(x - z)] - \varepsilon\right) \leq \exp\left(-\frac{n\varepsilon^2}{2\mathbb{E}[q_h^2(x - z)] + 2\|q\|_\infty h^{-d}\varepsilon/3}\right).$$

We get with $\varepsilon = \frac{1}{2}\mathbb{E}[q_h(x - z)]$, using $\mathbb{E}[q_h^2(x - z)] \leq \|q\|_\infty h^{-d}\mathbb{E}[q_h(x - z)]$, for the event $\mathcal{A}(x) = \{\frac{1}{n} \sum_{i=1}^n q_h(x - x_i) \leq \frac{1}{2}\mathbb{E}[q_h(x - z)]\}$:

$$\begin{aligned} \mathbb{P}(\mathcal{A}(x)) &\leq \exp\left(-\frac{\frac{n}{4}(\mathbb{E}[q_h(x - z)])^2}{2\mathbb{E}[q_h^2(x - z)] + \mathbb{E}[q_h(x - z)]h^{-d}\|q\|_\infty/3}\right) \\ &\leq \exp\left(-\frac{\frac{n}{4}\mathbb{E}[q_h(x - z)]}{(7/3)h^{-d}\|q\|_\infty}\right) \leq \frac{\|q\|_\infty}{nh^d\mathbb{E}[q_h(x - z)]} \cdot \frac{1}{e} \frac{28}{3} \leq \frac{4\|q\|_\infty}{nh^d\mathbb{E}[q_h(x - z)]}, \end{aligned} \quad (6.7)$$

where we have used $\alpha e^{-\alpha} \leq 1/e$ for $\alpha \geq 0$. We can now bound bias and variance.

Variance. For a fixed $x \in \mathcal{X}$, we get

$$\begin{aligned}\mathbb{E}\left[\sum_{i=1}^n \hat{w}_i(x)^2\right] &= \mathbb{E}\left[1_{\mathcal{A}(x)} \sum_{i=1}^n \hat{w}_i(x)^2\right] + \mathbb{E}\left[1_{\mathcal{A}(x)^c} \sum_{i=1}^n \hat{w}_i(x)^2\right] \\ &\leq \mathbb{P}(\mathcal{A}(x)) + \frac{4}{(n\mathbb{E}[q_h(x-z)])^2} \mathbb{E}\left[\sum_{i=1}^n q\left(\frac{1}{h}(x-x_i)\right)^2\right] \\ &\leq \frac{4\|q\|_\infty}{nh^d\mathbb{E}[q_h(x-z)]} + \frac{4\mathbb{E}[q_h(x-z)^2]}{n[\mathbb{E}q_h(x-z)]^2} \leq \frac{8\|q\|_\infty}{nh^d\mathbb{E}[q_h(x-z)]}.\end{aligned}$$

Moreover, we have $\mathbb{E}[q_h(x-z)] = \int_{\mathbb{R}^d} dp(x-hu)q(u)du = [p * q_h](x)$. This leads to an overall bound on the variance term as $\int_{\mathcal{X}} \mathbb{E}\left[\sum_{i=1}^n \hat{w}_i(x)^2\right] p(x)dx \leq \frac{8\|q\|_\infty}{nh^d} \int_{\mathcal{X}} \frac{p(x)}{[p * q_h](x)} dx$.

Bias term. We have a similar reasoning for the bias term. Indeed, we get for a given $x \in \mathcal{X}$, using the bound in Eq. (6.7):

$$\begin{aligned}&\mathbb{E}\left[\sum_{i=1}^n \hat{w}_i(x)\|x-x_i\|_2^2\right] \\ &= \mathbb{E}\left[1_{\mathcal{A}(x)} \sum_{i=1}^n \hat{w}_i(x)\|x-x_i\|_2^2\right] + \mathbb{E}\left[1_{\mathcal{A}(x)^c} \sum_{i=1}^n \hat{w}_i(x)\|x-x_i\|_2^2\right] \\ &\leq \mathbb{P}(\mathcal{A}(x)) \cdot \text{diam}(\mathcal{X})^2 + \frac{2}{n\mathbb{E}[q_h(x-z)]} \cdot n\mathbb{E}[q_h(x-z)\|x-z\|_2^2] \\ &\leq \frac{4\|q\|_\infty}{nh^d[q_h * p](x)} \cdot \text{diam}(\mathcal{X})^2 + \frac{2h^2}{[q_h * p](x)} \cdot \int_{\mathbb{R}^d} q(u)\|u\|_2^2 p(x-uh)du \\ &\leq \frac{4\|q\|_\infty}{nh^d[q_h * p](x)} \cdot \text{diam}(\mathcal{X})^2 + \frac{2h^2\|p\|_\infty}{[q_h * p](x)} \cdot \int_{\mathbb{R}^d} q(u)\|u\|_2^2 du.\end{aligned}$$

This leads to an overall bound on the bias term equal to $\int_{\mathcal{X}} \mathbb{E}\left[\sum_{i=1}^n \hat{w}_i(x)\|x-x_i\|_2^2\right] p(x)dx \leq \int_{\mathcal{X}} \frac{p(x)}{[q_h * p](x)} dx \cdot \left[\frac{4\|q\|_\infty}{nh^d} \text{diam}(\mathcal{X})^2 + 2h^2\|p\|_\infty \left(\int_{\mathbb{R}^d} q(u)\|u\|_2^2 du \right) \right]$.

Putting things together, we get that the excess risk $\int_{\mathcal{X}} \mathbb{E}[(\hat{f}(x) - f^*(x))^2] dp(x)$ is less than

$$\left[\frac{8\|q\|_\infty}{nh^d} \left(1 + \frac{1}{2} \text{diam}(\mathcal{X})^2 \right) + 2Bh^2\|p\|_\infty \left(\int_{\mathbb{R}^d} q(u)\|u\|_2^2 du \right) \right] \cdot \int_{\mathcal{X}} \frac{p(x)}{[q_h * p](x)} dx,$$

which is exactly the desired bound. ■

Exercise 6.4 Assume that the support \mathcal{X} of the density p of inputs is bounded and that p is strictly positive and continuously differentiable on \mathcal{X} . Show that for h small enough (with an explicit upper-bound), then $C_h = \int_{\mathcal{X}} \frac{p(x)}{[q_h * p](x)} dx \leq \frac{1}{2} \text{vol}(\mathcal{X})$.

Experiments. For the problem shown in Section 6.2, we plot in Figure 6.5 (right) training and testing errors averaged over 32 replications (with error bars showing the standard deviations), where we clearly see the trade-off in the choice of h .

6.4 Universal consistency (♦)

Above, we have required the following conditions on the weights:

- $\int_{\mathcal{X}} \mathbb{E} \left[\sum_{i=1}^n \hat{w}_i(x) d(x_i, x)^2 \right] dp(x) \rightarrow 0$ when n tends to infinity, to ensure that the bias goes to zero.
- $\int_{\mathcal{X}} \sum_{i=1}^n \mathbb{E}[\hat{w}_i(x)^2] dp(x) \rightarrow 0$ when n tends to infinity, to ensure that the variance goes to zero.

This was enough to show consistency when the target function is Lipschitz-continuous in \mathbb{R}^d . This also led to a precise rate of convergence, which turns out to be optimal for learning with target functions that are Lipschitz-continuous, and for which the curse of dimensionality cannot be avoided (see Chapter 12).

To show universal consistency, that is, consistency for any square-integrable functions, we need an extra (technical) assumption, which was first outlined in Stone's theorem (Stone, 1977), namely that there exists $c > 0$ such that for any non-negative integrable function $h : \mathcal{X} \rightarrow \mathbb{R}$, then

$$\int_{\mathcal{X}} \sum_{i=1}^n \mathbb{E}[\hat{w}_i(x)h(x_i)] dp(x) \leq c \cdot \int_{\mathcal{X}} h(x) dp(x). \quad (6.8)$$

Below, h will be the squared deviation between two functions.

⚠ Above, we only take the expectation with respect to the training data, while we use the integral notation to take the expectation with respect to the training distribution.

Then for any $\varepsilon > 0$, and for any target function $f^* \in L_2(dp(x))$, we can find a function g which is $B(\varepsilon)$ -Lipschitz-continuous and such that $\|f^* - g\|_{L_2(dp(x))} \leq \varepsilon$, because the set of Lipschitz-continuous functions is dense in $L_2(dp(x))$ (see, e.g., Ambrosio et al., 2013))

Then we have, for a given $x \in \mathcal{X}$:

$$\begin{aligned}
& \mathbb{E} \left(\left[\sum_{i=1}^n \hat{w}_i(x) [f^*(x_i) - f^*(x)] \right]^2 \right) \\
& \leq \mathbb{E} \left(\left[\sum_{i=1}^n \hat{w}_i(x) \left(|f^*(x_i) - g(x_i)| + |g(x_i) - g(x)| + |g(x) - f^*(x)| \right) \right]^2 \right) \\
& \leq 3\mathbb{E} \left(\left[\sum_{i=1}^n \hat{w}_i(x) |f^*(x_i) - g(x_i)| \right]^2 \right) + 3\mathbb{E} \left(\left[\sum_{i=1}^n \hat{w}_i(x) |g(x_i) - g(x)| \right]^2 \right) \\
& \quad + 3\mathbb{E} \left(\left[\sum_{i=1}^n \hat{w}_i(x) |g(x) - f^*(x)| \right]^2 \right) \text{ using the inequality } (a+b+c)^2 \leq 3a^2 + 3b^2 + 3c^2, \\
& \leq 3\mathbb{E} \left(\left[\sum_{i=1}^n \hat{w}_i(x) |f^*(x_i) - g(x_i)| \right]^2 \right) + 3\mathbb{E} \left(\left[\sum_{i=1}^n \hat{w}_i(x) B(\varepsilon) d(x, x_i) \right]^2 \right) \\
& \quad + 3\mathbb{E} \left(|g(x) - f^*(x)|^2 \right) \text{ since weights sum to one, and } g \text{ is Lipschitz-continuous,} \\
& \leq 3\mathbb{E} \left[\sum_{i=1}^n \hat{w}_i(x) |f^*(x_i) - g(x_i)|^2 \right] + 3B(\varepsilon)^2 \mathbb{E} \left(\sum_{i=1}^n \hat{w}_i(x) d(x, x_i)^2 \right) \\
& \quad + 3\mathbb{E} \left(|g(x) - f^*(x)|^2 \right) \text{ using Jensen's inequality on the second term,} \\
& \leq 3c \cdot \mathbb{E} [|f^*(x) - g(x)|^2] + 3B(\varepsilon)^2 \mathbb{E} \left(\sum_{i=1}^n \hat{w}_i(x) d(x, x_i)^2 \right) + 3\mathbb{E} \left(|g(x) - f^*(x)|^2 \right),
\end{aligned}$$

using Eq. (6.8). We can now integrate with respect to x to get

$$\int_{\mathcal{X}} \mathbb{E} \left(\left[\sum_{i=1}^n \hat{w}_i(x) [f^*(x_i) - f^*(x)] \right]^2 \right) dp(x) \leq 3c \cdot \varepsilon^2 + 3B(\varepsilon)^2 \int_{\mathcal{X}} \mathbb{E} \left(\sum_{i=1}^n \hat{w}_i(x) d(x, x_i)^2 \right) dp(x) + 3\varepsilon^2. \tag{6.9}$$

Proving universal consistency. We can then combine the bound above (which gives a bound on the bias) with Eq. (6.2), starting from the excess risk $\int_{\mathcal{X}} \mathbb{E}[(\hat{f}(x) - f^*(x))^2] dp(x)$ less than

$$\int_{\mathcal{X}} \mathbb{E} \left(\left[\sum_{i=1}^n \hat{w}_i(x) |f^*(x_i) - f^*(x)| \right]^2 \right) dp(x) + \sigma^2 \int_{\mathcal{X}} \mathbb{E} \left[\sum_{i=1}^n \hat{w}_i(x)^2 \right] dp(x),$$

which is the sum of a bias term and a variance term, and for which, together with Eq. (6.9), we can use the same tools for consistency as for Eq. (6.3).

To prove universal consistency, we fix a certain $\varepsilon > 0$, from which we obtain some Lipschitz constant $B(\varepsilon)$. For such a $B(\varepsilon)$, we know how to make the term $B(\varepsilon)^2 \int_{\mathcal{X}} \mathbb{E} \left(\sum_{i=1}^n \hat{w}_i(x) d(x, x_i)^2 \right) dp(x) - \sigma^2 \int_{\mathcal{X}} \mathbb{E} \left[\sum_{i=1}^n \hat{w}_i(x)^2 \right] dp(x)$ less than ε , by choosing appropriate hyperparameter and number of observations n (see previous sections). Thus, if the extra condition in Eq. (6.8) is

satisfied, these three methods are universally consistent. Note that in general, n has to grow unbounded when ε tends to zero, without any a priori bound.

We can now look at the three cases:

- Partitioning: We have then $c = 2$, and we get universal consistency. Indeed, using the same notations as in Section 6.2.2, we have for any fixed $x \in A_j$, $j \in J$, and f a non-negative function:

$$\begin{aligned} \sum_{i=1}^n \mathbb{E}[\hat{w}_i(x)f(x_i)] &= \mathbb{E}\left[1_{n_{A_j}>0} \frac{1}{n_{A_j}} \sum_{\substack{i \text{ s.t. } x_i \in A_j}} f(x_i) + 1_{n_{A_j}=0} \frac{1}{n} \sum_{i=1}^n f(x_i)\right] \\ &= \mathbb{E}\left[1_{n_{A_j}>0} \frac{1}{n_{A_j}} \sum_{\substack{i \text{ s.t. } x_i \in A_j}} \mathbb{E}[f(x_i)|x_i \in A_j] + 1_{n_{A_j}=0} \frac{1}{n} \sum_{i=1}^n f(x_i)\right] \\ &\leq \mathbb{E}[f(z)|z \in A_j] + \mathbb{E}[f(z)], \end{aligned}$$

where z is distributed as x . Thus, integrating with respect to x and summing over $j \in J$, we get:

$$\int_X \sum_{i=1}^n \mathbb{E}[\hat{w}_i(x)h(x_i)] dp(x) \leq \sum_{j \in J} \left(\mathbb{P}(A_j) \mathbb{E}[f(z)|z \in A_j] + \mathbb{P}(A_j) \cdot \mathbb{E}[f(z)] \right) = 2\mathbb{E}[f(z)],$$

which is exactly Eq. (6.8) with $c = 2$.

- Kernel regression: it can be shown using the same type of techniques outlined for consistency for Lipschitz-continuous functions.
- k -nearest neighbor: the condition in Eq. (6.8) is not easy to show and is often referred to as Stone's lemma. See [Biau and Devroye \(2015, Lemma 10.7\)](#).

6.5 Adaptivity (♦♦)

As shown above, all local averaging techniques achieve the same performance on Lipschitz-continuous functions, which is an unavoidable bad performance when d grows (curse of dimensionality). One extra order of smoothness, that is, on \mathbb{R}^d , two bounded derivatives, can be leveraged to lead to a convergence rate proportional to $n^{-4/(4+d)}$ ([Wasserman, 2006](#), Section 5.4). However, the higher smoothness of the target function does not seem to be easy to leverage, that is, even if the target function is very smooth, the local averaging techniques will not be able to attain better convergence rates. The impossibility comes from the bias term which is the square of $\sum_{i=1}^n \hat{w}_i(x)[f^*(x_i) - f^*(x)]$ in Section 6.3: when f^* is once differentiable, $f^*(x_i) - f^*(x) = O(\|x_i - x\|)$ and this is what we leveraged in the proofs;

when f^* is twice differentiable, by a Taylor expansion, $f^*(x_i) - f^*(x) = (x_i - x)^\top (f^*)'(x_i) + O(\|x_i - x\|^2)$, and we can choose weights so that $\sum_{i=1}^n \hat{w}_i(x)(x - x_i) = O(\|x - x_i\|^2)$ (this is possible because the components of $x - x_i$ may take positive and negative values, leading to potential cancellations, see exercise below); but when f is three-times differentiable or more, obtaining a term $O(\|x_i - x\|^3)$ that would come from a Taylor expansion, is only possible if the weights satisfy $\sum_{i=1}^n \hat{w}_i(x)(x - x_i)(x - x_i)^\top = O(\|x_i - x\|^3)$, which is not possible when the weights are non-negative as no cancellations are possible.

Positive-definite kernel methods will provide simple ways in Chapter 7, as well as neural networks in Chapter 9, to leverage smoothness. Among local averaging techniques, there are, however, ways to do it. For example, using locally linear regression, where one solves for any test point x ,

$$\inf_{\beta_1 \in \mathbb{R}^d, \beta_0 \in \mathbb{R}} \sum_{i=1}^n \hat{w}_i(x)(y_i - \beta_1^\top x_i - \beta_0)^2.$$

(note that the regular regressogram corresponds to setting $\beta_1 = 0$ above). In other words we solve

$$\inf_{\beta_1 \in \mathbb{R}^d, \beta_0 \in \mathbb{R}} \int_y (y - \beta_1^\top x - \beta_0)^2 d\hat{p}(y|x).$$

The running time is now $O(nd^2)$ per testing point as we have to solve a linear least-squares (see Chapter 3), but the performance, both empirical and theoretical ([Tsybakov, 2008](#)), improves. See an example with the regressogram weights in Figure 6.6.

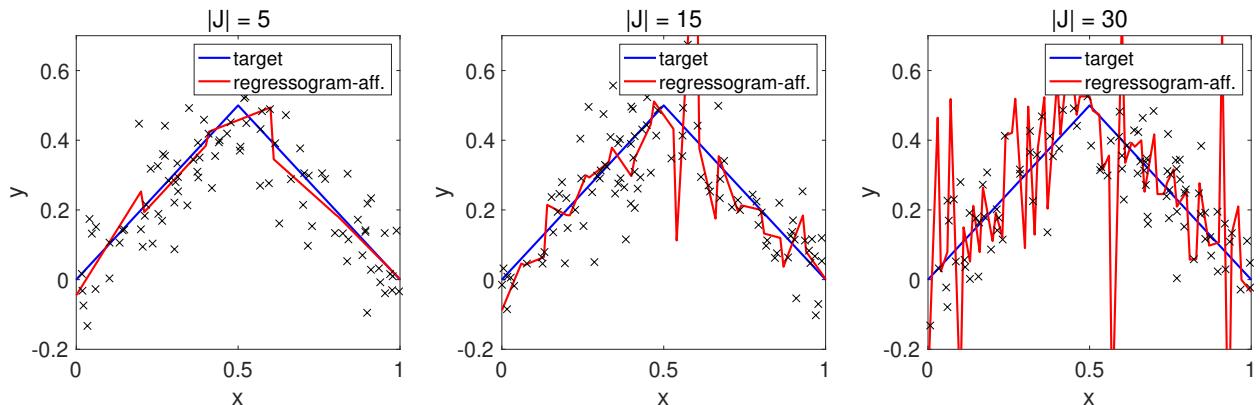


Figure 6.6: Locally linear regression, on the same data as Figure 6.2, for three values of the number $|J|$ of sets within in the partition. Notice the difference with Figure 6.2.

Exercise 6.5 (♦) For the Nadaraya Watson estimator, show that when the target function and the kernel are twice continuously differentiable, then the bias term is bounded by a constant times h^4 . Show that the optimal bandwidth selection leads to a rate proportional to $n^{-4/(4+d)}$.

Chapter 7

Kernel methods

Chapter summary

- Kernels and representer theorem: learning with infinite-dimensional linear models can be done in a time that depends on the number of observations using a kernel function.
- Kernels on \mathbb{R}^d : such models include polynomials and classical Sobolev spaces (functions with square-integrable partial derivatives).
- Algorithms: convex optimization algorithms can be applied with theoretical guarantees and many dedicated developments to avoid the quadratic complexity of computing the kernel matrix.
- Analysis of well-specified models: When the target function is in the associated function space, learning can be done with rates that are independent of dimension.
- Analysis of misspecified models: if the target function is not in the function space, the curse of dimensionality cannot be avoided in the worst-case situations of few existing derivatives of the target function, but the methods are adaptive to any amount of intermediate smoothness.
- Sharp analysis of ridge regression: for the square loss, a more involved analysis leads to optimal rates in various situations in \mathbb{R}^d .

In this chapter, we consider positive-definite kernel methods, with only a brief account of the main result. For more details, see [Schölkopf and Smola \(2001\)](#); [Shawe-Taylor and Cristianini \(2004\)](#); [Christmann and Steinwart \(2008\)](#).

7.1 Introduction

In this chapter, we study empirical risk minimization for linear models, that is, prediction functions $f_\theta : \mathcal{X} \rightarrow \mathbb{R}$ which are *linear in their parameters* θ , that is, of the form $f_\theta(x) = \langle \theta, \varphi(x) \rangle_{\mathcal{H}}$, where $\varphi : \mathcal{X} \rightarrow \mathcal{H}$ and \mathcal{H} is a Hilbert space (essentially a Euclidean space with potentially infinite dimension), and $\theta \in \mathcal{H}$. We will often use the notation $\langle \theta, \varphi(x) \rangle$ in this chapter instead of $\langle \theta, \varphi(x) \rangle_{\mathcal{H}}$ when this is not ambiguous.

The key difference with Chapter 3 on least-squares estimation is that (1) we are not restricted to the square loss (although many of the same concepts with play a role, in particular, in the analysis of ridge regression), and (2), we will explicitly allow infinite-dimensional models, thus extending the dimension-free bounds from Chapter 3. The notion of *kernel function* (or simply kernel) $k(x, y) = \langle \varphi(x), \varphi(y) \rangle_{\mathcal{H}}$ will be particularly fruitful.

Why is this relevant? The study of infinite-dimensional linear methods is important for several reasons:

- Understanding linear models in finite but very large input dimensions requires tools from the infinite-dimensional analysis.
- Kernel methods lead to simple and stable algorithms, with theoretical guarantees and adaptivity to the smoothness of the target function (as opposed to local averaging techniques). They can be applied in high dimensions, with good practical performance (note that for supervised learning problems with many observations in domains such as computer vision and natural language processing, they do not achieve the state of the art anymore, which is achieved by neural networks presented in Chapter 9).
- They can be easily applied when input observations are not vectors.
- They are useful to understand other models such as neural networks (see Chapter 9).



The type of kernel we consider here is different from the ones in Chapter 6. The ones here are “positive definite;” the ones from Chapter 6 are “non-negative”. See more details in <https://francisbach.com/cursed-kernels/>.

7.2 Representer theorem

Dealing with infinite-dimensional models seems impossible at first because algorithms cannot be run in infinite dimensions. In this section, we show how the kernel function plays a crucial role in achieving lower-dimensional algorithms.

As a motivation, we consider the optimization problem coming from machine learning with linear models, with data $(x_i, y_i) \in \mathcal{X} \times \mathcal{Y}$, $i = 1, \dots, n$:

$$\min_{\theta \in \mathcal{H}} \quad \frac{1}{n} \sum_{i=1}^n \ell(y_i, \langle \varphi(x_i), \theta \rangle) + \frac{\lambda}{2} \|\theta\|^2, \quad (7.1)$$

assuming the loss function ℓ is already from $\mathcal{Y} \times \mathbb{R} \rightarrow \mathbb{R}$ and not from $\mathcal{Y} \times \mathcal{Y} \rightarrow \mathbb{R}$ (e.g., hinge loss, logistic loss or least-squares, see Chapter 4).

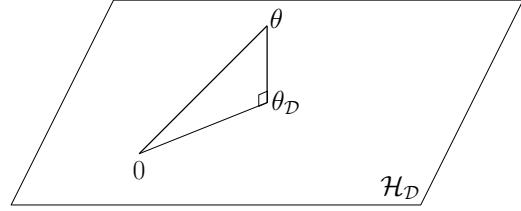
The key property of the objective function in Eq. (7.1) is that it accesses the input observations $x_1, \dots, x_n \in \mathcal{X}$, only through dot-products $\langle \theta, \varphi(x_i) \rangle$, $i = 1, \dots, n$, and that we penalize using the Hilbert norm $\|\theta\|$. The following theorem is crucial and has a particularly simple proof.

Theorem 7.1 (Representer theorem (Kimeldorf and Wahba, 1971)) *Let $\varphi : \mathcal{X} \rightarrow \mathcal{H}$. Let $(x_1, \dots, x_n) \in \mathcal{X}^n$, and assume that the functional $\Psi : \mathbb{R}^{n+1} \rightarrow \mathbb{R}$ is strictly increasing with respect to the last variable, then the infimum of $\Psi(\langle \theta, \varphi(x_1) \rangle, \dots, \langle \theta, \varphi(x_n) \rangle, \|\theta\|^2)$ can be obtained by restricting to a vector θ of the form*

$$\theta = \sum_{i=1}^n \alpha_i \varphi(x_i),$$

with $\alpha \in \mathbb{R}^n$.

Proof Let $\theta \in \mathcal{H}$, and $\mathcal{H}_{\mathcal{D}} = \left\{ \sum_{i=1}^n \alpha_i \varphi(x_i), \alpha \in \mathbb{R}^n \right\} \subset \mathcal{H}$, the linear span of the feature vectors. Let $\theta_{\mathcal{D}} \in \mathcal{H}_{\mathcal{D}}$ and $\theta_{\perp} \in \mathcal{H}_{\mathcal{D}}^{\perp}$ be such that $\theta = \theta_{\mathcal{D}} + \theta_{\perp}$, a decomposition which is using the Hilbertian structure of \mathcal{H} . Then $\forall i \in \{1, \dots, n\}$, $\langle \theta, \varphi(x_i) \rangle = \langle \theta_{\mathcal{D}}, \varphi(x_i) \rangle + \langle \theta_{\perp}, \varphi(x_i) \rangle$ with $\langle \theta_{\perp}, \varphi(x_i) \rangle = 0$, by definition of the orthogonal.



From the Pythagorean theorem, we get: $\|\theta\|^2 = \|\theta_{\mathcal{D}}\|^2 + \|\theta_{\perp}\|^2$. Therefore we have:

$$\begin{aligned} \Psi(\langle \theta, \varphi(x_1) \rangle, \dots, \langle \theta, \varphi(x_n) \rangle, \|\theta\|^2) &= \Psi(\langle \theta_{\mathcal{D}}, \varphi(x_1) \rangle, \dots, \langle \theta_{\mathcal{D}}, \varphi(x_n) \rangle, \|\theta_{\mathcal{D}}\|^2 + \|\theta_{\perp}\|^2) \\ &\geq \Psi(\langle \theta_{\mathcal{D}}, \varphi(x_1) \rangle, \dots, \langle \theta_{\mathcal{D}}, \varphi(x_n) \rangle, \|\theta_{\mathcal{D}}\|^2), \end{aligned}$$

with equality if and only if $\theta_{\perp} = 0$ (since Ψ is strictly increasing with respect to the last variable). Thus

$$\inf_{\theta \in \mathcal{H}} \Psi(\langle \theta, \varphi(x_1) \rangle, \dots, \langle \theta, \varphi(x_n) \rangle, \|\theta\|^2) = \inf_{\theta \in \mathcal{H}_{\mathcal{D}}} \Psi(\langle \theta, \varphi(x_1) \rangle, \dots, \langle \theta, \varphi(x_n) \rangle, \|\theta\|^2),$$

which is exactly the desired result. \blacksquare

This implies that the minimizer of Eq. (7.1) can be found among the vectors of the form $\theta = \sum_{i=1}^n \alpha_i \varphi(x_i)$:

Corollary 7.1 (Representer theorem for supervised learning) *For $\lambda > 0$, the infimum of $\frac{1}{n} \sum_{i=1}^n \ell(y_i, \langle \theta, \varphi(x_i) \rangle) + \frac{\lambda}{2} \|\theta\|^2$ can be obtained by restricting to a vector θ of the form $\theta = \sum_{i=1}^n \alpha_i \varphi(x_i)$, with $\alpha \in \mathbb{R}^n$.*

It is important to note that there is no assumption on the loss function ℓ . In particular, no convexity is assumed. This is to be contrasted to the use of duality in Section 7.4, where convexity will play a major role and similar α 's will be defined (but with some notable differences).

Given Corollary 7.1, we can reformulate the learning problem. We will need the *kernel function* k , which is the dot product between feature vectors:

$$k(x, x') = \langle \varphi(x), \varphi(x') \rangle.$$

We have:

$$\forall j \in \{1, \dots, n\}, \langle \theta, \varphi(x_j) \rangle = \sum_{i=1}^n \alpha_i k(x_i, x_j) = (K\alpha)_j$$

where $K \in \mathbb{R}^{n \times n}$ is the *kernel matrix*, such that $K_{ij} = \langle \varphi(x_i), \varphi(x_j) \rangle = k(x_i, x_j)$, and

$$\|\theta\|^2 = \sum_{i=1}^n \sum_{j=1}^n \alpha_i \alpha_j \langle \varphi(x_i), \varphi(x_j) \rangle = \sum_{i=1}^n \sum_{j=1}^n \alpha_i \alpha_j K_{ij} = \alpha^\top K \alpha.$$

We can then write:

$$\inf_{\theta \in \mathcal{H}} \frac{1}{n} \sum_{i=1}^n \ell(y_i, \langle \theta, \varphi(x_i) \rangle) + \frac{\lambda}{2} \|\theta\|^2 = \inf_{\alpha \in \mathbb{R}^n} \frac{1}{n} \sum_{i=1}^n \ell(y_i, (K\alpha)_i) + \frac{\lambda}{2} \alpha^\top K \alpha. \quad (7.2)$$

For a test point $x \in \mathcal{X}$, we have $f(x) = \sum_{i=1}^n \alpha_i k(x, x_i)$.

Thus, the input observations are summarized in the kernel matrix and the kernel function, regardless of the dimension of \mathcal{H} . Moreover, explicitly computing the feature vector $\varphi(x)$ is never needed! This is the *kernel trick*. This kernel trick allows to:

- replace the search space \mathcal{H} by \mathbb{R}^n ; this is interesting computationally when the dimension of \mathcal{H} is very large (see more details in Section 7.4),
- separate the representation problem (design of kernels on a set \mathcal{X}) and the design of algorithms and their analysis (which only use the kernel matrix K); this is interesting because a wide range of kernels can be defined for many data types (see more details in Section 7.3).

Minimum norm interpolation. The representer theorem can be extended to interpolating estimator with essentially the same proof (see proposition below).

Proposition 7.1 *Given $x_1, \dots, x_n \in \mathcal{X}$, and $y \in \mathbb{R}^n$ such that there exists at least one $\theta \in \mathcal{H}$ such that $y_i = \langle \theta, \varphi(x_i) \rangle$ for all $i \in \{1, \dots, n\}$, then among all these $\theta \in \mathcal{H}$ that interpolate the data, the one of minimum norm can be expressed as $\theta = \sum_{i=1}^n \alpha_i \varphi(x_i)$, with $\alpha \in \mathbb{R}^n$ is such that $y = K\alpha$ (this system must then have a solution).*

7.3 Kernels

In the section above, we have introduced the kernel function $k : \mathcal{X} \times \mathcal{X} \rightarrow \mathbb{R}$ as obtained from a dot product $k(x, x') = \langle \varphi(x), \varphi(x') \rangle$. The associated kernel matrix is then a matrix of dot-products (often called a “Gram matrix”) and is thus symmetric positive semi-definite, that is, all of its eigenvalues are non-negative, or $\forall \alpha \in \mathbb{R}^n$, $\alpha^\top K \alpha \geq 0$. It turns out that this simple property is enough to impose the existence of a feature function.

⚠ If $\mathcal{H} = \mathbb{R}^d$, and $\Phi \in \mathbb{R}^{n \times d}$ is the matrix of features (design matrix in the context of regression) with i -th row composed of $\varphi(x_i)$, then $K = \Phi \Phi^\top \in \mathbb{R}^{n \times n}$ is the kernel matrix, while $\frac{1}{n} \Phi^\top \Phi \in \mathbb{R}^{d \times d}$ is the empirical covariance matrix.

Definition 7.1 (Positive definite kernels) *A function $k : \mathcal{X} \times \mathcal{X} \rightarrow \mathbb{R}$ is a positive definite kernel if and only if all kernel matrices are symmetric positive semi-definite.*

The following important theorem dates back to Aronszajn (1950) and comes with an elegant constructive proof. Note the total absence of assumptions on the set \mathcal{X} .

Theorem 7.2 (Aronszajn, 1950) *k is a positive definite kernel if and only if there exists a Hilbert space \mathcal{H} , and a function $\varphi : \mathcal{X} \rightarrow \mathcal{H}$ such that $\forall x, x' \in \mathcal{X}$, $k(x, x') = \langle \varphi(x), \varphi(x') \rangle_{\mathcal{H}}$.*

Partial proof We first assume that $k(x, x') = \langle \varphi(x), \varphi(x') \rangle_{\mathcal{H}}$. Then for any $\alpha \in \mathbb{R}^n$, and points $x_1, \dots, x_n \in \mathcal{X}$, we have:

$$\alpha^\top K \alpha = \sum_{i,j=1}^n \alpha_i \alpha_j \langle \varphi(x_i), \varphi(x_j) \rangle_{\mathcal{H}} = \left\| \sum_{i=1}^n \alpha_i \varphi(x_i) \right\|_{\mathcal{H}}^2 \geq 0.$$

Thus k is a positive definite kernel.

For the other direction, we consider a positive-definite kernel, and we will construct a space of functions explicitly from \mathcal{X} to \mathbb{R} with a dot-product. We define the set $\mathcal{H}' \subset \mathbb{R}^{\mathcal{X}}$ as the set of linear combinations of kernel functions $\sum_{i=1}^n \alpha_i k(\cdot, x_i)$ for any integer n , any set of n points and any $\alpha \in \mathbb{R}^n$. This is a vector space on which we can define a dot-product through

$$\left\langle \sum_{i=1}^n \alpha_i k(\cdot, x_i), \sum_{j=1}^m \beta_j k(\cdot, x'_j) \right\rangle = \sum_{i=1}^n \sum_{j=1}^m \alpha_i \beta_j k(x_i, x'_j). \quad (7.3)$$

We first check that this is a well-defined function on $\mathcal{H}' \times \mathcal{H}'$, that is, the value does not depend on the chosen representation as a linear combination of kernel functions. Indeed, if we denote $f = \sum_{i=1}^n \alpha_i k(\cdot, x_i)$, then the dot-product is equal to $\sum_{j=1}^m \beta_j f(x'_j)$ and depends only on the values of f , and not on its representation (and similarly for the function on the right of the dot-product).

This dot-product is bi-linear and always non-negative when applied to the same function (that is, in Eq. (7.3) above, when $\alpha = \beta$ and the points x_i 's and the x'_j are the same, we get a positive number because of the positivity of the kernel k). Moreover, it satisfies the two properties for any $f \in \mathcal{H}'$, $x, x' \in \mathcal{X}$:

$$\langle k(\cdot, x), f \rangle = f(x) \text{ and } \langle k(\cdot, x), k(\cdot, x') \rangle = k(x, x').$$

These are called reproducing properties and correspond to an explicit construction of the feature map $\varphi(x) = k(\cdot, x)$.

The space \mathcal{H}' is called “pre-Hilbertian” because it is not complete.¹ It can be “completed” into a Hilbert space \mathcal{H} with the same reproducing property. See Aronszajn (1950); Berlinet and Thomas-Agnan (2004) for more details. ■

We can make the following observations:

- \mathcal{H} is called the “feature space,” and φ the “feature map,” that goes from the “input space” \mathcal{X} to the feature space \mathcal{H} .

¹See https://en.wikipedia.org/wiki/Complete_metric_space for definitions.

- No assumption is needed about the input space \mathcal{X} , and no regularity assumption is needed for k . Up to isomorphisms, the feature map and space happen to be unique. The particular space of functions we built is called the *reproducing kernel Hilbert space (RKHS)* associated with k , for which $\varphi(x) = k(\cdot, x)$.
- A classical intuitive interpretation of the identity $\langle k(\cdot, x), f \rangle = f(x)$ is that the function evaluation is the dot-product with a function (this is, in fact, another characterization). If $L_2(\mathbb{R}^d)$ was an RKHS, this would mean that there exists a function $k : \mathcal{X} \times \mathcal{X} \rightarrow \mathbb{R}$ such that $\int_{\mathbb{R}^d} k(x, x') f(x') dx' = f(x)$. In other words, $k(x, x') dx'$ would be a Dirac measure at x , which is impossible (as Dirac measures have no density with respect to the Lebesgue measure). Thus $L_2(\mathbb{R}^d)$ is a Hilbert space that is too large to be an RKHS.
- Given a positive-definite kernel k , we can thus associate it to some feature map φ such that $k(x, y) = \langle \varphi(x), \varphi(y) \rangle_{\mathcal{H}}$, but also to a *space of functions on \mathcal{X} with a given norm*, either directly through the RKHS above or by looking at all functions f_θ of the form $f_\theta(x) = \langle \theta, \varphi(x) \rangle_{\mathcal{H}}$, with a regularization term $\|\theta\|_{\mathcal{H}}^2$. These two views are equivalent.

! From now on, we will denote elements of the Hilbert space \mathcal{H} through the notation $f \in \mathcal{H}$ to highlight the fact that we are considering a space of functions from \mathcal{X} to \mathbb{R} , except for optimization algorithms in Section 7.4, where will use the notation $\langle \theta, \varphi(x) \rangle_{\mathcal{H}}$ instead of $f(x)$.

Kernels = features and functions. A positive-definite kernel thus defines a feature map and a space of functions. Sometimes, the feature map is easy to find, and sometimes it is not. In the next section, we will look at the main examples and describe the associated spaces of functions (and the corresponding norms).

Exercise 7.1 *The sum and (pointwise) product of kernels are kernels. What are their associated feature spaces and feature maps?*

We now look at different ways of building the kernels, by starting first from the feature vector (e.g., linear kernels), from the kernel and explicit feature map (polynomial kernel), from the norm (translation-invariant kernel on $[0, 1]$), or from the kernel without explicit features (translation-invariant kernel on \mathbb{R}^d).

7.3.1 Linear and polynomial kernels

We start with the most obvious kernels on $\mathcal{X} = \mathbb{R}^d$, for which feature maps are easily found.

Linear kernel. We define $k(x, x') = x^\top x'$. It corresponds to a function space composed of linear functions $f_\theta(x) = \theta^\top x$, with an ℓ_2 -penalty $\|\theta\|_2^2$. The kernel trick can be useful when the input data have huge dimension d but are quite sparse (many zeros), such as in text processing, so that the dot-product $x^\top x'$ can be computed in time $o(d)$.

Polynomial kernel. For r a positive integer, the kernel $k(x, x') = (x^\top x')^r$ can be expanded as (with the binomial theorem²):

$$k(x, x') = \left(\sum_{i=1}^d x_i x'_i \right)^r = \sum_{\alpha_1 + \dots + \alpha_d = r} \binom{r}{\alpha_1, \dots, \alpha_d} \underbrace{(x_1 x'_1)^{\alpha_1} \cdots (x_d x'_d)^{\alpha_d}}_{(x_1^{\alpha_1} \cdots x_d^{\alpha_d})((x'_1)^{\alpha_1} \cdots (x'_d)^{\alpha_d})},$$

where the sum is over all non-negative integer vectors $(\alpha_1, \dots, \alpha_d)$. We have an explicit feature map: $\varphi(x) = ((\binom{r}{\alpha_1, \dots, \alpha_d})^{\frac{1}{2}} x_1^{\alpha_1} \cdots x_d^{\alpha_d})_{\alpha_1 + \dots + \alpha_d = r}$, and the set of functions is the set of degree- r homogeneous³ polynomials on \mathbb{R}^d , which has dimension $\binom{d+r-1}{r}$.

When d and r grow, the feature space dimension grows as d^r , an explicit representation is not desirable, and the kernel trick can be advantageous. Note, however, that the associated norm (which penalizes coefficients of the polynomials) is hard to interpret (as a small change in a single high-order coefficient can lead to significant changes).

Exercise 7.2 Show that the kernel $k(x, y) = (1 + x^\top y)^r$ corresponds to the set of all monomials $x_1^{\alpha_1} \cdots x_d^{\alpha_d}$ such that $\alpha_1 + \cdots + \alpha_d \leq r$. Show that the dimension of the feature space is $\binom{d+r}{r}$.

7.3.2 Translation-invariant kernels on $[0, 1]$

We consider $\mathcal{X} = [0, 1]$, and kernels of the form $k(x, x') = q(x - x')$ with a function $q : [0, 1] \rightarrow \mathbb{R}$, which is 1-periodic. We will show how they emerge from penalties on the Fourier coefficients of functions. We will use the fact that complex-valued squared integrable functions, which are 1-periodic, can be expanded in Fourier series, that is, $q(x) = \sum_{m \in \mathbb{Z}} e^{2im\pi x} \hat{q}_m$, with $\hat{q}_m = \int_0^1 q(x) e^{-2im\pi x} dx \in \mathbb{C}$, for $m \in \mathbb{Z}$. The function q is real-valued if and only if for all $m \in \mathbb{Z}$, $\hat{q}_{-m} = \hat{q}_m^*$ (the complex conjugate of \hat{q}_m).

When presenting translation-invariant kernels, we can choose to start from the kernel or from the associated squared norm. In this section, we start from the squared norm, while in the next one, we start from the kernel.

²See https://en.wikipedia.org/wiki/Binomial_theorem.

³A function $f : \mathbb{R}^d \rightarrow \mathbb{R}$ is said homogeneous if there exists $s \in \mathbb{R}_+$ such that for all $x \in \mathbb{R}^d$, and $\lambda \in \mathbb{R}_+$, $f(\lambda x) = \lambda^s f(x)$.

Given a 1-periodic function f decomposed into its Fourier series $f(x) = \sum_{m \in \mathbb{Z}} e^{2im\pi x} \hat{f}_m$, we consider the penalty

$$\sum_{m \in \mathbb{Z}} c_m |\hat{f}_m|^2,$$

with $c \in \mathbb{R}_+^{\mathbb{Z}}$; this penalty can be interpreted through a feature map and the ℓ_2 -norm on $\mathbb{C}^{\mathbb{Z}}$. Indeed, it corresponds to the feature vector $\varphi(x)_m = \frac{e^{2im\pi x}}{\sqrt{c_m}}$, and $\theta \in \mathbb{C}^{\mathbb{Z}}$, such that $\theta_m = \hat{f}_m \sqrt{c_m}$ (we can easily consider complex-valued features instead of real-valued features if Hermitian dot-products are considered), so that $f(x) = \langle \theta, \varphi(x) \rangle$ and $\sum_{m \in \mathbb{Z}} |\theta_m|^2$ is equal to the norm $\sum_{m \in \mathbb{Z}} c_m |\hat{f}_m|^2$.

Thus the associated kernel is

$$k(x, x') = \sum_{m \in \mathbb{Z}} \varphi(x)_m \varphi(x')_m^* = \sum_{m \in \mathbb{Z}} \frac{e^{2im\pi x}}{\sqrt{c_m}} \frac{e^{-2im\pi x'}}{\sqrt{c_m}} = \sum_{m \in \mathbb{Z}} \frac{1}{c_m} e^{2im\pi(x-x')},$$

which is thus of the form $q(x - x')$ for a 1-periodic function q .

What we showed above is that any penalty of the form $\sum_{m \in \mathbb{Z}} c_m |\hat{f}_m|^2$ defines a squared RKHS norm as soon as c_m is strictly positive for all $m \in \mathbb{Z}$, and $\sum_{m \in \mathbb{Z}} \frac{1}{c_m}$ is finite. The kernel function is then of the form $k(x, y) = q(x - y)$ with q being 1-periodic, and such that the Fourier series has non-negative real values $\hat{q}_m = c_m^{-1}$. In the other direction, all such kernels are positive-definite (see an extension to \mathbb{R}^d in Section 7.3.3).

Penalization of derivatives. For certain penalties based on c , there is a natural link with penalties on derivatives, as if f is s -times differentiable with squared integrable derivative, we have $f^{(s)}(x) = \sum_{m \in \mathbb{Z}} (2im\pi)^s e^{2im\pi x} \hat{f}_m$, and thus, from Parseval's theorem (which states that the squared L_2 -norm of a function is equal to the sum of the square modulus of its Fourier coefficients):

$$\int_0^1 |f^{(s)}(x)|^2 dx = (2\pi)^{2s} \sum_{m \in \mathbb{Z}} m^{2s} |\hat{f}_m|^2.$$

In this chapter, we will consider penalizing such derivatives, leading to Sobolev spaces on $[0, 1]$. The following examples are often considered:

- **Bernoulli polynomials:** we can consider $c_0 = 1$ and $c_m = |m|^{2s}$ for $m \neq 0$, for which the associated norm is $\|f\|_{\mathcal{H}}^2 = \frac{1}{(2\pi)^{2s}} \int_0^1 |f^{(s)}(x)|^2 dx + \left(\int_0^1 f(x) dx \right)^2$. The corresponding kernel $k(x, x')$ can then be written as

$$k(x, x') = \sum_{m \in \mathbb{Z}} c_m^{-1} e^{2im\pi(x-x')} = 1 + \sum_{m \geq 1} \frac{2 \cos[2\pi m(x-x')]}{m^{2s}}.$$

In order to have an expression for q in closed form we notice that if we define $\{x\} = x - \lfloor x \rfloor \in [0, 1)$ the fractional part of x , the function $x \mapsto \{x\}$ has (by integration by part) an m -th Fourier coefficient equal to $\int_0^1 e^{-2im\pi x} x dx = \frac{i}{2m\pi}$. Similarly, the s -th power of $\{x\}$ has an m -th Fourier coefficient which is an order s polynomial in m^{-1} . This implies that $k(x, x')$ has to be an order s polynomial in $\{x - x'\}$.

For $s = 1$, we have $k(x, x) = 1 + 2 \sum_{m \geq 1} m^{-2} = 1 + \pi^2/3$; moreover by using the Fourier series expansion $\{t\} = \frac{1}{2} - \frac{1}{2\pi} \sum_{m \geq 1} \frac{2\sin[2\pi mt]}{m}$, and integrating, we get

$$k(x, x') = 2\pi^2\{x - x'\}^2 - 2\pi^2\{x - x'\} + \pi^2/3 + 1 = q(x - x'),$$

with q plotted in Figure 7.1.

For $s \geq 1$, we have the closed-form expression $k(x, x') = 1 + (-1)^{s-1} \frac{(2\pi)^{2s}}{(2s)!} B_{2s}(\{x - x'\})$, where B_{2s} the $(2s)$ -th Bernoulli polynomial,⁴ from which we can “check” the computation above since $B_2(t) = t^2 - t + 1/6$.

Exercise 7.3 Show that for $s = 2$, $k(x, x') = q(x - x')$ with $q(t) = 1 - \frac{(2\pi)^4}{24} \left(\{t\}^4 - 2\{t\}^3 + \{t\}^2 - \frac{1}{30} \right)$.

- **Periodic exponential kernel:** we can consider $c_m = 1 + \alpha^2|m|^2$, for which we also have a closed-form formula, with the penalty $\|f\|_{\mathcal{H}}^2 = \frac{\alpha^2}{(2\pi)^2} \int_0^1 |f'(x)|^2 dx + \int_0^1 |f(x)|^2 dx$.

Exercise 7.4 (♦♦♦) Show that we have $k(x, x') = \sum_{m \in \mathbb{Z}} \frac{e^{2im\pi(x-x')}}{1+\alpha^2|m|^2} = q(x - x')$ for $q(t) = \frac{\pi}{\alpha} \frac{\cosh \frac{\pi}{\alpha}(1-2|\{t+1/2\}-1/2|)}{\sinh \frac{\pi}{\alpha}}$. Hint: use the Cauchy residue formula.⁵

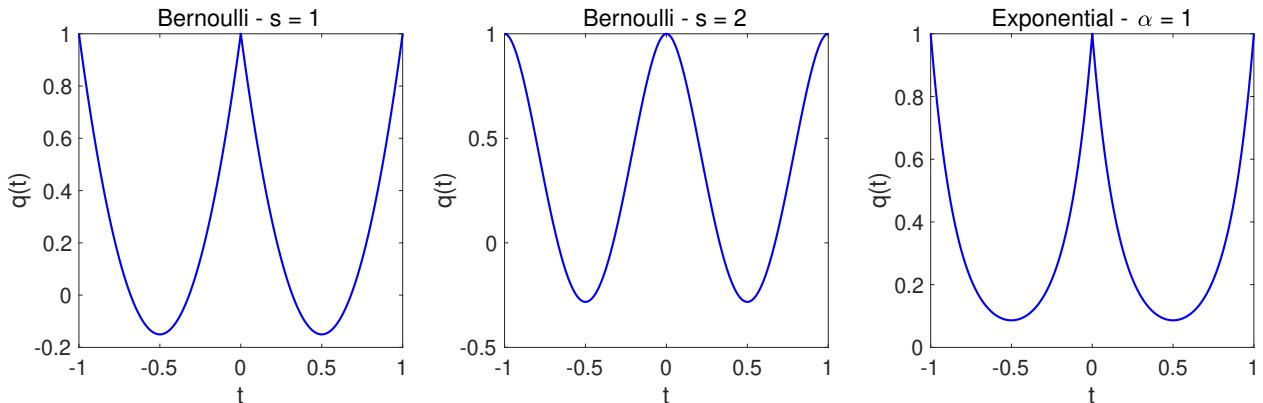


Figure 7.1: Translation-invariant kernels on $[0, 1]$, of the form $k(x, x') = q(x - x')$, with q 1-periodic, for the kernels based on Bernoulli polynomials, and the periodic exponential kernel. Kernels are normalized so that $k(x, x) = 1$.

⁴See https://en.wikipedia.org/wiki/Bernoulli_polynomials.

⁵See <https://francisbach.com/cauchy-residue-formula/>.

These kernels are mainly used for their simplicity and explicit feature map, which are simpler than the kernels most used below (with similar links with Sobolev spaces). Note also that for the uniform distribution on $[0, 1]$, the Fourier basis will be an orthogonal eigenbasis of the covariance operator with eigenvalues c_m^{-1} (see Section 7.6.6).

We saw that for the kernel $q(x - x')$ with Fourier series \hat{q}_m for q , the associated norm is $\sum_{m \in \mathbb{Z}} \frac{|\hat{f}_m|^2}{\hat{q}_m}$. We now extend this to Fourier transforms (instead of Fourier series).

7.3.3 Translation-invariant kernels on \mathbb{R}^d

We consider $\mathcal{X} = \mathbb{R}^d$, and a kernel of the form $k(x, x') = q(x - x')$ with a function $q : \mathbb{R}^d \rightarrow \mathbb{R}$, which we refer to as translation-invariant as they are invariant by the addition of the same constant to both arguments. The following theorem gives conditions under which we obtain a positive definite kernel.

Theorem 7.3 (Böchner (Reed and Simon, 1978)) *The kernel k is positive definite if and only if q is the Fourier transform of a non-negative Borel measure. Consequently, if $q \in L^1(dx)$ and its Fourier transform only has non-negative real values, then k is positive definite.*

Partial proof We only give the proof of the consequence, which is the only one we need. Since q is integrable, $\hat{q}(\omega) = \int_{\mathbb{R}^d} e^{-i\omega^\top x} q(x) dx$ is defined on \mathbb{R}^d and continuous, and we have through the inverse Fourier transform formula:

$$q(x - x') = \frac{1}{(2\pi)^d} \int_{\mathbb{R}^d} \hat{q}(\omega) e^{i(x-x')^\top \omega} d\omega.$$

Let $x_1, \dots, x_n \in \mathbb{R}^d$, let $\alpha_1, \dots, \alpha_n \in \mathbb{R}$. We have:

$$\begin{aligned} \sum_{s,j=1}^n \alpha_s \alpha_j k(x_s, x_j) &= \sum_{s,j=1}^n \alpha_s \alpha_j q(x_s - x_j) = \frac{1}{(2\pi)^d} \sum_{s,j=1}^n \alpha_s \alpha_j \int_{\mathbb{R}^d} e^{i\omega^\top (x_s - x_j)} \hat{q}(\omega) d\omega \\ &= \frac{1}{(2\pi)^d} \int_{\mathbb{R}^d} \left(\sum_{s,j=1}^n \alpha_s \alpha_j e^{i\omega^\top x_s} (e^{i\omega^\top x_j})^* \right) \hat{q}(\omega) d\omega \\ &= \frac{1}{(2\pi)^d} \int_{\mathbb{R}^d} \left| \sum_{s=1}^n \alpha_s e^{i\omega^\top x_s} \right|^2 \hat{q}(\omega) d\omega \geq 0, \end{aligned}$$

which shows the positive-definiteness. See also Varadhan (2001, Theorem 2.7) for a proof of the other direction. ■

Construction of the associated norm. We give an intuitive (non-rigorous) reasoning: if q is in $L^1(dx)$, then $\hat{q}(\omega)$ exists and, we have an explicit representation as

$$k(x, x') = \frac{1}{(2\pi)^d} \int_{\mathbb{R}^d} \sqrt{\hat{q}(\omega)} e^{i\omega^\top x} (\sqrt{\hat{q}(\omega)} e^{i\omega^\top x'})^* d\omega = \int_{\mathbb{R}^d} \varphi(x)_\omega \varphi(x')_\omega^* d\omega,$$

which is of the form $\langle \varphi(x), \varphi(y) \rangle$, with $\varphi(x)_\omega = \frac{1}{(2\pi)^{d/2}} \sqrt{\hat{q}(\omega)} e^{i\omega^\top x}$. If we consider $f(x) = \int_{\mathbb{R}^d} \varphi(x)_\omega \theta_\omega d\omega = \langle \varphi(x), \theta \rangle$, then $\theta_\omega = \frac{1}{(2\pi)^{d/2}} \hat{f}(\omega) / \sqrt{\hat{q}(\omega)}$, and the squared norm of θ is equal to $\frac{1}{(2\pi)^d} \int_{\mathbb{R}^d} \frac{|\hat{f}(w)|^2}{\hat{q}(\omega)} d\omega$, where \hat{f} denotes the Fourier transform of f . Therefore, the norm of a function $f \in \mathcal{H}$ is (for a formal proof, see [Schölkopf and Smola, 2001](#)):

$$\|f\|_{\mathcal{H}}^2 = \frac{1}{(2\pi)^d} \int_{\mathbb{R}^d} \frac{|\hat{f}(w)|^2}{\hat{q}(\omega)} d\omega.$$

Note the similarity with the penalty for the kernel on $[0, 1]$ (see more similarity below).

Link with derivatives. When f has partial derivatives, then the Fourier transform of $\frac{\partial f}{\partial x_j}$ is equal to $i\omega_j$ times the Fourier transform of f . This leads to, using Parseval's theorem, $\frac{1}{(2\pi)^d} \int_{\mathbb{R}^d} |\omega_j|^2 |\hat{f}(w)|^2 d\omega = \int_{\mathbb{R}^d} \left| \frac{\partial f}{\partial x_j}(x) \right|^2 dx$, which extends to higher order derivatives:

$$\frac{1}{(2\pi)^d} \int_{\mathbb{R}^d} |\omega_1^{\alpha_1} \cdots \omega_d^{\alpha_d}|^2 |\hat{f}(w)|^2 d\omega = \int_{\mathbb{R}^d} \left| \frac{\partial^\alpha f}{\partial x_1^{\alpha_1} \cdots \partial x_d^{\alpha_d}}(x) \right|^2 dx.$$

This will allow us to find corresponding norms by expanding $\hat{q}(\omega)^{-1}$ as sums of monomials. We now consider the main classical examples.

Exponential kernel. This is the kernel $q(x - x') = \exp(-\alpha \|x - x'\|_2)$, for which the Fourier transform can be computed as $\hat{q}(\omega) = 2^d \pi^{(d-1)/2} \Gamma((d+1)/2) \frac{\alpha}{(\alpha^2 + \|\omega\|_2^2)^{(d+1)/2}}$.

See [Rasmussen and Williams \(2006, page 84\)](#). Thus, $\hat{q}(\omega)^{-1}$ is a sum of monomials, and looking at their orders, we see that the corresponding RKHS norm (that is, the norm on the space of functions on \mathbb{R}^d that our kernel defines) is penalizing all derivatives up to total order $(d+1)/2$, that is for all $\alpha \in \mathbb{N}^d$ such that $\alpha_1 + \cdots + \alpha_d \leq (d+1)/2$, which is a Sobolev space (fractional for d even).⁶

In particular, for $d = 1$, we have $\hat{q}(\omega) = \frac{2\alpha}{\alpha^2 + \omega^2}$, and thus

$$\begin{aligned} \|f\|_{\mathcal{H}}^2 &= \frac{1}{2\pi} \int_{\mathbb{R}} \frac{|\hat{f}(w)|^2}{\hat{q}(\omega)} d\omega = \frac{\alpha}{2} \frac{1}{2\pi} \int_{\mathbb{R}} |\hat{f}(\omega)|^2 d\omega + \frac{1}{2\alpha} \frac{1}{2\pi} \int_{\mathbb{R}} |\omega \hat{f}(\omega)|^2 d\omega \\ &= \frac{\alpha}{2} \int_{\mathbb{R}} |f(x)|^2 dx + \frac{1}{2\alpha} \int_{\mathbb{R}} |f'(x)|^2 dx, \end{aligned}$$

⁶See https://en.wikipedia.org/wiki/Sobolev_space.

and we recover the Sobolev space of functions with squared-integrable derivatives.

Gaussian kernel. This is the kernel $q(x - x') = \exp(-\alpha \|x - x'\|_2^2)$, for which the Fourier transform can be computed as $\hat{q}(\omega) = \left(\frac{\pi}{\alpha}\right)^{d/2} \exp(-\|\omega\|_2^2/(4\alpha))$. By expanding $\hat{q}(\omega)^{-1}$ through its power series as $\hat{q}(\omega)^{-1} = \left(\frac{\pi}{\alpha}\right)^{d/2} \sum_{s=0}^{\infty} \frac{\|\omega\|_2^{2s}}{(4\alpha)^s s!}$, this corresponds to an RKHS norm which is penalizing all derivatives. Note that all members of this RKHS (the associated function space) are infinitely differentiable and thus much smoother than functions coming from the exponential kernel (the RKHS is smaller).

Matern kernels. More generally, one can define a series of kernels so that $\hat{q}(\omega)$ is proportional to $(\alpha^2 + \|\omega\|_2^2)^{-s}$ for $s > d/2$, to ensure integrability of the Fourier transform. These so-called “Matern kernels” all correspond to Sobolev spaces of order s and can be computed in closed form; see [Rasmussen and Williams \(2006, page 84\)](#). A key fact is that to be an RKHS, a Sobolev space has to have many derivatives when d grows; in particular, having only first-order derivatives ($s = 1$) only leads to an RKHS for $d = 1$, and having $s = 0$ never does.

For $s = \frac{d+3}{2}$, we have $k(x, x') \propto (1 + \sqrt{3}\alpha \|x - x'\|_2) \exp(-\sqrt{3}\alpha \|x - x'\|_2)$, and for $s = \frac{d+5}{2}$, we have $k(x, x') \propto (1 + \sqrt{5}\alpha \|x - x'\|_2 + \frac{5}{3}\alpha^2 \|x - x'\|_2^2) \exp(-\sqrt{5}\alpha \|x - x'\|_2)$. General values s also lead to closed-form formulas (through Bessel functions).

Density in $L_2(\mathbb{R}^d)$. For all the kernels below, the set \mathcal{H} is dense in $L_2(\mathbb{R}^d)$ (the set of square-integrable functions with respect to the Lebesgue measure), meaning that all functions in $L_2(\mathbb{R}^d)$ can be approached (with respect to their corresponding norm) by a function in \mathcal{H} . This is made quantitative in Section [7.5.2](#).

⚠ In this chapter, we will consider two spaces of integrable functions, with respect to the Lebesgue measure (which is not a probability measure), which we denote $L_2(\mathbb{R}^d)$, and with respect to the probability measure of the input data, which we denote $L_2(p)$. If p has a density with respect to the Lebesgue measure and this density $\frac{dp}{dx}(x)$ is uniformly bounded, then $L_2(\mathbb{R}^d) \subset L_2(p)$; more precisely, $\|f\|_{L_2(p)} \leq \left\| \frac{dp}{dx} \right\|_{\infty}^{1/2} \|f\|_{L_2(\mathbb{R}^d)}$. However, the converse is not true, simply because being an element of $L_2(\mathbb{R}^d)$ imposes a zero limit at infinity, which being an element of $L_2(p)$ does not impose (moreover, non zero constants are in $L_2(p)$ but not in $L_2(\mathbb{R}^d)$).

Examples of members of RKHS. Below, we sampled $n = 10$ random points in $[-1, 1]$ with 10 random responses, and we look for the function $f \in \mathcal{H}$ such that $f(x_i) = y_i$ for all $i \in \{1 \dots, n\}$ and with minimum norm. Given the representer theorem, we can write

$f(x) = \sum_{i=1}^n \alpha_i k(x, x_i)$, and the interpolation condition implies that $K\alpha = y$, and thus $y = K^{-1}\alpha$.

We consider several kernels in Figure 7.2, going from close to piecewise affine interpolation to infinitely differentiable functions (for the Gaussian kernel).

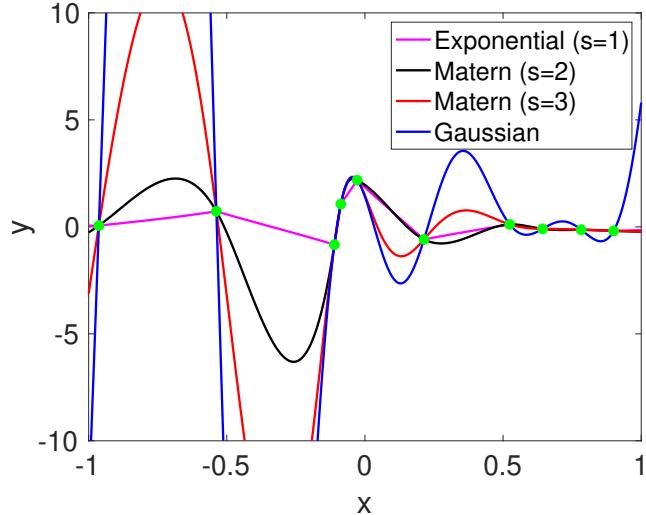


Figure 7.2: Examples of functions in the reproducing kernel Hilbert spaces (RKHS) for several kernels. All functions are the minimum norm interpolators of the green points.

7.3.4 Beyond vectorial input spaces (♦)

While the theoretical analysis of kernel methods focuses a lot on kernels on \mathbb{R}^d and their link with differentiability properties of the target function, kernels can be applied to a wide variety of problems with various input types. We give below classic examples (see more details by [Shawe-Taylor and Cristianini, 2004](#)).

- Set of subsets of a given set V : for example, the function k defined as $k(A, B) = \frac{|A \cap B|}{|A \cup B|}$ is a positive definite kernel.
- Text documents / web pages: with the usual “bag of words” assumption, we represent a text document or a web page by considering a vocabulary of “words” (this could be groups of letters, single original words, or groups of words or letters), and counting the number of occurrences of this word in the corresponding document. This gives a typically high-dimensional feature vector $\varphi(x)$ (with dimension the size of the vocabulary). Using linear functions on this feature provides cheap and stable predictors on such data types (better models that take into account the word order can be obtained, such as neural networks, at the expense of significantly more computational resources). See, e.g., [Joulin et al. \(2017\)](#) for examples.

- Sequences: given some finite alphabet \mathcal{A} , we consider the set \mathcal{X} of finite sequences in \mathcal{A} with arbitrary length. A classical infinite-dimensional feature space is indexed by \mathcal{X} itself, and for $y \in \mathcal{X}$, $\varphi(x)_y$ is equal to 1 if y is a subsequence of x (we could also count the number of times the subsequence y appears in x , or we could add a weight that depends on y , e.g., to penalize longer subsequences). This kernel has an infinite-dimensional feature space, but for two sequences x and x' , we can enumerate all subsequences of x and x' and compare them in polynomial time (there exist much faster algorithms, see [Gusfield \(1997\)](#)). These kernels have many applications in bioinformatics.

The same techniques can be extended to more general combinatorial objects such as trees and graphs (see [Shawe-Taylor and Cristianini, 2004](#)).

- Images: before neural networks took over in the years 2010s with the use of large amounts of data, several kernels were designed for images, with often a “bag-of-words” assumption that provides for free invariance by translation. The key is what to consider as “words”, i.e., the presence of specific local patterns in the image and the regions under which this assumption is made. See [Zhang et al. \(2007\)](#) for details.

7.4 Algorithms

In this section, we briefly mention algorithms aimed at solving

$$\min_{f \in \mathcal{H}} \frac{1}{n} \sum_{i=1}^n \ell(y_i, f(x_i)) + \frac{\lambda}{2} \|f\|_{\mathcal{H}}^2, \quad (7.4)$$

for ℓ being convex with respect to its second variable. We assume that for all $i \in \{1, \dots, n\}$, $k(x_i, x_i) = \|\varphi(x_i)\|^2 \leq R^2$.

Representer theorem. We can directly apply the representer theorem, as done in Eq. (7.2) and try to solve

$$\min_{\alpha \in \mathbb{R}^n} \frac{1}{n} \sum_{i=1}^n \ell(y_i, (K\alpha)_i) + \frac{\lambda}{2} \alpha^\top K \alpha,$$

which is a convex optimization problem since ℓ is assumed convex with respect to the second variable, and K is positive-semidefinite.

In the special case of the square loss (ridge regression), this leads to

$$\min_{\alpha \in \mathbb{R}^n} \frac{1}{2n} \|y - K\alpha\|_2^2 + \frac{\lambda}{2} \alpha^\top K \alpha,$$

and setting the gradient to zero, we get $(K^2 + n\lambda K)\alpha = Ky$, with a solution $\alpha = (K + n\lambda I)^{-1}y$.

However, in general (for the square loss and beyond), it is an ill-conditioned optimization problem because K often has very small eigenvalues (more on this later). When the loss is smooth, the Hessians are equal to $\frac{1}{n}K \text{Diag}(h)K + \lambda K$, where $h \in \mathbb{R}^n$ is a vector of second-order derivatives of ℓ , so that the Hessians are ill-conditioned.

A better alternative is to first compute a square root of K as $K = \Phi\Phi^\top$, where $\Phi \in \mathbb{R}^{n \times m}$, and m the rank of K , and solve

$$\min_{\beta \in \mathbb{R}^m} \frac{1}{n} \sum_{i=1}^n \ell(y_i, (\Phi\beta)_i) + \frac{\lambda}{2} \|\beta\|_2^2,$$

with $\beta = \Phi^\top\alpha$. Note that this corresponds to an explicit feature space representation (that is, the rows of Φ correspond to features in \mathbb{R}^n for the corresponding data point). For ridge regression, the objective function's Hessian is equal to $\frac{1}{n}\Phi^\top\Phi + \lambda I$, which is well-conditioned because its lowest eigenvalue is greater than λ and is thus directly controlled by regularization.

Computing a square root can be done in several ways (through Cholesky decomposition or SVD) ([Golub and Loan, 1996](#)), in running time $O(m^2n)$.

Column sampling. Approximate square roots are a very useful tool, and among various algorithms, approximating $K \in \mathbb{R}^{n \times n}$ from a subset of its columns can be done as $K \approx K(V, I)K(I, I)^{-1}K(I, V)$, where $K(A, B)$ is the sub-matrix of K obtained by taking rows from the set $A \subset \{1, \dots, n\}$ and columns from $B \subset \{1, \dots, n\}$, and $V = \{1, \dots, n\}$. See below for an illustration when $I = \{1, \dots, m\}$ and a partition of the kernel matrix.

| | |
|-----------|-----------|
| $K(I, I)$ | $K(I, J)$ |
| $K(J, I)$ | $K(J, J)$ |

This corresponds to an approximate square root $\Phi = K(V, I)K(I, I)^{-1/2} \in \mathbb{R}^{n \times m}$, with $m = |I|$, and it can be computed in time $O(m^2n)$ (computing the entire kernel matrix is not even needed). Then, the complexity is typically $O(m^2n)$ instead of $O(n^3)$ (e.g., when using matrix inversion for ridge regression, for faster algorithms, see below), and is thus linear in n .

Exercise 7.5 (♦) Show that column sampling corresponds to approximating optimally each $\varphi(x_j)$, $j \notin I$, by a linear combination of $\varphi(x_i)$, $i \in I$.

This approximation technique, often called “Nyström approximation,” can be analyzed when the columns are chosen randomly ([Rudi et al., 2015](#)).

Random features. Some kernels have a special form that leads to specific approximation schemes, that is,

$$k(x, x') = \int_{\mathcal{V}} \varphi(x, v) \varphi(x', v) d\mu(v),$$

where μ is a probability distribution on some space \mathcal{V} and $\varphi(x, v) \in \mathbb{R}$. We can then approximate the expectation by an empirical average

$$\hat{k}(x, x') = \frac{1}{m} \sum_{i=1}^m \varphi(x, v_i) \varphi(x', v_i),$$

where the v_i 's are sampled i.i.d. from μ . We can thus use an explicit feature representation $\hat{\varphi}(x) = (\frac{1}{\sqrt{m}} \varphi(x, v_i))_{i \in \{1, \dots, m\}}$, and solve

$$\min_{\beta \in \mathbb{R}^m} \frac{1}{n} \sum_{i=1}^n \ell(y_i, \hat{\varphi}(x_i)^\top \beta) + \frac{\lambda}{2} \|\beta\|_2^2.$$

For this scheme to make sense, the number m of random features has to be significantly smaller than n , which is often sufficient in practice (see an analysis by [Rudi and Rosasco, 2017](#)).

⚠ Note that dimension reduction is performed independently of the input data (that is, the random feature functions $\varphi(\cdot, v_i)$ are selected before the data are observed, as opposed to column sampling, which is a data-dependent dimension reduction scheme).

The two classic examples are:

- **Translation-invariant kernels:** $k(x, y) = q(x - y) = \frac{1}{(2\pi)^d} \int_{\mathbb{R}^d} \hat{q}(\omega) e^{i\omega^\top (x-y)} d\omega$, for which we can take $\varphi(x, \omega) = \sqrt{q(0)} e^{i\omega^\top x} \in \mathbb{C}$, where ω is sampled from the distribution with density $\frac{1}{(2\pi)^d} \frac{\hat{q}(\omega)}{q(0)}$, which is a Gaussian distribution for the Gaussian kernel. Alternatively, one can use a real-valued feature (instead of a complex-valued one) by using $\sqrt{2} \cos(\omega^\top x + b)$ with b sampled uniformly in $[0, 2\pi]$ ([Rahimi and Recht, 2008](#)).
- **Neural networks with random weights:** we can start from an expectation, for which the sampled features are classical, e.g., $\varphi(x, v) = \sigma(v^\top x)$ for some function

$\sigma : \mathbb{R} \rightarrow \mathbb{R}$. For the “rectified linear unit”, that is, $\sigma(\alpha) = \max\{0, \alpha\}$, and for v sampled uniformly on the sphere, we have (proof left as an exercise) $k(x, x') = \frac{\|x\|_2 \|x'\|_2}{2(d+1)\pi} [(\pi - \eta) \cos \eta + \sin \eta]$, where $\cos \eta = \frac{x^\top x'}{\|x\|_2 \|x'\|_2}$ (Le Roux and Bengio, 2007). Therefore, we can view a neural network with a large number of hidden neurons, with random input weights and not optimized as a kernel method. See a thorough discussion in Chapter 9.

Dual algorithms (♦). For the next two algorithms, we go back to the notation $f(x) = \langle \varphi(x), \theta \rangle$ with $\theta \in \mathcal{H}$ because it is more adapted (and is a direct infinite-dimensional extension of the algorithms from Chapter 5). To solve $\min_{\theta \in \mathcal{H}} \frac{1}{n} \sum_{i=1}^n \ell(y_i, \langle \varphi(x_i), \theta \rangle) + \frac{\lambda}{2} \|\theta\|^2$, for a loss which is convex with respect to the second variable, we can derive a Lagrange dual in the following way (for an introduction to Lagrange duality, see Boyd and Vandenberghe, 2004). We start by reformulating the problem as a constrained problem:

$$\begin{aligned} & \min_{\theta \in \mathcal{H}} \frac{1}{n} \sum_{i=1}^n \ell(y_i, \langle \varphi(x_i), \theta \rangle) + \frac{\lambda}{2} \|\theta\|^2 \\ &= \min_{\theta \in \mathcal{H}, u \in \mathbb{R}^n} \frac{1}{n} \sum_{i=1}^n \ell(y_i, u_i) + \frac{\lambda}{2} \|\theta\|^2 \text{ such that } \forall i \in \{1, \dots, n\}, \langle \varphi(x_i), \theta \rangle = u_i \end{aligned}$$

By Lagrange duality, this is equal to (with λ added on top of the regular multiplier α for convenience):

$$\begin{aligned} & \max_{\alpha \in \mathbb{R}^n} \min_{\theta \in \mathcal{H}, u \in \mathbb{R}^n} \frac{1}{n} \sum_{i=1}^n \ell(y_i, u_i) + \frac{\lambda}{2} \|\theta\|^2 + \lambda \sum_{i=1}^n \alpha_i (u_i - \langle \varphi(x_i), \theta \rangle) \\ &= \max_{\alpha \in \mathbb{R}^n} \left\{ \frac{1}{n} \sum_{i=1}^n \min_{u_i \in \mathbb{R}} \{ \ell(y_i, u_i) + n\lambda\alpha_i u_i \} + \min_{\theta \in \mathcal{H}} \left\{ \frac{\lambda}{2} \|\theta\|^2 - \lambda \sum_{i=1}^n \alpha_i \langle \varphi(x_i), \theta \rangle \right\} \right\} \text{ by reordering,} \\ &= \max_{\alpha \in \mathbb{R}^n} \frac{1}{n} \sum_{i=1}^n \min_{u_i \in \mathbb{R}} \{ \ell(y_i, u_i) + n\lambda\alpha_i u_i \} - \frac{1}{2\lambda} \left\| \sum_{i=1}^n \alpha_i \varphi(x_i) \right\|^2 \text{ with } \theta = \sum_{i=1}^n \alpha_i \varphi(x_i), \\ &= \max_{\alpha \in \mathbb{R}^n} \frac{1}{n} \sum_{i=1}^n \min_{u_i \in \mathbb{R}} \{ \ell(y_i, u_i) + n\lambda\alpha_i u_i \} - \frac{1}{2\lambda} \alpha^\top K \alpha, \end{aligned}$$

with $\theta = \sum_{i=1}^n \alpha_i \varphi(x_i)$ at optimum. Since the functions $\alpha_i \mapsto \min_{u_i \in \mathbb{R}} \{ \ell(y_i, u_i) + n\lambda\alpha_i u_i \}$ are concave (as minima of affine functions), this is a concave maximization problem.

Note the similarity with the representer theorem (existence of $\alpha \in \mathbb{R}^n$ such that $\theta = \sum_{i=1}^n \alpha_i \varphi(x_i)$) and the dissimilarity (one is a minimization problem, one is maximization problem). Moreover, when the loss is smooth, one can show that the function $\alpha_i \mapsto$

$\min_{u_i \in \mathbb{R}} \{\ell(y_i, u_i) + n\lambda\alpha_i u_i\}$ is a strongly concave function, and thus relatively easy to optimize (in other words, the associated condition numbers are smaller than when using the representer theorem).

Exercise 7.6 (a) For ridge regression, compute the dual problem and compare the condition number of the primal problem and the condition number of the dual problem; (b) compare the two formulations to using normal equations as in Chapter 3, and relate the two using the matrix inversion lemma $(\Phi\Phi^\top + n\lambda I)^{-1}\Phi = \Phi(\Phi^\top\Phi + n\lambda I)^{-1}$.

SGD (♦). When minimizing an expectation

$$\min_{\theta \in \mathcal{H}} \mathbb{E}[\ell(y, \langle \varphi(x), \theta \rangle)] + \frac{\lambda}{2} \|\theta\|^2$$

as in Chapter 5, the stochastic gradient algorithm leads to the recursion

$$\theta_t = \theta_{t-1} - \gamma_t [\ell'(y_t, \langle \varphi(x_t), \theta_{t-1} \rangle) \varphi(x_t) + \lambda \theta_{t-1}],$$

where (x_t, y_t) is an i.i.d. sample from the distribution defining the expectation, and ℓ' is the derivative with respect to the second variable.

When initializing at $\theta_0 = 0$, θ_t is a linear combination of all $\varphi(x_i)$, $i = 1, \dots, t$, and thus we can write

$$\theta_t = \sum_{i=1}^t \alpha_i^{(t)} \varphi(x_i),$$

with $\alpha^{(0)} = 0$, and the recursion in α as

$$\alpha_i^{(t)} = (1 - \gamma_t \lambda) \alpha_i^{(t-1)} \text{ for } i \in \{1, \dots, t-1\}, \text{ and } \alpha_t^{(t)} = -\gamma_t \ell' \left(y_t, \sum_{i=1}^{t-1} \alpha_i^{(t-1)} k(x_t, x_i) \right).$$

The complexity after t iterations is $O(t^2)$ kernel evaluations. The convergence rates from Chapter 5 apply. More precisely, if the loss is G -Lipschitz continuous, then, for $F(\theta) = \mathbb{E}[\ell(y, \langle \varphi(x), \theta \rangle)] + \frac{\lambda}{2} \|\theta\|^2$, we have, for the averaged iterate $\bar{\theta}_t$ (from Theorem 5.5):

$$\mathbb{E}[F(\bar{\theta}_t)] - \inf_{\theta \in \mathcal{H}} F(\theta) \leq \frac{2G^2 R^2 (1 + \log t)}{\lambda t}.$$



When doing a single pass with $t = n$, then $F(\theta)$ is the regularized expected risk, and we obtain a generalization bound, leading to $\mathbb{E}[\mathcal{R}(f_{\bar{\theta}_t})] \leq \frac{G^2 R^2}{\lambda n} + \inf_{f \in \mathcal{H}} \{\mathcal{R}(f) + \frac{\lambda}{2} \|f\|_{\mathcal{H}}^2\}$. These bounds are similar to the ones in Section 7.5 below (which assume a regularized empirical risk minimizer is available).

“Kernelization” of linear algorithms. Beyond supervised learning, many unsupervised learning algorithms can be “kernelized,” such as principal component analysis, K -means, or canonical correlation analysis. Indeed, these algorithms can be cast only through the matrices of dot-products between observations and can thus be applied after the feature transformation $\varphi : \mathcal{X} \rightarrow \mathcal{H}$, and run implicitly only using the kernel function $k(x, x') = \langle \varphi(x), \varphi(x') \rangle$. See Schölkopf and Smola (2001); Shawe-Taylor and Cristianini (2004) for details and exercises below.

Exercise 7.7 We consider n observations x_1, \dots, x_n in a set \mathcal{X} equipped with a positive definite kernel and feature map $\varphi : \mathcal{X} \rightarrow \mathcal{H}$. Show that the largest eigenvector of the empirical non-centered covariance operator $\frac{1}{n} \sum_{i=1}^n \varphi(x_i) \otimes \varphi(x_i)$ is proportional to $\sum_{i=1}^n \alpha_i \varphi(x_i)$ where $\alpha \in \mathbb{R}^n$ is an eigenvector of the $n \times n$ kernel matrix associated with the largest eigenvalue.

Exercise 7.8 Show that the K -means clustering algorithm⁷ can be expressed only using dot-products.

Exercise 7.9 We consider a probability distribution p on a set \mathcal{X} equipped with a positive definite kernel k with feature map $\varphi : \mathcal{X} \rightarrow \mathcal{H}$. For a function f which is linear in φ , we want to approximate $\int_{\mathcal{X}} f(x) dp(x)$ from a linear combination $\sum_{i=1}^n \alpha_i f(x_i)$ with $\alpha \in \mathbb{R}^n$.

(a) Show that

$$\left| \int_{\mathcal{X}} f(x) dp(x) - \sum_{i=1}^n \alpha_i f(x_i) \right| \leq \|f\| \cdot \left\| \int_{\mathcal{X}} \varphi(x) dp(x) - \sum_{i=1}^n \alpha_i \varphi(x_i) \right\|.$$

(b) Express the square of the right-hand side with the kernel function, and show how to minimize with respect to $\alpha \in \mathbb{R}^n$.

(c) Show that if the points x_1, \dots, x_n are sampled i.i.d. from p and $\alpha_i = 1/n$ for all i , then $\mathbb{E} \left\| \int_{\mathcal{X}} \varphi(x) dp(x) - \sum_{i=1}^n \alpha_i \varphi(x_i) \right\|^2 \leq \frac{1}{n} \mathbb{E}[k(x, x)]$.

7.5 Generalization guarantees - Lipschitz-continuous losses

In this section, we consider a G -Lipschitz-continuous loss function, and consider a minimizer $\hat{f}_D^{(c)}$ of the constrained problem

$$\min_{f \in \mathcal{H}} \frac{1}{n} \sum_{i=1}^n \ell(y_i, f(x_i)) \text{ such that } \|f\|_{\mathcal{H}} \leq D, \quad (7.5)$$

⁷See https://en.wikipedia.org/wiki/K-means_clustering.

and the unique minimizer $\hat{f}_\lambda^{(r)}$ of the regularized problem

$$\min_{f \in \mathcal{H}} \frac{1}{n} \sum_{i=1}^n \ell(y_i, f(x_i)) + \frac{\lambda}{2} \|f\|_{\mathcal{H}}^2. \quad (7.6)$$

We denote by $\mathcal{R}(f) = \mathbb{E}[\ell(y, f(x))]$ the expected risk, and by f^* one of its minimizers (which we assume to be square integrable). We assume $k(x, x) \leq R^2$ almost surely.

We can first relate the excess risk to the L_2 -norm of $f - f^*$, as

$$\begin{aligned} \mathcal{R}(f) - \mathcal{R}(f^*) &\leq \mathbb{E}[|\ell(y, f(x)) - \ell(y, f^*(x))|] \leq G \mathbb{E}[|f(x) - f^*(x)|] \\ &\leq G \sqrt{\mathbb{E}[|f(x) - f^*(x)|^2]} = G \|f - f^*\|_{L_2(p)}, \end{aligned}$$

that is, the excess risk is dominated by the $L_2(p)$ -norm of $f - f^*$. For $\mathcal{X} = \mathbb{R}^d$, and probability measures with bounded density with respect to the Lebesgue measure, we have shown that $\|f\|_{L_2(p)} \leq \left\| \frac{dp}{dx} \right\|_\infty^{1/2} \|f\|_{L_2(\mathbb{R}^d)}$, so we can replace in upper-bounds $G \|f - f^*\|_{L_2(p)}$ by $G \left\| \frac{dp}{dx} \right\|_\infty^{1/2} \|f - f^*\|_{L_2(\mathbb{R}^d)}$.

7.5.1 Risk decomposition

Constrained problem. Dimension-free results from Chapter 4 (Prop. 4.5), based on Rademacher complexities, immediately apply, and we obtain that the estimation error is bounded from above by $\frac{4GDR}{\sqrt{n}}$, leading to:

$$\mathbb{E}[\mathcal{R}(\hat{f}_D^{(c)})] - \mathcal{R}(f^*) \leq \frac{4GDR}{\sqrt{n}} + G \inf_{\|f\|_{\mathcal{H}} \leq D} \|f - f^*\|_{L_2(p)},$$

(the first term is the **estimation error**, the second term is the **approximation error**).

To find the optimal D (to balance estimation and approximation error), we can minimize the bound with respect to D , leading to:

$$\begin{aligned} \inf_{D \geq 0} \frac{4GRD}{\sqrt{n}} + G \inf_{\|f\|_{\mathcal{H}} \leq D} \|f - f^*\|_{L_2(p)} &= \inf_{f \in \mathcal{H}} \frac{4GR\|f\|_{\mathcal{H}}}{\sqrt{n}} + G \|f - f^*\|_{L_2(p)} \\ &\leq 2G \sqrt{\inf_{f \in \mathcal{H}} \left\{ \|f - f^*\|_{L_2(p)}^2 + \frac{16R^2}{n} \|f\|_{\mathcal{H}}^2 \right\}}. \end{aligned}$$

Note that the suggested D is then proportional to $\frac{\sqrt{n}}{R} \sqrt{\inf_{f \in \mathcal{H}} \left\{ \|f - f^*\|_{L_2(p)}^2 + \frac{16R^2}{n} \|f\|_{\mathcal{H}}^2 \right\}}$ (as shown below, a good regularization parameter to achieve this bound is proportional to $1/\sqrt{n}$).

Overall, we need to understand how the deterministic quantity

$$A(\lambda, f^*) = \inf_{f \in \mathcal{H}} \left\{ \|f - f^*\|_{L_2(p)}^2 + \lambda \|f\|_{\mathcal{H}}^2 \right\}$$

goes to zero when λ goes to zero. A few situations are possible:

- If the target function f^* happens to be in \mathcal{H} , then $A(\lambda, f^*) = \lambda \|f^*\|_{\mathcal{H}}^2$, and thus it tends to zero as $O(\lambda)$. This is the best-case scenario and requires that the target function is sufficiently regular (with at least $d/2$ derivatives for $\mathcal{X} = \mathbb{R}^d$). Then, using it with $\lambda = \mu^* = \frac{16R^2}{n}$ above, the overall excess risk goes to zero as $O(1/\sqrt{n})$.
- The target function f^* is not in \mathcal{H} , but can be approached arbitrary closely in $L_2(p)$ -norm by a function in \mathcal{H} ; in other words, f^* is in the closure of \mathcal{H} in $L_2(p)$. In this situation, $A(\lambda, f^*)$ goes to zero as λ goes to zero, but without an explicit rate if no further assumptions are made.

For $\mathcal{X} = \mathbb{R}^d$, and $dp(x)$ with a bounded density with respect to the Lebesgue measure, and for the translation-invariant kernels from Section 7.3.3, this closure includes all of $L_2(\mathbb{R}^d)$, so this case includes most potential functions. See Section 7.5.2 for explicit rates.

- Otherwise, denoting $\Pi_{\bar{\mathcal{H}}}(f^*)$ the orthogonal projection in $L_2(p)$ of f^* on the closure of \mathcal{H} , by the Pythagorean theorem, $A(\lambda, f^*) = A(\lambda, \Pi_{\bar{\mathcal{H}}}(f^*)) + \|f^* - \Pi_{\bar{\mathcal{H}}}(f^*)\|_{L_2(p)}^2$, that is, there is an incompressible error due to a choice of function space which is not large enough.

Note that we will use the same reasoning for neural networks in Section 9.3.7.

Regularized problem (♦). For the regularized problem, we can use the bound from Chapter 4 (Prop. 4.6):

$$\mathbb{E}[\mathcal{R}(\hat{f}_\lambda^{(r)})] - \mathcal{R}(f^*) \leq \frac{32G^2R^2}{\lambda n} + \inf_{f \in \mathcal{H}} \left\{ G\|f - f^*\|_{L_2(p)} + \frac{\lambda}{2}\|f\|_{\mathcal{H}}^2 \right\}.$$

We can now minimize the bound with respect to λ as $\lambda^* = \frac{8RG}{\sqrt{n}}$, to obtain the bound:

$$G \inf_{f \in \mathcal{H}} \left\{ \|f - f^*\|_{L_2(p)} + \frac{8R}{\sqrt{n}}\|f\|_{\mathcal{H}} \right\} \leq 2G \sqrt{\inf_{f \in \mathcal{H}} \left\{ \|f - f^*\|_{L_2(p)}^2 + \frac{64R^2}{n}\|f\|_{\mathcal{H}}^2 \right\}},$$

which is the same bound as for the constrained problem but on a more commonly used optimization problem in practice.

7.5.2 Approximation error for translation-invariant kernels on \mathbb{R}^d

We first start with analyzing the approximation error of kernel methods for translation invariant kernels. Given a distribution $dp(x)$, the goal is to compute

$$A(\lambda, f^*) = \inf_{f \in \mathcal{H}} \|f - f^*\|_{L_2(p)}^2 + \lambda \|f\|_{\mathcal{H}}^2,$$

where f^* is the target function (e.g., the minimizer of the test risk), which we assume squared-integrable. If $A(\lambda, f^*)$ tends to zero when λ tends to zero for any fixed f^* , then kernel-based supervised learning leads to universally consistent algorithms.

We assume that $\|f - f^*\|_{L_2(p)}^2 \leq C \|f - f^*\|_{L_2(\mathbb{R}^d)}^2$ (e.g., with $C = \|dp/dx\|_\infty$ where dp/dx is the density of p). Moreover, for simplicity, we assume that $\|f^*\|_{L_2(\mathbb{R}^d)}$ is finite (that is, f^* has to go to zero at infinity). We now give bounds on

$$\tilde{A}(\lambda, f^*) = \inf_{f \in \mathcal{H}} \|f - f^*\|_{L_2(\mathbb{R}^d)}^2 + \lambda \|f\|_{\mathcal{H}}^2,$$

keeping in mind that $A(\lambda, f^*) \leq C \tilde{A}(\lambda/C, f^*)$. Remember from Section 7.5.1 that if $f^* \in \mathcal{H}$ (best case scenario), then $\tilde{A}(\lambda, f^*) = \lambda \|f^*\|_{\mathcal{H}}^2$.

Explicit approximation. We have, for translation-invariant kernels, an explicit formulation of the norm $\|\cdot\|_{\mathcal{H}}$ as $\|f\|_{\mathcal{H}}^2 = \frac{1}{(2\pi)^d} \int_{\mathbb{R}^d} \frac{|\hat{f}(\omega)|^2}{\hat{q}(\omega)} d\omega$, and thus

$$\tilde{A}(\lambda, f^*) = \inf_{\hat{f} \in L_2(\mathbb{R}^d)} \frac{1}{(2\pi)^d} \int_{\mathbb{R}^d} \left[|\hat{f}(\omega) - \hat{f}^*(\omega)|^2 + \lambda \frac{|\hat{f}(\omega)|^2}{\hat{q}(\omega)} \right] d\omega.$$

The optimization can be performed independently for each ω , and this is a quadratic problem. Setting the derivative with respect to $\hat{f}(\omega)$ to zero leads to $0 = 2(\hat{f}(\omega) - \hat{f}^*(\omega)) + 2\lambda \frac{\hat{f}(\omega)}{\hat{q}(\omega)}$, and thus $\hat{f}_\lambda(\omega) = \frac{\hat{f}^*(\omega)}{1 + \lambda \hat{q}(\omega)^{-1}}$. In terms of the objective function, we get:

$$\tilde{A}(\lambda, f^*) = \frac{1}{(2\pi)^d} \int_{\mathbb{R}^d} \left[|\hat{f}^*(\omega)|^2 \left(1 - \frac{1}{1 + \lambda \hat{q}(\omega)^{-1}} \right) \right] d\omega = \frac{1}{(2\pi)^d} \int_{\mathbb{R}^d} \left[|\hat{f}^*(\omega)|^2 \frac{\lambda}{\hat{q}(\omega) + \lambda} \right] d\omega.$$

When λ goes to zero, we see that for each ω , $\hat{f}_\lambda(\omega)$ tends to $\hat{f}(\omega)$. By the dominated convergence theorem, $\tilde{A}(\lambda, f^*)$ goes to zero when λ goes to zero.

Without further assumptions, it is impossible to obtain a convergence rate (otherwise, the no-free lunch theorem from Chapter 2 would be invalidated). However, this is possible when assuming regularity properties for f^* .

Sobolev spaces (♦). If we assume that

$$\frac{1}{(2\pi)^d} \int_{\mathbb{R}^d} (1 + \|\omega\|_2^2)^t |\hat{f}^*(\omega)|^2 d\omega < +\infty \quad (7.7)$$

for some $t > 0$, that is, f^* with squared integrable partial derivatives up to order t , then we can further bound:

$$\tilde{A}(\lambda, f^*) \leq \frac{1}{(2\pi)^d} \int_{\mathbb{R}^d} (1 + \|\omega\|_2^2)^t |\hat{f}^*(\omega)|^2 d\omega \times \sup_{\omega \in \mathbb{R}^d} \left\{ \frac{\lambda}{\hat{q}(\omega) + \lambda} \frac{1}{(1 + \|\omega\|_2^2)^t} \right\}.$$

If we now assume $\hat{q}(\omega) \propto (1 + \|\omega\|_2^2)^{-s}$ (Matern kernels), with $s > d/2$ to get an RKHS, then with $t \geq s$, $f^* \in \mathcal{H}$, and have $\tilde{A}(\lambda, f^*) = \lambda \|f^*\|_{\mathcal{H}}^2$. With $t < s$, that is the function is not inside the RKHS \mathcal{H} , then we get a bound proportional to (using $a + b \geq \frac{t}{s}a + (1 - \frac{t}{s})b \geq a^{t/s}b^{1-t/s}$):

$$\sup_{\omega \in \mathbb{R}^d} \left\{ \frac{\lambda}{\hat{q}(\omega) + \lambda} \frac{1}{(1 + \|\omega\|_2^2)^t} \right\} \leq \sup_{\omega \in \mathbb{R}^d} \left\{ \frac{\lambda}{\hat{q}(\omega)^{t/s} \lambda^{1-t/s}} \frac{1}{(1 + \|\omega\|_2^2)^t} \right\} = O(\lambda^{t/s}).$$

Exercise 7.10 (♦) Find an upper-bound of $\tilde{A}(\lambda, f^*)$ for the same assumption on f^* but with the Gaussian kernel.



There are two regularities: $t \geq 0$ for the target function, and $s > d/2$ for the kernel.

Putting things together. Thus, for Lipschitz-continuous losses and target functions that satisfy Eq. (7.7), we get an expected excess risk of the order $\sqrt{\tilde{A}(R^2/n, f^*)} = O(\frac{1}{n^{t/(2s)}})$, when $t \leq s$. For example, when $t = 1$, that is, only first order derivatives are assumed to be square integrable, then for $s = d/2 + 1/2$ (exponential kernel), we obtain a rate of $O(\frac{1}{n^{1/(d+1)}})$, which is similar to the rate obtained with local averaging techniques in Chapter 6 (note here that we are in Lipschitz-loss set-up, which leads to worse rates, see the square loss in Section 7.6). Thus kernel methods do not escape the curse of dimensionality (which is unavoidable anyway). However, with the proper choice of the regularization parameter, they can benefit from extra smoothness of the target function: in the very favorable case, where $f^* \in \mathcal{H}$, that is $t \geq s$, then we obtain a dimension-independent rate of $1/\sqrt{n}$. In intermediate scenarios, the rates are in between. This is why kernel methods are said to be *adaptive to the smoothness* of the target function.

Approximation bounds (♦). In some analysis set-ups (such as those explored in Chapter 9), it is required to approximate some f^* up to ε with the minimum possible RKHS norm. This can be done as follows.

A bound on the quantity $A(\lambda, f^*) = \inf_{f \in \mathcal{H}} \{\|f - f^*\|_{L_2(p)}^2 + \lambda \|f\|_{\mathcal{H}}^2\}$ of the form $c\lambda^\alpha$ for $\alpha \in (0, 1)$ leads to the following bound:

$$\begin{aligned} & \inf_{f \in \mathcal{H}} \|f\|_{\mathcal{H}}^2 \text{ such that } \|f - f^*\|_{L_2(p)} \leq \varepsilon \\ &= \inf_{f \in \mathcal{H}} \sup_{\mu \geq 0} \|f\|_{\mathcal{H}}^2 + \mu(\|f - f^*\|_{L_2(p)}^2 - \varepsilon^2) \text{ using Lagrangian duality,} \\ &= \sup_{\mu \geq 0} \mu A(\mu^{-1}, f^*) - \mu \varepsilon^2 \leq \sup_{\mu \geq 0} \mu c \mu^{-\alpha} - \mu \varepsilon^2. \end{aligned}$$

The optimal μ is such that $(1-\alpha)c\mu^{-\alpha} = \varepsilon^2$, leading to an approximation bound proportional to $\varepsilon^{2(1-1/\alpha)} = \varepsilon^{-2(1-\alpha)/\alpha}$.

Applied to $\alpha = t/s$ like before, this leads to an RKHS norm proportional to $\varepsilon^{-(1-\alpha)/\alpha}$ to get an error less than $\|f - f^*\|_{L_2(\mathbb{R}^d)}$. So when $t = 1$ (single derivative for the target function), and $s > d/2$ (for the Sobolev kernel), we get a norm of the order $\varepsilon^{-(1/\alpha-1)} = \varepsilon^{-(s-1)} \geq \varepsilon^{-d/2+1}$, which explodes exponentially in dimension, which is another way of formulating the curse of dimensionality.

7.6 Theoretical analysis of ridge regression (♦)

In this section, we provide finer results for ridge regression used within kernel methods. Compared to the analysis performed in Section 3.6, there are three difficulties:

- (1) we go from fixed design to random design: this will require finer probabilistic arguments to relate population and empirical covariance operators,
- (2) we need to go infinite-dimensional: in terms of notations, this will mean not using transposes of matrices, but dot-products, which is a minor modification,
- (3) the infimum of the expected risk over linear functions parameterized by $\theta \in \mathcal{H}$ may not be attained by an element of \mathcal{H} , but by an element of its closure in $L_2(p)$. This is important, as this allows access to a potentially large set of functions and requires more care.

7.6.1 Kernel ridge regression as a “linear” estimator

We consider n i.i.d. observations $(x_i, y_i) \in \mathcal{X} \times \mathbb{R}$, and we aim at minimizing, for $\lambda > 0$,

$$\frac{1}{n} \sum_{i=1}^n (y_i - f(x_i))^2 + \lambda \|f\|_{\mathcal{H}}^2.$$

Like local averaging methods in Chapter 6, the ridge regression estimator happens to be a “linear” estimator that depends linearly on the response vector (but of course non-linearly in x in general). Indeed, using the representer theorem from Eq. (7.2), the estimator is $f(x) = \sum_{i=1}^n \alpha_i k(x, x_i)$, with $\alpha \in \mathbb{R}^n$ defined as $\alpha = (K + n\lambda I)^{-1}y$, where $K \in \mathbb{R}^{n \times n}$ is the kernel matrix. We can then write

$$f(x) = \sum_{i=1}^n \hat{w}_i(x) y_i,$$

with $\hat{w}(x) = (K + n\lambda I)^{-1}q(x) \in \mathbb{R}^n$, where $q(x) \in \mathbb{R}^n$ is defined as $q_i(x) = k(x, x_i)$. The smoothing matrix H is then equal to $H = K(K + n\lambda I)^{-1}$.

The key differences with local averaging are that (a) the weights do not sum to one, that is, $\sum_{i=1}^n \hat{w}_i(x)$ may be different from one, and (b) the weights are not constrained to be non-negative. While the first difference can be removed using centering (see exercise below), the second one is more fundamental: allowing the weights to be negative will enable the adaptivity to smoothness, which local averaging methods missed (see Section 6.5).

Exercise 7.11 We consider the optimization problem $\frac{1}{2n}\|y - \Phi\theta - \eta 1_n\|_2^2 + \frac{\lambda}{2}\|\theta\|_2^2$, where $\Phi \in \mathbb{R}^{n \times d}$ is the design matrix obtained from feature map φ and data points x_1, \dots, x_b , and $y \in \mathbb{R}^n$, and $1_n \in \mathbb{R}^n$ is the vector of all ones. Show that the optimal value of θ and η are: $\theta = \Phi^\top \alpha$, and $\eta = \frac{1}{n} 1_n^\top (y - \Phi\theta)$, with $\alpha = \Pi_n (\Pi_n K \Pi_n + n\lambda I)^{-1} \Pi_n y$, and $\Pi_n = I - \frac{1}{n} 1_n 1_n^\top$. Show that the prediction function $f(x) = \varphi(x)^\top \theta + \eta$ is of the form $\sum_{i=1}^n \hat{w}_i(x) y_i$ with weights that sum to one.

Exercise 7.12 (♦) For x_1, \dots, x_n equally spaced in $[0, 1]$ and for a translation-invariant kernel from Section 7.3.2, compute the eigenvalues of the kernel matrix and the smoothing matrix.

7.6.2 Bias and variance decomposition (♦)

Beyond fixed-design finite-dimensional analysis. In Chapter 3, we considered ridge regression in the fixed design setting (where the input data are assumed deterministic) and a finite-dimensional feature space \mathcal{H} , and obtained in Prop. 3.7 the following *exact* expression

of the excess risk of the ridge regression estimator $\hat{\theta}_\lambda$, assuming $y_i = \langle \theta_*, \varphi(x_i) \rangle + \varepsilon_i$, with ε_i independent from x_i , and where $\mathbb{E}[\varepsilon_i] = 0$, $\mathbb{E}[\varepsilon_i^2] = \sigma^2$:

$$\mathbb{E}[(\hat{\theta}_\lambda - \theta_*)^\top \hat{\Sigma}(\hat{\theta}_\lambda - \theta_*)] = \lambda^2 \theta_*^\top (\hat{\Sigma} + \lambda I)^{-2} \hat{\Sigma} \theta_* + \frac{\sigma^2}{n} \text{tr} [\hat{\Sigma}^2 (\hat{\Sigma} + \lambda I)^{-2}]. \quad (7.8)$$

For the random design assumption (which is the usual machine learning setting), we first need to obtain a value for the expected risk. Moreover, to apply to infinite dimensional \mathcal{H} where the minimizer has a potentially infinite norm, we need to replace the matrix notation.

Modeling assumptions. We assume that

$$y_i = f^*(x_i) + \varepsilon_i,$$

with for simplicity $\mathbb{E}[\varepsilon_i|x_i] = 0$, and $\mathbb{E}[\varepsilon_i^2|x_i] \leq \sigma^2$ almost surely, for some target function $f^* \in L_2(p)$, so that $f^*(x) = \mathbb{E}[y|x]$ is exactly the conditional expectation of $y|x$.

 The target function f^* may not be in \mathcal{H} . All dot-products will always be in \mathcal{H} , while we will specify the corresponding space for norms.

We thus consider the optimization problem:

$$\min_{f \in \mathcal{H}} \frac{1}{n} \sum_{i=1}^n (y_i - f(x_i))^2 + \lambda \|f\|_{\mathcal{H}}^2, \quad (7.9)$$

with the solution found with algorithms in Section 7.4.

 The theoretical analysis of kernel methods typically does not involve the parameters $\alpha \in \mathbb{R}^n$ obtained from the representer theorem.

We have, with $\hat{\Sigma} = \frac{1}{n} \sum_{i=1}^n \varphi(x_i) \otimes \varphi(x_i)$ a self-adjoint operator from \mathcal{H} to \mathcal{H} (the empirical covariance operator), a cost function equal to

$$\frac{1}{n} \sum_{i=1}^n y_i^2 + \langle f, \hat{\Sigma} f \rangle - 2 \left\langle \frac{1}{n} \sum_{i=1}^n y_i \varphi(x_i), f \right\rangle + \lambda \langle f, f \rangle,$$

leading to the minimizer \hat{f}_λ of Eq. (7.9) equal to:

$$\hat{f}_\lambda = (\hat{\Sigma} + \lambda I)^{-1} \frac{1}{n} \sum_{i=1}^n y_i \varphi(x_i) = (\hat{\Sigma} + \lambda I)^{-1} \frac{1}{n} \sum_{i=1}^n f^*(x_i) \varphi(x_i) + (\hat{\Sigma} + \lambda I)^{-1} \frac{1}{n} \sum_{i=1}^n \varepsilon_i \varphi(x_i).$$

We can now compute the (expected) excess risk equal to $\mathbb{E}[\|\hat{f}_\lambda - f^*\|_{L_2(p)}^2]$ as (using that $\mathbb{E}(\varepsilon_i|x_i) = 0$):

$$\begin{aligned} & \mathbb{E}[\|\hat{f}_\lambda - f^*\|_{L_2(p)}^2] \\ = & \mathbb{E}\left[\|(\widehat{\Sigma} + \lambda I)^{-1} \frac{1}{n} \sum_{i=1}^n \varepsilon_i \varphi(x_i)\|_{L_2(p)}^2\right] + \mathbb{E}\left[\|(\widehat{\Sigma} + \lambda I)^{-1} \frac{1}{n} \sum_{i=1}^n f^*(x_i) \varphi(x_i) - f^*\|_{L_2(p)}^2\right]. \end{aligned}$$

The first term is the usual **variance** term (that depends on the noise on top of the optimal predictions). In contrast, the second is the **bias** term (which depends on the regularity of the target function). Before developing the probabilistic argument, we give simplified upper bounds of the two terms.

On top of the non-centered empirical covariance operator $\widehat{\Sigma} = \frac{1}{n} \sum_{i=1}^n \varphi(x_i) \otimes \varphi(x_i)$, we will need its expectation, the covariance operator (from \mathcal{H} to \mathcal{H})

$$\Sigma = \mathbb{E}[\varphi(x) \otimes \varphi(x)],$$

for the corresponding distribution of the x_i 's. A key property relates the $L_2(p)$ -norm and the RKHS norm, that is, that for $g \in \mathcal{H}$,

$$\|g\|_{L_2(p)}^2 = \int_X g(x)^2 dp(x) = \int_X \langle g, \varphi(x) \rangle^2 dp(x) = \int_X \langle g, \varphi(x) \otimes \varphi(x) g \rangle dp(x) = \langle g, \Sigma g \rangle = \|\Sigma^{1/2} g\|_{\mathcal{H}}^2. \quad (7.10)$$

Variance term. Starting from $\text{variance} = \mathbb{E}\left[\|(\widehat{\Sigma} + \lambda I)^{-1} \frac{1}{n} \sum_{i=1}^n \varepsilon_i \varphi(x_i)\|_{L_2(p)}^2\right]$, the variance term can be upper-bounded as follows (first using independence and zero means of the variables ε_i). Below, we use the property that for symmetric matrices such that $A \succcurlyeq 0$ and $B \preccurlyeq C$, we have $\text{tr}[AB] \leq \text{tr}[AC]$, and Eq. (7.10):

$$\begin{aligned} & \mathbb{E}\left[\|(\widehat{\Sigma} + \lambda I)^{-1} \frac{1}{n} \sum_{i=1}^n \varepsilon_i \varphi(x_i)\|_{L_2(p)}^2\right] \\ = & \frac{1}{n^2} \sum_{i=1}^n \mathbb{E}\left[\text{tr}\left((\widehat{\Sigma} + \lambda I)^{-1} \Sigma (\widehat{\Sigma} + \lambda I)^{-1} \varepsilon_i^2 \varphi(x_i) \otimes \varphi(x_i)\right)\right] \\ \leq & \frac{\sigma^2}{n} \mathbb{E}\left[\text{tr}\left((\widehat{\Sigma} + \lambda I)^{-1} \Sigma (\widehat{\Sigma} + \lambda I)^{-1} \widehat{\Sigma}\right)\right] \text{ using } \mathbb{E}[\varepsilon_i^2|x_i] \leq \sigma^2, \\ \leq & \frac{\sigma^2}{n} \mathbb{E}\left[\text{tr}\left((\widehat{\Sigma} + \lambda I)^{-1} \Sigma\right)\right] \text{ using } (\widehat{\Sigma} + \lambda I)^{-1} \widehat{\Sigma} \preccurlyeq I. \end{aligned} \quad (7.11)$$

This will be the main expression we will bound later.

Bias term. We first assume that $f^* \in \mathcal{H}$, that is, the model is well-specified. Then, writing $f^*(x_i) = \langle f^*, \varphi(x_i) \rangle$ (which is possible because $f^* \in \mathcal{H}$), the bias term is equal to

$$\text{bias} = \mathbb{E}\left[\|(\widehat{\Sigma} + \lambda I)^{-1} \frac{1}{n} \sum_{i=1}^n f^*(x_i) \varphi(x_i) - f^*\|_{L_2(p)}^2\right] \quad (7.12)$$

$$= \mathbb{E}\left[\|(\widehat{\Sigma} + \lambda I)^{-1} \frac{1}{n} \sum_{i=1}^n \langle f^*, \varphi(x_i) \rangle \varphi(x_i) - f^*\|_{L_2(p)}^2\right] \quad (7.13)$$

$$= \mathbb{E}\left[\|(\widehat{\Sigma} + \lambda I)^{-1} \widehat{\Sigma} f^* - f^*\|_{L_2(p)}^2\right]$$

$$= \mathbb{E}\left[\|\lambda \Sigma^{1/2} (\widehat{\Sigma} + \lambda I)^{-1} f^*\|_{\mathcal{H}}^2\right] = \lambda^2 \mathbb{E}\left[\langle f^*, (\widehat{\Sigma} + \lambda I)^{-1} \Sigma (\widehat{\Sigma} + \lambda I)^{-1} f^* \rangle\right], \quad (7.14)$$

where we have used Eq. (7.10) above to re-introduce the operator Σ . This will be the main expression we will bound later.

Upper-bound on excess risk. We have thus shown the following proposition:

Proposition 7.2 *When $f^* \in \mathcal{H}$, the excess risk of the ridge regression estimator is upper-bounded by:*

$$\mathbb{E}\left[\|\hat{f}_\lambda - f^*\|_{L_2(p)}^2\right] \leq \frac{\sigma^2}{n} \mathbb{E}\left[\text{tr}((\widehat{\Sigma} + \lambda I)^{-1} \Sigma)\right] + \lambda^2 \mathbb{E}\left[\langle f^*, (\widehat{\Sigma} + \lambda I)^{-1} \Sigma (\widehat{\Sigma} + \lambda I)^{-1} f^* \rangle\right]. \quad (7.15)$$

Given the expression of the expected variance in Eq. (7.11) and of the expected bias in Eq. (7.14), we notice that both the empirical and expected covariance operators appear and that it would be important to replace the empirical one with the expected one. This is possible with extra multiplicative factors, which we now show. Then we will bound the two terms separately and show how balancing them leads to interesting learning bounds.

7.6.3 Relating empirical and population covariance operators

We follow Mourtada and Rosasco (2022) and derive simple relationships between the empirical covariance operator $\widehat{\Sigma}$ and the population operator Σ , by showing the following lemma dealing with expectations; for high probability bounds, see, e.g., Rudi et al. (2015); Rudi and Rosasco (2017), as well as the end of Section 7.6.4.

Lemma 7.1 (Mourtada and Rosasco, 2022) *Assuming i.i.d. data $x_1, \dots, x_n \in \mathcal{X}$, and bounded features $\|\varphi(x)\|_{\mathcal{H}} \leq R$ for all $x \in \mathcal{X}$; we have, for all $g \in \mathcal{H}$:*

$$\mathbb{E}\left[\text{tr}((\widehat{\Sigma} + \lambda I)^{-1} \Sigma)\right] \leq \left(1 + \frac{R^2}{\lambda n}\right) \text{tr}((\Sigma + \lambda I)^{-1} \Sigma) \quad (7.16)$$

$$\mathbb{E}\left[\langle g, (\widehat{\Sigma} + \lambda I)^{-1} \Sigma (\widehat{\Sigma} + \lambda I)^{-1} g \rangle\right] \leq \lambda^{-1} \left(1 + \frac{R^2}{\lambda n}\right)^2 \langle g, (\Sigma + \lambda I)^{-1} \Sigma g \rangle. \quad (7.17)$$

Proof (♦) The main idea is to introduce a $(n+1)$ -th independent observation from the same distribution, write $\Sigma = \mathbb{E}[\varphi(x_{n+1}) \otimes \varphi(x_{n+1})]$, and use the fact that the observations are “exchangeable”, that is, they can be permuted without changing their joint distribution.

We denote $C = \sum_{i=1}^{n+1} \varphi(x_i) \otimes \varphi(x_i)$, and using the matrix inversion lemma (Section 1.1.3),

$$\begin{aligned} (C + n\lambda I)^{-1} \varphi(x_{n+1}) &= (n\widehat{\Sigma} + n\lambda I + \varphi(x_{n+1}) \otimes \varphi(x_{n+1}))^{-1} \varphi(x_{n+1}) \\ &= \frac{1}{1 + \langle \varphi(x_{n+1}), (n\widehat{\Sigma} + n\lambda I)^{-1} \varphi(x_{n+1}) \rangle} (n\widehat{\Sigma} + n\lambda I)^{-1} \varphi(x_{n+1}). \end{aligned} \quad (7.18)$$

Finally, we will use $c = \langle \varphi(x_{n+1}), (n\widehat{\Sigma} + n\lambda I)^{-1} \varphi(x_{n+1}) \rangle \leq \frac{R^2}{\lambda n}$. To prove Eq. (7.16), we use Eq. (7.18) above to express $(\widehat{\Sigma} + \lambda I)^{-1} \varphi(x_{n+1})$ in terms of $(C + n\lambda I)^{-1} \varphi(x_{n+1})$, to get:

$$\begin{aligned} \mathbb{E} \left[\text{tr} ((\widehat{\Sigma} + \lambda I)^{-1} \Sigma) \right] &= \mathbb{E} \left[\text{tr} ((\widehat{\Sigma} + \lambda I)^{-1} \varphi(x_{n+1}) \otimes \varphi(x_{n+1})) \right] \\ &= \mathbb{E} \left[\langle \varphi(x_{n+1}), (\widehat{\Sigma} + \lambda I)^{-1} \varphi(x_{n+1}) \rangle \right] \\ &= n \mathbb{E} \left[(1+c) \langle \varphi(x_{n+1}), (C + n\lambda I)^{-1} \varphi(x_{n+1}) \rangle \right] \\ &\leq \left(1 + \frac{R^2}{\lambda n} \right) \mathbb{E} \left[\langle \varphi(x_{n+1}), (C + n\lambda I)^{-1} \varphi(x_{n+1}) \rangle \right]. \end{aligned}$$

Thus, using that the variables (x_1, \dots, x_{n+1}) are exchangeable:

$$\begin{aligned} \mathbb{E} \left[\text{tr} ((\widehat{\Sigma} + \lambda I)^{-1} \Sigma) \right] &\leq \left(1 + \frac{R^2}{\lambda n} \right) \frac{1}{n+1} \sum_{i=1}^{n+1} \mathbb{E} \left[\langle \varphi(x_i), (C + n\lambda I)^{-1} \varphi(x_i) \rangle \right] \\ &= \left(1 + \frac{R^2}{\lambda n} \right) \frac{1}{n+1} \mathbb{E} \left[\text{tr} (C(C + n\lambda I)^{-1}) \right] \text{ since } C = \sum_{i=1}^{n+1} \varphi(x_i) \otimes \varphi(x_i) \\ &\leq \left(1 + \frac{R^2}{\lambda n} \right) \frac{1}{n+1} [\text{tr} (\mathbb{E}[C](\mathbb{E}[C] + n\lambda I)^{-1})] \text{ by Jensen's inequality,}^8 \\ &= \left(1 + \frac{R^2}{\lambda n} \right) \frac{1}{n+1} \text{tr} ((n+1)\Sigma((n+1)\Sigma + n\lambda I)^{-1}) \\ &\leq \left(1 + \frac{R^2}{\lambda n} \right) \text{tr} (\Sigma(\Sigma + \lambda I)^{-1}), \text{ which is exactly Eq. (7.16).} \end{aligned}$$

To prove Eq. (7.17), we use the same technique, that is,

$$\begin{aligned} \mathbb{E} \left[(\widehat{\Sigma} + \lambda I)^{-1} \Sigma (\widehat{\Sigma} + \lambda I)^{-1} \right] &= \mathbb{E} \left[(\widehat{\Sigma} + \lambda I)^{-1} \varphi(x_n) \otimes \varphi(x_n) (\widehat{\Sigma} + \lambda I)^{-1} \right] \\ &= n^2 (1+c)^2 [(C + n\lambda I)^{-1} \varphi(x_{n+1})] \otimes [(C + n\lambda I)^{-1} \varphi(x_{n+1})]. \end{aligned}$$

This leads to:

$$\begin{aligned}
& \mathbb{E}[\langle g, (\widehat{\Sigma} + \lambda I)^{-1} \Sigma (\widehat{\Sigma} + \lambda I)^{-1} g \rangle] \\
&= n^2 \mathbb{E}[(1+c)^2 \langle (C + n\lambda I)^{-1} \varphi(x_{n+1}), g \rangle^2] \\
&\leq n^2 \left(1 + \frac{R^2}{\lambda n}\right)^2 \mathbb{E}[\langle (C + n\lambda I)^{-1} \varphi(x_{n+1}), g \rangle^2] \\
&= \frac{n^2}{n+1} \left(1 + \frac{R^2}{\lambda n}\right)^2 \mathbb{E}[\langle g, (C + n\lambda I)^{-1} C (C + n\lambda I)^{-1} g \rangle] \text{ by exchangeability,} \\
&\leq \frac{1}{\lambda} \frac{n}{n+1} \left(1 + \frac{R^2}{\lambda n}\right)^2 \mathbb{E}[\langle g, C(C + n\lambda I)^{-1} g \rangle] \\
&\leq \frac{1}{\lambda} \frac{n}{n+1} \left(1 + \frac{R^2}{\lambda n}\right)^2 \langle g, \mathbb{E}[C](\mathbb{E}[C] + n\lambda I)^{-1} g \rangle \text{ by Jensen's inequality,} \\
&= \frac{1}{\lambda} n \left(1 + \frac{R^2}{\lambda n}\right)^2 \langle g, \Sigma((n+1)\Sigma + n\lambda I)^{-1} g \rangle \leq \lambda^{-1} \left(1 + \frac{R^2}{\lambda n}\right)^2 \langle g, (\Sigma + \lambda I)^{-1} \Sigma g \rangle.
\end{aligned}$$

■

7.6.4 Analysis for well-specified problems (♦)

In this section, we assume that $f^* \in \mathcal{H}$. We have the following result for the excess risk, whose proof consists in applying Lemma 7.1 to Eq. (7.15).

Proposition 7.3 (Well-specified model kernel ridge regression) *Assume i.i.d. data $(x_i, y_i) \in \mathcal{X} \times \mathbb{R}$, for $i = 1, \dots, n$, and $y_i = f^*(x_i) + \varepsilon_i$, with $\mathbb{E}[\varepsilon_i | x_i] = 0$ and $\mathbb{E}[\varepsilon_i^2 | x_i] \leq \sigma^2$, and $f^* \in \mathcal{H}$. Assume $\|\varphi(x)\|_{\mathcal{H}} \leq R$. We have:*

$$\mathbb{E}[\|\hat{f}_\lambda - f^*\|_{L_2(p)}^2] \leq \frac{\sigma^2}{n} \left(1 + \frac{R^2}{\lambda n}\right) \text{tr}((\Sigma + \lambda I)^{-1} \Sigma) + \lambda \left(1 + \frac{R^2}{\lambda n}\right)^2 \langle f^*, \Sigma(\Sigma + \lambda I)^{-1} f^* \rangle. \quad (7.19)$$

This is to be contrasted with Eq. (7.8): we obtain a similar result with $\widehat{\Sigma}$ replaced by Σ , but with some extra multiplicative constants that are close to one if $R^2/(\lambda n)$ is small. We can further bound $\text{tr}((\Sigma + \lambda I)^{-1} \Sigma) \leq \frac{R^2}{\lambda}$ and $\langle f^*, \Sigma(\Sigma + \lambda I)^{-1} f^* \rangle \leq \langle f^*, f^* \rangle$, to get the bound

$$\mathbb{E}[\|\hat{f}_\lambda - f^*\|_{L_2(p)}^2] \leq \sigma^2 \frac{R^2}{\lambda n} \left(1 + \frac{R^2}{\lambda n}\right) + \lambda \left(1 + \frac{R^2}{\lambda n}\right)^2 \|f^*\|_{\mathcal{H}}^2,$$

which is a random design version of the developments in the proof of Prop. 3.8.

Bounds in high-probability (♦♦). Instead of obtaining bounds in expectation (with respect to the training data), we can obtain high-probability bounds, as briefly shown below for the simplest bound; see, more refined bounds by Rudi et al. (2015); Rudi and Rosasco (2017).

Proposition 7.4 (High-probability bound for kernel ridge regression) *Assume i.i.d. data $(x_i, y_i) \in \mathcal{X} \times \mathbb{R}$, for $i = 1, \dots, n$, and $y_i = f^*(x_i) + \varepsilon_i$, with $\mathbb{E}[\varepsilon_i | x_i] = 0$ and $\varepsilon_i^2 \leq \sigma^2$ almost surely, and $f^* \in \mathcal{H}$. Assume $\|\varphi(x)\|_{\mathcal{H}} \leq R$ and $n \geq (\frac{4}{3} + \frac{R^2}{8\lambda}) \log \frac{14R^2}{\lambda\delta}$. We have, with probability greater than $1 - \delta$,*

$$\|\hat{f}_\lambda - f^*\|_{L_2(p)}^2 \leq \frac{8\sigma^2 R^2}{\lambda n} + 4\lambda \|f^*\|_{\mathcal{H}}^2 + \frac{16\sigma^2 R^2}{\lambda n} \log \frac{2}{\delta}. \quad (7.20)$$

Proof We first apply Prop. 1.7 with $M_i = \Sigma(\Sigma + \lambda I)^{-1} - (\Sigma + \lambda I)^{-1/2}\varphi(x_i)\otimes\varphi(x_i)(\Sigma + \lambda I)^{-1/2}$, for which we have $V = \frac{R^2}{\lambda}\Sigma(\Sigma + \lambda I)^{-1}$, $\sigma^2 = \frac{R^2}{\lambda}$, $c = 1$, and $t = 1$, leading to

$$\lambda_{\max}[(\Sigma + \lambda I)^{-1/2}(\Sigma - \hat{\Sigma})(\Sigma + \lambda I)^{-1/2}] \leq \frac{1}{2}$$

with probability greater than $1 - 7\frac{R^2}{\lambda} \exp[-\frac{n}{4/3+R^2/(8\lambda)}]$, as soon as $\frac{1}{2} \geq \frac{1}{3n} + \frac{R}{\sqrt{\lambda n}}$. This probability is greater than $1 - \delta/2$ as soon as $n \geq (4/3 + R^2/(8\lambda)) \log \frac{14R^2}{\lambda\delta}$.

This implies $\Sigma - \hat{\Sigma} \leq \frac{1}{2}(\Sigma + \lambda I)$, $\frac{1}{2}(\Sigma + \lambda I) \leq \hat{\Sigma} + \lambda I$, and thus $(\hat{\Sigma} + \lambda I)^{-1} \leq 2(\Sigma + \lambda I)^{-1}$. Using the Łojasiewicz inequality (Lemma 5.1) on the regularized empirical risk $\hat{\mathcal{R}}_\lambda(f) = \frac{1}{2n}\langle f - f^*, \hat{\Sigma}(f - f^*) \rangle - \langle \frac{1}{n} \sum_{i=1}^m \varepsilon_i \varphi(x_i), f \rangle + \frac{\lambda}{2} \|f\|_{\mathcal{H}}^2$, we get:

$$\hat{\mathcal{R}}_\lambda(f^*) - \hat{\mathcal{R}}_\lambda(\hat{f}_\lambda) \leq \frac{1}{2\lambda} \|\hat{\mathcal{R}}'_\lambda(f^*)\|_{\mathcal{H}}^2.$$

Using $\hat{\mathcal{R}}_\lambda(f^*) - \hat{\mathcal{R}}_\lambda(\hat{f}_\lambda) = \frac{1}{2}\langle f^* - \hat{f}_\lambda, (\hat{\Sigma} + \lambda I)(f^* - \hat{f}_\lambda) \rangle \geq \frac{1}{4}\langle f^* - \hat{f}_\lambda, (\Sigma + \lambda I)(f^* - \hat{f}_\lambda) \rangle = \frac{1}{4}\|\hat{f}_\lambda - f^*\|_{L_2(p)}^2$, we get

$$\|\hat{f}_\lambda - f^*\|_{L_2(p)}^2 \leq \frac{2}{\lambda} \left\| \frac{1}{n} \sum_{i=1}^m \varepsilon_i \varphi(x_i) + \lambda f^* \right\|_{\mathcal{H}}^2 \leq \frac{4}{\lambda} \left\| \frac{1}{n} \sum_{i=1}^n \varepsilon_i \varphi(x_i) \right\|_{\mathcal{H}}^2 + 4\lambda \|f^*\|_{\mathcal{H}}^2.$$

We thus need a high-probability bound for $\left\| \frac{1}{n} \sum_{i=1}^n \varepsilon_i \varphi(x_i) \right\|_{\mathcal{H}}$, which we can obtain, with probability greater than $1 - \delta/2$, from McDiarmid's inequality, as

$$\left\| \frac{1}{n} \sum_{i=1}^n \varepsilon_i \varphi(x_i) \right\|_{\mathcal{H}} \leq \frac{R\sigma}{\sqrt{n}} \left(1 + \sqrt{2 \log \frac{2}{\delta}} \right).$$

■

Before analyzing the last proposition and balancing bias and variance, we show how this can be applied beyond well-specified models.

7.6.5 Analysis beyond well-specified problems (♦)

In the bound in Eq. (7.19), the only term that requires potentially that $f^* \in \mathcal{H}$ is the bias term $\lambda \langle f^*, (\Sigma + \lambda I)^{-1} \Sigma f^* \rangle$. The key to an extension to all functions f^* in the closure of \mathcal{H} is the following simple lemma.

Lemma 7.2 *Given the covariance operator Σ and any function $f^* \in \mathcal{H}$, then*

$$\lambda \langle f^*, (\Sigma + \lambda I)^{-1} \Sigma f^* \rangle = \inf_{f \in \mathcal{H}} \left\{ \|f - f^*\|_{L_2(p)}^2 + \lambda \|f\|_{\mathcal{H}}^2 \right\}.$$

Proof The optimization problem above can be written as, using Eq. (7.10), $\inf_{f \in \mathcal{H}} \left\{ \|\Sigma^{1/2}(f - f^*)\|_{\mathcal{H}}^2 + \lambda \|f\|_{\mathcal{H}}^2 \right\}$, with solution $f = (\Sigma + \lambda I)^{-1} \Sigma f^*$ and we can simply put back the value in the objective function to get the desired result. ■

Target function in the closure of \mathcal{H} . By using a limiting argument, we can extend the formula of the bias term in Prop. 7.3 to the general case of $f^* \in L_2(p)$ with Eq. (7.21), in the closure of \mathcal{H} in $L_2(p)$ (because all functions in the closure can be approached by a function in \mathcal{H}), leading to

$$(1 + \frac{R^2}{\lambda n})^2 \inf_{f \in \mathcal{H}} \left\{ \|f - f^*\|_{L_2(p)}^2 + \lambda \|f\|_{\mathcal{H}}^2 \right\}, \quad (7.21)$$

For translation-invariant kernels in \mathbb{R}^d (which are dense in $L_2(\mathbb{R}^d)$), this allows estimating any target function.

Final result. Combining the two cases above, we can now show the upper bound for kernel ridge regression in the potentially misspecified case.

Proposition 7.5 (Mis-specified model kernel ridge regression) *Assume i.i.d. data $(x_i, y_i) \in \mathcal{X} \times \mathbb{R}$, for $i = 1, \dots, n$, and $y_i = f^*(x_i) + \varepsilon_i$, with $\mathbb{E}[\varepsilon_i | x_i] = 0$ and $\mathbb{E}[\varepsilon_i^2 | x_i] \leq \sigma^2$. Assume $\|\varphi(x)\|_{\mathcal{H}} \leq R$ and f^* in the closure of \mathcal{H} in $L_2(p)$. We have:*

$$\mathbb{E}[\|\hat{f}_\lambda - f^*\|_{L_2(p)}^2] \leq \frac{\sigma^2}{n} \left(1 + \frac{R^2}{\lambda n}\right) \text{tr}((\Sigma + \lambda I)^{-1} \Sigma) + \left(1 + \frac{R^2}{\lambda n}\right)^2 \inf_{f \in \mathcal{H}} \left\{ \|f - f^*\|_{L_2(p)}^2 + \lambda \|f\|_{\mathcal{H}}^2 \right\}. \quad (7.22)$$



Be careful with homogeneity of formulas; e.g., $\frac{R^2}{\lambda n}$ is indeed a constant.

7.6.6 Balancing bias and variance (\spadesuit)

We can now balance the bias and variance term in the following upper-bound on the expected excess risk,

$$\frac{\sigma^2}{n} \left(1 + \frac{R^2}{\lambda n}\right) \text{tr}((\Sigma + \lambda I)^{-1} \Sigma) + \left(1 + \frac{R^2}{\lambda n}\right)^2 \inf_{f \in \mathcal{H}} \left\{ \|f - f^*\|_{L_2(p)}^2 + \lambda \|f\|^2\right\}.$$

For this section, we will assume that $\mathcal{X} = \mathbb{R}^d$ and that the target function belongs to a Sobolev kernel of order $t > 0$, while the RKHS is a Sobolev space of order $s > d/2$.

We have seen in Section 7.5.2 that the bias term is of order $\left(1 + \frac{R^2}{\lambda n}\right)^2 \lambda^{t/s}$ when $s \geq t$. For the variance term, we need to study the so-called “degrees of freedom”.

Degrees of freedom. This is the quantity $\text{tr}[\Sigma(\Sigma + \lambda I)^{-1}]$, which is decreasing in λ , from $+\infty$ for $\lambda = 0$ to 0 for $\lambda = +\infty$. If we know that the eigenvalues $(\lambda_m)_{m \geq 0}$ of the covariance operator satisfy

$$\lambda_m \leq C(m+1)^{-\alpha},$$

for $\alpha > 1$, then one has:

$$\begin{aligned} \text{tr}[\Sigma(\Sigma + \lambda I)^{-1}] &= \sum_{m \geq 0} \frac{\lambda_m}{\lambda_m + \lambda} \leq \sum_{m \geq 0} \frac{1}{1 + \lambda C^{-1}(m+1)^\alpha} \leq \int_0^\infty \frac{1}{1 + \lambda C^{-1}t^\alpha} \\ &\leq \int_0^\infty \lambda^{-1/\alpha} C^{1/\alpha} \frac{1}{\alpha} u^{1/\alpha-1} \frac{du}{1+u} \text{ with the change of variable } u = \lambda C^{-1}t^\alpha, \\ &\leq O(\lambda^{-1/\alpha}). \end{aligned}$$

It turns out that if the distribution of inputs has a bounded density with respect to the Lebesgue measure, then for our chosen Sobolev space, we have $\alpha = 2s/d$ (see, e.g., Harchaoui et al., 2008, Appendix D).

Balancing terms (Sobolev spaces). We thus need to balance $\lambda^{t/s}$ with $\frac{1}{n} \lambda^{-1/\alpha}$, leading to an optimal λ proportional to $n^{-(1/\alpha+t/s)^{-1}}$, and a rate proportional to $\frac{1}{n^{\alpha t/(\alpha t+s)}}$. This rate is only achievable through our analysis when $\frac{R^2}{n\lambda}$ remains bounded, that is, essentially $\lambda \geq R^2/n$, thus, $\frac{1}{\alpha} + \frac{t}{s} \geq 1$.

For $\alpha = 2s/d$, we obtain the rate $\frac{1}{n^{2t/(2t+d)}}$, which is valid as long as $\frac{d}{2} + t \geq s \geq t$. We can make the following observations:

- Except for the constraint $\frac{d}{2} + t \geq s \geq t$, the upper-bound on the rate obtained after optimizing over λ does not depend on the kernel.
- We obtain some form of adaptivity, that is, the rate improves with the regularity of the target function, from the slow rate $\frac{1}{n^{2/(2+d)}}$ when $t = 1$ (recovering the same rate as for local averaging methods in Chapter 6), and that can only be achieved when $s \leq d/2 + 1$, e.g., with the exponential kernel), to the rate $\frac{1}{n^{2s/(2s+d)}}$ when $t = s$, the rate is then always better than $1/\sqrt{n}$ because of the constraint $s > d/2$.
- In order to allow for regularization parameters λ which are less than $1/n$, other assumptions are needed. See, e.g., [Pillaud-Vivien et al. \(2018\)](#) and references therein.

7.7 Experiments

We consider one-dimensional problems to highlight the adaptivity of kernel methods to the regularity of the target function, with one smooth target and one non-smooth target, and three kernels: exponential kernel corresponding to the Sobolev space of order 1 (top of Figure 7.3), Matern kernel corresponding to the Sobolev space of order 3 (middle), and Gaussian kernel (bottom). In the right plots, dotted lines are affine fits to the log-log learning curves. The regularization parameter for ridge regression is selected to minimize expected risk, and learning curves are obtained by averaging over 20 replications. See results in Figure 7.3. The data

We observe adaptivity for the three kernels: learning is possible even with irregular functions, and the rates are better for smooth target functions. We also note that for kernels with smaller feature spaces (Matern and Gaussian), the performance on the non-smooth target function is worse than for the large feature space (exponential kernel). As highlighted by [Bach \(2013\)](#), this drop in performance is primarily due to a numerical issue (the eigenvalues of the kernel matrice decay exponentially fast, and finite precision arithmetic prevents the use of regularization parameters that are too small).

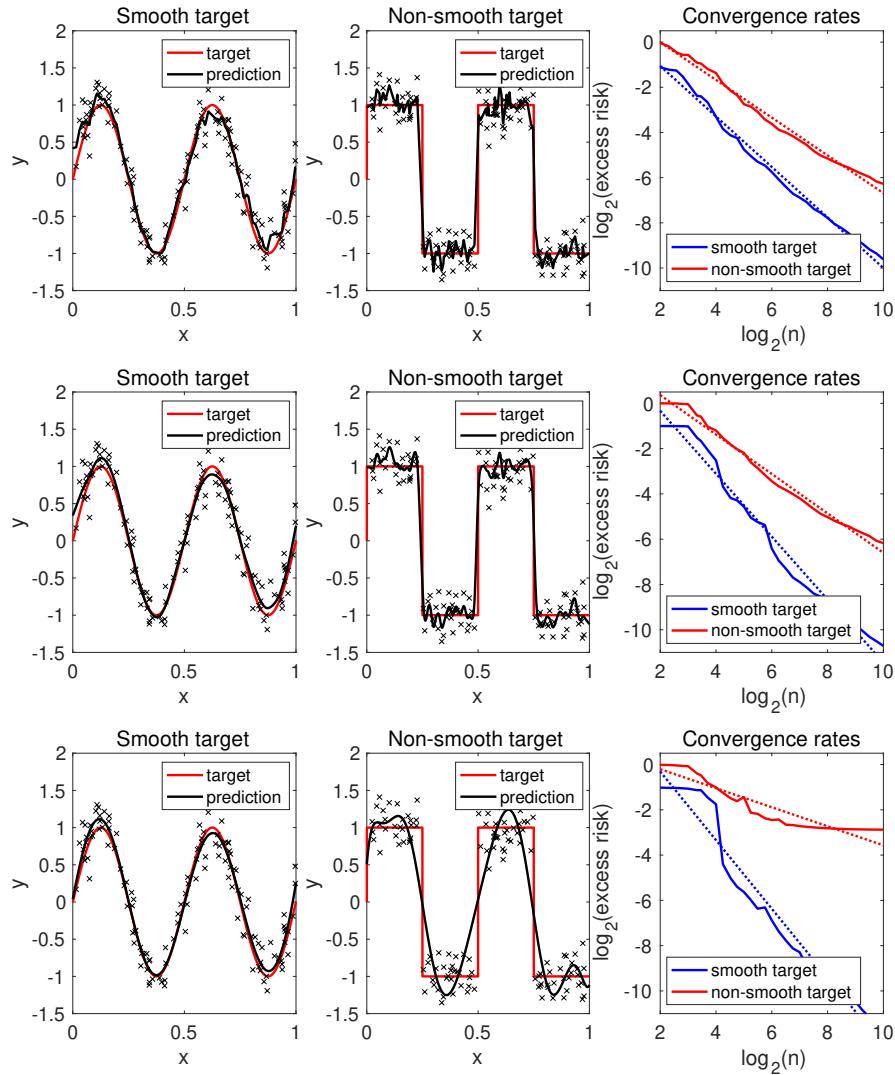


Figure 7.3: Comparison of three kernels, Sobolev space of order 1 (top), Matern kernel corresponding to the Sobolev space of order 3 (middle), and Gaussian kernel (bottom). We consider two different target functions and plot on the right plots the excess risks.

Chapter 8

Sparse methods

Chapter summary

Model selection can be performed by adding a specific penalty on top of the empirical risk.
- ℓ_0 -penalty: For fixed design linear regression, if the optimal predictor has k non-zeros, then we can replace the rate $\frac{\sigma^2 d}{n}$ by $\frac{\sigma^2 k \log d}{n}$ with an ℓ_0 -penalty on the square loss (which is computationally hard).

- ℓ_1 -penalty: With few assumptions, we can get a slow rate proportional to $\sqrt{\frac{\log d}{n}}$ with an ℓ_1 -penalty and efficient algorithms, while fast rates require strong assumptions on the design matrix in the fixed design setting. In the random design setting, fast rates can be obtained with invertible population covariance matrices.

8.1 Introduction

In previous chapters, we have seen the strong effect of the dimensionality of the input space \mathcal{X} on the generalization performance of supervised learning methods in two settings:

- When the target function f^* was only assumed to be Lipschitz-continuous on $\mathcal{X} = \mathbb{R}^d$, we saw that the excess risk for k -nearest-neighbors, Nadaraya-Watson estimation (Chapter 6), or positive kernel methods (Chapter 7), was scaling as $n^{-2/(d+2)}$.
- When the target function is linear in some features $\varphi(x) \in \mathbb{R}^d$, then the excess risk for unregularized least-squares was scaling as d/n .

In these two situations, when d is too large (of course, much larger in the linear case), efficient learning is generally impossible.

To improve upon these rates, we study two techniques in this book. The first one is regularization, e.g., by the ℓ_2 -norm, that allows obtaining dimension-independent bounds that cannot improve over the bounds above in the worst-case but are typically adaptive to additional regularity (see Chapter 3 and Chapter 7).

In this chapter, we consider another framework, namely *variable selection*, whose aim is to build predictors that depend only on a small number of variables. The key difficulty is that the identity of the selected variables is not known in advance.

In practice, variable selection is used in mainly two ways:

- The original set of features is already large (for example, in text or web data).
 - Given some input $x \in \mathcal{X}$, a large-dimensional feature vector $\varphi(x)$ is built where features are added that could potentially help predict the response, but from which we expect only a small number to be relevant.
- ⚠ If no good predictor with a small number of active variables exists, these methods are not supposed to work better.

In this chapter, we focus on linear methods, where we assume that we have a feature vector $\varphi(x) \in \mathbb{R}^d$, and we aim to minimize

$$\mathbb{E}[\ell(y, \varphi(x)^\top \theta)]$$

with respect to $\theta \in \mathbb{R}^d$, for some loss function $\ell : \mathcal{Y} \times \mathbb{R} \rightarrow \mathbb{R}$. We will consider two variable selection techniques, namely the penalization by $\|\theta\|_0$ the number of non-zeros in θ (often called abusively the “ ℓ_0 -norm”), or the ℓ_1 -norm. See extensions in Section 8.5.

Main focus on least-squares. These two types of penalties can be applied to all losses, but in this chapter, for simplicity, we will primarily consider the square loss, and in most cases, the fixed design setting (see the classical set-up in Section 3.5), and assume that we have n observations $(x_i, y_i) \in \mathcal{X} \times \mathcal{Y}$, such that there exists $\theta_* \in \mathbb{R}^d$ for which for $i \in \{1, \dots, n\}$,

$$y_i = \varphi(x_i)^\top \theta_* + \varepsilon_i,$$

where x_i is assumed deterministic, and ε_i has zero mean and variance σ^2 (we also assume independence from x_i , and sometimes stronger regularity, such as bounded almost surely, or Gaussian). The goal is then to find $\theta \in \mathbb{R}^d$, such that

$$\frac{1}{n} \|\Phi(\theta - \theta_*)\|_2^2 = (\theta - \theta_*)^\top \widehat{\Sigma}(\theta - \theta_*)$$

is as small as possible, where $\Phi \in \mathbb{R}^{n \times d}$ is the design matrix and $\widehat{\Sigma} = \frac{1}{n}\Phi^\top\Phi$ the non-centered empirical covariance matrix. We recall from Chapter 3 that for the ordinary least-squares estimator, the expectation of this excess risk is less than $\sigma^2 d/n$. This is the best possible performance if we make no assumption on θ_* . In this chapter, we assume that θ_* is sparse, that is, only a few of its components are non-zero, or in other words, $\|\theta_*\|_0 = k$ is small compared to d .

8.1.1 Dedicated proof technique for constrained least-squares

In this chapter, we consider a more refined proof technique¹ that can extend to constrained versions of least-squares (while our technique in Chapter 3 heavily relies on having a closed form for the estimator, which is not possible in constrained or regularized cases except in few instances, such as ridge regression).

We denote by $\hat{\theta}$ a minimizer of $\frac{1}{n}\|y - \Phi\theta\|_2^2$ with the constraint that $\theta \in \Theta$, for some subset Θ of \mathbb{R}^d . If $\theta_* \in \Theta$, then we have, by optimality of $\hat{\theta}$:

$$\|y - \Phi\hat{\theta}\|_2^2 \leq \|y - \Phi\theta_*\|_2^2.$$

By expanding with $y = \Phi\theta_* + \varepsilon$, we get $\|\varepsilon - \Phi(\hat{\theta} - \theta_*)\|_2^2 \leq \|\varepsilon\|_2^2$, leading to, by expanding the norms:

$$\|\varepsilon\|_2^2 - 2\varepsilon^\top\Phi(\hat{\theta} - \theta_*) + \|\Phi(\hat{\theta} - \theta_*)\|_2^2 \leq \|\varepsilon\|_2^2,$$

and thus

$$\|\Phi(\hat{\theta} - \theta_*)\|_2^2 \leq 2\varepsilon^\top\Phi(\hat{\theta} - \theta_*).$$

We can write it as

$$\|\Phi(\hat{\theta} - \theta_*)\|_2^2 \leq 2\|\Phi(\hat{\theta} - \theta_*)\|_2 \cdot \varepsilon^\top \left(\frac{\Phi(\hat{\theta} - \theta_*)}{\|\Phi(\hat{\theta} - \theta_*)\|_2} \right).$$

This reformulation is difficult to deal with because $\hat{\theta}$ also appears on the right side of the equation. Like done for upper-bounding estimation errors in Chapter 4, we can maximize with respect to $\theta \in \Theta$, which leads to

$$\|\Phi(\hat{\theta} - \theta_*)\|_2^2 \leq 2\|\Phi(\hat{\theta} - \theta_*)\|_2 \cdot \sup_{\theta \in \Theta} \varepsilon^\top \left(\frac{\Phi(\theta - \theta_*)}{\|\Phi(\theta - \theta_*)\|_2} \right), \quad (8.1)$$

where $\hat{\theta}$ has disappeared from the right-hand side. Finally, we get:

$$\|\Phi(\hat{\theta} - \theta_*)\|_2^2 \leq 4 \sup_{\theta \in \Theta} \left[\varepsilon^\top \left(\frac{\Phi(\theta - \theta_*)}{\|\Phi(\theta - \theta_*)\|_2} \right) \right]^2. \quad (8.2)$$

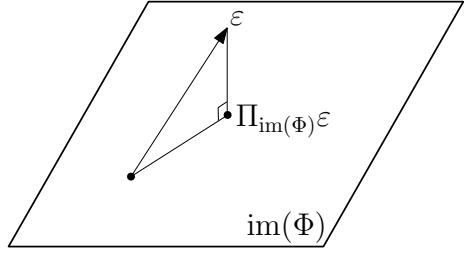
¹Taken from Philippe Rigollet's lecture notes, see <http://www-math.mit.edu/~rigollet/PDFs/RigNotes17.pdf>. See also Rigollet and Tsybakov (2007) for an example of application.

This inequality is true almost surely, and we can take expectation (with respect to ε) to obtain bounds. Therefore, in this chapter, we will compute expectations of maxima of quadratic forms in ε .

For example, when $\Theta = \mathbb{R}^d$ (no constraints), we get, by taking $z = \frac{\Phi(\theta - \theta_*)}{\|\Phi(\theta - \theta_*)\|_2}$, with $\Pi_\Phi = \Pi_{\text{im}(\Phi)}$ the orthogonal projector on the image space $\text{im}(\Phi)$ (which has dimension $\text{rank}(\Phi)$):

$$\mathbb{E}[\|\Phi(\hat{\theta} - \theta_*)\|_2^2] \leq 4\mathbb{E}\left[\sup_{z \in \text{im}(\Phi), \|z\|_2=1} [\varepsilon^\top z]^2\right].$$

By a simple geometric argument (see below),



we have

$$\sup_{z \in \text{im}(\Phi), \|z\|_2=1} [\varepsilon^\top z]^2 = \sup_{z \in \text{im}(\Phi), \|z\|_2=1} [(\Pi_\Phi \varepsilon)^\top z]^2 = \|\Pi_\Phi \varepsilon\|^2,$$

leading to

$$\mathbb{E}[\|\Phi(\hat{\theta} - \theta_*)\|_2^2] \leq 4\mathbb{E}[\|\Pi_\Phi \varepsilon\|^2] = 4\sigma^2 \mathbb{E} \text{tr}(\Pi_\Phi^2) = 4\sigma^2 \text{rank}(\Phi).$$

We thus get, up to a constant 4, the excess risk as $\sigma^2 d/n$, which is worse than the direct computation from Chapter 3 (Prop. 3.5) but allows extensions to more complex situations.

This reasoning also allows getting high probability bounds by adding assumptions on the noise ε . Finally, this also extends to penalized problems (see Section 8.2.2).

8.1.2 Probabilistic and combinatorial lemmas

We start with two small probabilistic lemmas:

Lemma 8.1 *If $z \in \mathbb{R}^n$ has a Gaussian distribution with mean 0 and covariance matrix $\sigma^2 I$, then, if $s < \frac{1}{2\sigma^2}$, $\mathbb{E}[e^{s\|z\|_2^2}] = (1 - 2\sigma^2 s)^{-n/2}$.*

Proof We have, for $\sigma = 1$ (from which we can derive the result for all σ), and $s < 1/2$ (using independence among the components of z):

$$\begin{aligned}\mathbb{E}[e^{s\|z\|_2^2}] &= \mathbb{E}[e^{s\sum_{i=1}^n z_i^2}] = \prod_{i=1}^n \mathbb{E}[e^{sz_i^2}] = \frac{1}{(2\pi)^{n/2}} \prod_{i=1}^n \int_{-\infty}^{\infty} e^{(s-\frac{1}{2})z_i^2} dz_i \\ &= \frac{1}{(2\pi)^{n/2}} \prod_{i=1}^n \sqrt{2\pi} (1-2s)^{-1/2} = (1-2s)^{-n/2}.\end{aligned}$$

■

Lemma 8.2 Let u_1, \dots, u_m be m random variables which are *potentially dependent*, and $s > 0$. Then, $\mathbb{E}[\max\{u_1, \dots, u_m\}] \leq \frac{1}{s} \log \left(\sum_{i=1}^m \mathbb{E}[e^{su_i}] \right)$.

Proof Following the reasoning from Section 1.2.4 in Chapter 1, for any $s \in \mathbb{R}$,

$$\mathbb{E}[\max\{u_1, \dots, u_m\}] \leq \frac{1}{s} \log (\mathbb{E}[e^{s \max\{u_1, \dots, u_m\}}]) = \frac{1}{s} \log (\mathbb{E}[\max\{e^{su_1}, \dots, e^{su_m}\}]),$$

which is thus less than $\frac{1}{s} \log (\sum_{i=1}^m \mathbb{E}[e^{su_i}])$. ■

The previous two lemmas can be combined to upper-bound the expectation of squared norms of Gaussian random variables: if $z_1, \dots, z_m \in \mathbb{R}^n$ are centered (that is, zero-mean) Gaussian random vectors which are potentially dependent, but for which the covariance matrix of z_i has eigenvalues less than σ^2 , we have for $s = \frac{1}{4\sigma^2}$, and Lemma 8.1, $\mathbb{E}[e^{s\|z\|_2^2}] \leq 2^{n/2}$, and from Lemma 8.2,

$$\mathbb{E}[\max\{\|z_1\|_2^2, \dots, \|z_m\|_2^2\}] \leq 4\sigma^2 \log(m2^{n/2}) = 2n\sigma^2 \log(2) + 4\sigma^2 \log(m),$$

which is to be compared to the expectation of each argument of the max, which is less than $\sigma^2 n$. We pay an additive factor proportional to $\sigma^2 \log(m)$. This will be applied to $m \propto d^k$, leading to the additional term in $\sigma^2 k \log(d)$ for methods based on the ℓ_0 -penalty. The term in d^k comes from the following lemma.

Lemma 8.3 Let $d > 0$ and $k \in \{1, \dots, d\}$. Then $\log \binom{d}{k} \leq k(1 + \log \frac{d}{k})$.

Proof By recursion on k , the inequality is trivial for $k = 1$, and if $\binom{d}{k-1} \leq \left(\frac{ed}{k-1}\right)^{k-1}$, then

$$\binom{d}{k} = \binom{d}{k-1} \frac{d-k}{k} \leq \left(\frac{ed}{k-1}\right)^{k-1} \frac{d}{k} \leq \left(\frac{ed}{k}\right)^{k-1} \left(1 + \frac{1}{k-1}\right)^{k-1} \frac{d}{k} \leq \left(\frac{ed}{k}\right)^{k-1} e \frac{d}{k} = \left(\frac{ed}{k}\right)^k,$$

where we use for $\alpha > 0$, $(1 + \frac{1}{\alpha})^\alpha = \exp(\alpha \log(1 + 1/\alpha)) \leq \exp(1) = e$. ■

We now consider two types of variable selection frameworks, one based on ℓ_0 -penalties and one based on ℓ_1 -penalties.

8.2 Variable selection by ℓ_0 penalty

In this section, we assume that the target vector θ_* has k non-zero components, that is, $\|\theta_*\|_0 = k$. We denote by $A = \text{supp}(\theta_*)$ the “support” of θ_* , that is, the subset of $\{1, \dots, d\}$ composed of j such that $(\theta_*)_j \neq 0$. We have $|A| = k$.

Price of adaptivity. If we knew the set A , then we could simply perform least-squares with the design matrix $\Phi_A \in \mathbb{R}^{n \times |A|}$, where Φ_B denotes the sub-matrix of Φ obtained by keeping only the columns from B , with an excess risk proportional to $\sigma^2 k/n$ (this is what we call the “oracle” in Section 8.4). Thus, as long as k is small compared to n , we can estimate θ_* correctly, regardless of the potentially large value of d .

However, we do not know A in advance, and we have to estimate it. We will see that this will lead to an extra factor of $\log(\frac{d}{k}) \leq \log d$ due to the potentially large number of models with k variables.

8.2.1 Assuming k is known

We start by assuming that the cardinality k is known in advance, and we consider Gaussian noise for simplicity (this extends to sub-Gaussian noise as well, see note below).

Proposition 8.1 (Model selection - known k) *Assume $y = \Phi\theta_* + \varepsilon$, with $\varepsilon \in \mathbb{R}^n$ a vector with independent Gaussian components of zero mean and variance σ^2 , with $\|\theta_*\|_0 \leq k$, for $k \leq d/2$. Let $\hat{\theta}$ be the minimizer of $\|y - \Phi\theta\|_2^2$ with the constraint that $\|\theta\|_0 \leq k$. Then, the (fixed design) excess risk is upper-bounded as:*

$$\mathbb{E}[(\hat{\theta} - \theta_*)^\top \widehat{\Sigma}(\hat{\theta} - \theta_*)] = \mathbb{E}\left[\frac{1}{n} \|\Phi(\hat{\theta} - \theta_*)\|_2^2\right] \leq 32\sigma^2 \frac{k}{n} \left(\log\left(\frac{d}{k}\right) + 1 \right).$$

Proof For any θ such that $\|\theta\|_0 \leq k$, we have $\|\theta - \theta_*\|_0 \leq 2k$. Thus we have, using the bounding technique from Section 8.1.1:

$$\begin{aligned} \|\Phi(\hat{\theta} - \theta_*)\|_2^2 &\leq 4 \sup_{\theta \in \mathbb{R}^d, \|\theta\|_0 \leq k} \left[\varepsilon^\top \left(\frac{\Phi(\theta - \theta_*)}{\|\Phi(\theta - \theta_*)\|_2} \right) \right]^2 \text{ from Eq. (8.2),} \\ &\leq 4 \sup_{\theta \in \mathbb{R}^d, \|\theta - \theta_*\|_0 \leq 2k} \left[\varepsilon^\top \left(\frac{\Phi(\theta - \theta_*)}{\|\Phi(\theta - \theta_*)\|_2} \right) \right]^2 \text{ from the discussion above,} \\ &= 4 \sup_{B \subset \{1, \dots, n\}, |B| \leq 2k} \sup_{\text{supp}(\theta - \theta_*) = B} \left[\varepsilon^\top \left(\frac{\Phi(\theta - \theta_*)}{\|\Phi(\theta - \theta_*)\|_2} \right) \right]^2 \end{aligned}$$

by separating by supports. Thus, using the same argument as in Section 8.1.1,

$$\begin{aligned} \|\Phi(\hat{\theta} - \theta_*)\|_2^2 &\leq 4 \sup_{B \subset \{1, \dots, n\}, |B| \leq 2k} \sup_{z \in \text{im}(\Phi_B), \|z\|_2=1} [\varepsilon^\top z]^2 \\ &\leq 4 \sup_{B \subset \{1, \dots, n\}, |B| \leq 2k} \|\Pi_{\Phi_B} \varepsilon\|^2 \leq 4 \sup_{B \subset \{1, \dots, n\}, |B|=2k} \|\Pi_{\Phi_B} \varepsilon\|^2, \end{aligned}$$

because $\|\Pi_{\Phi_B} \varepsilon\|^2$ is non-decreasing in B .

The random variable $\|\Pi_{\Phi_B} \varepsilon\|^2$ has an expectation which is less than $2k$. Given that there are $\binom{d}{2k} \leq \left(\frac{ed}{2k}\right)^{2k}$ sets B of cardinality $2k$ (bound from Lemma 8.3), we should expect, with concentration inequalities from Section 8.1.2, that we pay a price of $\log \left(\frac{ed}{2k}\right)^{2k} \approx k \log \frac{d}{k}$. We will make this reasoning formal.

Indeed, $\Pi_{\Phi_B} \varepsilon$ is normally distributed with isotropic covariance matrix of dimension $|B| \leq 2k$, and thus we have for $s\sigma^2 < 1/2$, from Lemma 8.1:

$$\mathbb{E}[e^{s\|\Pi_{\Phi_B} \varepsilon\|^2}] \leq (1 - 2\sigma^2 s)^{-k}.$$

Thus, with $s = 1/(4\sigma^2)$, for which $(1 - 2\sigma^2 s)^{-k} = 2^k$, we get, from Lemma 8.2:

$$\begin{aligned} \mathbb{E}[\|\Phi(\hat{\theta} - \theta_*)\|_2^2] &\leq 16\sigma^2 \log \left(\binom{d}{2k} 2^k \right) \\ &\leq 16\sigma^2 \log \left(\left(\frac{ed}{2k} \right)^{2k} 2^k \right) = 16\sigma^2 \left(2k \log \left(\frac{d}{k} \right) + (2 - \log 2)k \right). \end{aligned}$$

This leads to the desired result. ■

We can make the following observations:

- The result extends beyond Gaussian noise, that is, for all sub-Gaussian ε_i , for which $\mathbb{E}[e^{s\varepsilon_i}] \leq e^{s^2\tau^2}$ for all $s > 0$ (for some $\tau > 0$), or, equivalently $\mathbb{P}(|\varepsilon_i| > t) = O(e^{-ct^2})$ for some $c > 0$.
- The result extends if the minimization of the empirical risk is only done approximately.
- This result is not improvable by any algorithm (polynomial time or not), see, e.g., Giraud (2014, Theorem 2.3) and Chapter 12.

Algorithms. In terms of algorithms, essentially all subsets of size k have to be looked at for exact minimization, with a cost proportional to $O(d^k)$, which is a problem when k gets large. There are, however, two simple algorithms that only come with guarantees when such fast rates are available for ℓ_1 -regularization (see Section 8.3.3, and [Zhang, 2009](#)).

- **Greedy algorithm:** starting from the empty set, variables are added one by one, maximizing the resulting cost reduction. This is often referred to as orthogonal matching pursuit.
- **Iterative sorting:** Starting from $\theta_0 = 0$, the iterative algorithm goes as follows at iteration t ; the upper bound (based on the L -smoothness of the quadratic loss, with $L = \lambda_{\max}(\frac{1}{n}\Phi^\top\Phi)$, see Chapter 5):

$$\frac{1}{n}\|y - \Phi\theta_{t-1}\|_2^2 - \frac{2}{n}(y - \Phi\theta_{t-1})^\top\Phi(\theta - \theta_{t-1}) + \lambda_{\max}(\frac{1}{n}\Phi^\top\Phi)\|\theta - \theta_{t-1}\|_2^2$$

on the cost function $\frac{1}{n}\|y - \Phi\theta\|_2^2$ is built and minimized with respect to $\|\theta\|_0 \leq k$ to obtain θ_t . This is done (proof left as an exercise) by computing the unconstrained minimizer $\theta_{t-1} + \frac{1}{\lambda_{\max}(\frac{1}{n}\Phi^\top\Phi)}\frac{1}{n}\Phi^\top(y - \Phi\theta_{t-1})$, and selecting the k largest components.

8.2.2 Estimating k (♦)

In practice, regardless of the computational cost, one also needs to estimate k . A classical idea to consider penalized least-squares and minimize

$$\frac{1}{n}\|y - \Phi\theta\|_2^2 + \lambda\|\theta\|_0. \quad (8.3)$$

This is a hard problem to solve, which essentially requires looking at all 2^d subsets. For a well-chosen λ , this (almost) leads to the same performance as if k were known.

Proposition 8.2 (Model selection - ℓ_0 -penalty) *Assume $y = \Phi\theta_* + \varepsilon$, with $\varepsilon \in \mathbb{R}^n$ a vector with independent Gaussian components of zero mean and variance σ^2 , with $\|\theta_*\|_0 \leq k$. Let $\hat{\theta}$ be a minimizer of Eq. (8.3). Then, for $\lambda = \frac{8\sigma^2}{n} \log(2d)$, we have:*

$$\mathbb{E}\left[\frac{1}{n}\|\Phi(\hat{\theta} - \theta_*)\|_2^2\right] \leq \frac{16k\sigma^2}{n}[2 + \log(d)] + \frac{16\sigma^2}{n}.$$

Proof We follow the same proof technique than in Section 8.1.1, but now for regularized problems. We have by optimality of $\hat{\theta}$:

$$\|y - \Phi\hat{\theta}\|_2^2 + n\lambda\|\hat{\theta}\|_0 \leq \|y - \Phi\theta_*\|_2^2 + n\lambda\|\theta_*\|_0,$$

which leads to, using the inequality $2ab \leqslant 2a^2 + \frac{1}{2}b^2$, and the same arguments that led to Eq. (8.1):

$$\begin{aligned}\|\Phi(\hat{\theta} - \theta_*)\|_2^2 &\leqslant 2\|\Phi(\hat{\theta} - \theta_*)\|_2 \cdot \varepsilon^\top \left(\frac{\Phi(\hat{\theta} - \theta_*)}{\|\Phi(\hat{\theta} - \theta_*)\|_2} \right) + n\lambda\|\theta_*\|_0 - n\lambda\|\hat{\theta}\|_0 \\ &\leqslant 2\left(\varepsilon^\top \left(\frac{\Phi(\hat{\theta} - \theta_*)}{\|\Phi(\hat{\theta} - \theta_*)\|_2} \right)\right)^2 + \frac{1}{2}\|\Phi(\hat{\theta} - \theta_*)\|_2^2 + n\lambda\|\theta_*\|_0 - n\lambda\|\hat{\theta}\|_0,\end{aligned}$$

leading to, by taking the supremum over $\theta \in \mathbb{R}^d$:

$$\|\Phi(\hat{\theta} - \theta_*)\|_2^2 \leqslant \sup_{\theta \in \mathbb{R}^d} \left\{ 4\left(\varepsilon^\top \left(\frac{\Phi(\theta - \theta_*)}{\|\Phi(\theta - \theta_*)\|_2} \right)\right)^2 + 2n\lambda\|\theta_*\|_0 - 2n\lambda\|\theta\|_0 \right\}.$$

We then take the supremum by layers, as $\sup_{\theta \in \mathbb{R}^d} = \sup_{k' \in \{1, \dots, d\}} \sup_{|B|=k'} \sup_{\text{supp}(\theta)=B}$, that is, using the same derivations as for Prop. 8.1 (A is the support of θ_*):

$$\begin{aligned}&\mathbb{E}[\|\Phi(\hat{\theta} - \theta_*)\|_2^2] \\ &\leqslant \mathbb{E}\left[\sup_{k' \in \{1, \dots, d\}} \sup_{|B|=k'} \sup_{\text{supp}(\theta)=B} \left\{ 4\left(\varepsilon^\top \left(\frac{\Phi(\theta - \theta_*)}{\|\Phi(\theta - \theta_*)\|_2} \right)\right)^2 + 2n\lambda\|\theta_*\|_0 - 2n\lambda k' \right\} \right] \\ &\leqslant 2n\lambda\|\theta_*\|_0 + 4\mathbb{E}\left[\sup_{k' \in \{1, \dots, d\}} \sup_{|B|=k'} \left\{ \|\Pi_{\Phi_{A \cup B}} \varepsilon\|^2 - \frac{n\lambda}{2}k' \right\} \right].\end{aligned}$$

We thus get with the same reasoning as in Section 8.2.1 (based on the probabilistic lemmas from Section 8.1.2), using $s = \frac{1}{4\sigma^2}$ within Lemma 8.2:

$$\begin{aligned}&\mathbb{E}[\|\Phi(\hat{\theta} - \theta_*)\|_2^2] \\ &\leqslant 2n\lambda\|\theta_*\|_0 + 16\sigma^2 \log \left(\sum_{k'=1}^d \binom{d}{k'} 2^{k'+\|\theta^*\|_0} \exp \left(-\frac{n\lambda k'}{8\sigma^2} \right) \right) \\ &\leqslant 2n\lambda\|\theta_*\|_0 + 16\sigma^2\|\theta^*\|_0 \log(2) + 16\sigma^2 \log \left(\sum_{k'=1}^d \binom{d}{k'} \exp \left(k' \left(\log(2) - \frac{n\lambda}{8\sigma^2} \right) \right) \right) \\ &\leqslant (2n\lambda + 16\log(2)\sigma^2)\|\theta_*\|_0 + 16\sigma^2 d \log \left(1 + \exp \left(\log(2) - \frac{n\lambda}{8\sigma^2} \right) \right).\end{aligned}$$

In order to find a good regularization parameter, we can then approximately minimize the bound above with respect to λ . We obtain a good balance of the two terms by having $-\log d = \log(2) - \frac{n\lambda}{8\sigma^2}$, that is, $\lambda = \frac{8\sigma^2}{n} \log(2d)$, for which we get:

$$\mathbb{E}[\|\Phi(\hat{\theta} - \theta_*)\|_2^2] \leqslant (2n\lambda + 16\log(2)\sigma^2)\|\theta_*\|_0 + 16\sigma^2 \leqslant 16\sigma^2((\log(d) + 2)\|\theta_*\|_0 + 1),$$

and get the desired result. ■

We can make the following observations:

- The penalty proportional to $\|\theta\|_0 \log d$ is often referred to as the “BIC penalty”.
- Note that we need to know σ^2 in advance to compute λ , which can be a problem in practice. See [Giraud et al. \(2012\)](#) for more details and alternative formulations.
- The three most important aspects are that: (1) the bound does not require any assumption on the design matrix Φ , (2) we observe a positive high-dimensional phenomenon, where d only appears as $\frac{\log d}{n}$, but (3) only exponential-time algorithms are possible for solving the problem with guarantees (see algorithms below).

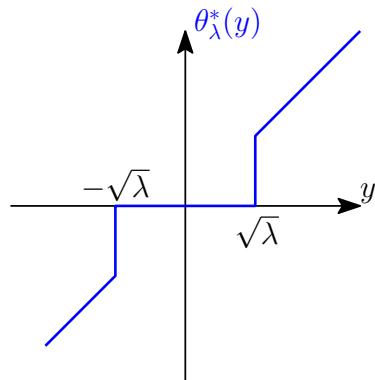
Exercise 8.1 (♦) With a penalty proportional to $\|\theta\|_0 \log \frac{d}{\|\theta\|_0}$, show the same bound than for k known.

Algorithms. We can extend the two algorithms from Section 8.2.1 for the penalized case:

- **Forward-backward algorithm to minimize a function of a set B :** Starting from the empty set $B = \emptyset$, at every step of the algorithm, one tries both a forward algorithm (adding a node to B) and a backward algorithm (removing a node from B), and only perform a step if it decreases the overall cost function. See an analysis by [Zhang \(2011\)](#).
- **Iterative hard-thresholding:** compared to the constrained case, we minimize

$$\frac{1}{n} \|y - \Phi \theta_{t-1}\|_2^2 - \frac{2}{n} (y - \Phi \theta_{t-1})^\top \Phi (\theta - \theta_{t-1}) + \lambda_{\max} \left(\frac{1}{n} \Phi^\top \Phi \right) \|\theta - \theta_{t-1}\|_2^2 + \lambda \|\theta\|_0,$$

which can also be computed in closed form (by iterative hard thresholding). That is, with $\theta_t = \theta_{t-1} + \frac{1}{\lambda_{\max}(\Phi^\top \Phi)} \Phi^\top (y - \Phi \theta_{t-1})$, all components $(\theta_t)_j$ such that $|(\theta_t)_j|^2 \geq \frac{\lambda}{\lambda_{\max}(\Phi^\top \Phi)}$, are left unchanged and all others are set to zero. Indeed, for one-dimensional problems, the minimizer of $|\theta - y|^2 + \lambda 1_{\theta \neq 0}$ is $\theta_\lambda^*(y) = 0$ if $|y|^2 \leq \lambda$ and $\theta_\lambda^*(y) = y$ otherwise (see below).



This is referred to as “iterative hard thresholding” (while for the ℓ_1 -norm, this will be iterative *soft* thresholding) because a component is either kept intact or set exactly to zero, leading to a discontinuous behavior. See an analysis by [Blumensath and Davies \(2009\)](#).

8.3 High-dimensional estimation through ℓ_1 -regularization

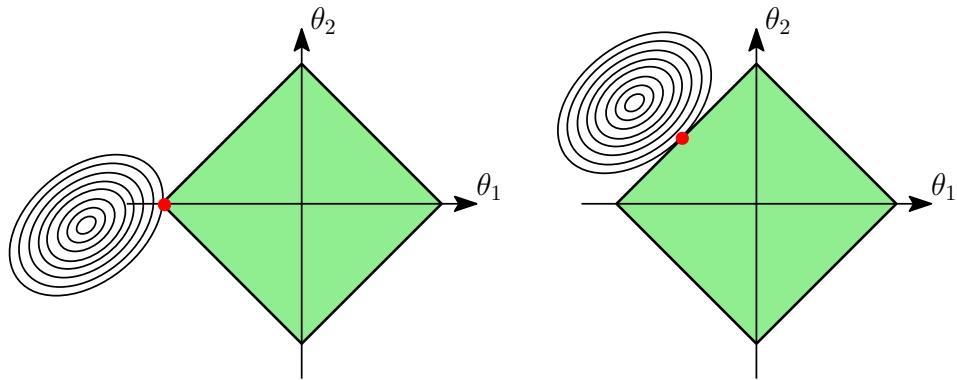
We now consider a computationally efficient alternative to ℓ_0 -penalties, namely using ℓ_1 -penalties, by minimizing, for the square loss:

$$\frac{1}{2n} \|y - \Phi\theta\|_2^2 + \lambda \|\theta\|_1. \quad (8.4)$$

This is a convex optimization problem on which algorithms from Chapter 5 can be applied (see instances below). It is often referred to as the “Lasso” problem, for “least absolute shrinkage and selection operator” ([Tibshirani, 1996](#)).

8.3.1 Intuition and algorithms

Sparsity-inducing effect. As opposed to the squared ℓ_2 -norm used in ridge regression, the ℓ_1 -norm is non-differentiable, and its non-differentiability is not limited to $\theta = 0$ but occurs in many other points. To see this, we can look at the ℓ_1 -ball and its different geometry compared to the ℓ_2 -ball. This is directly relevant to situations where we constrain the value of the norm instead of penalizing by it.



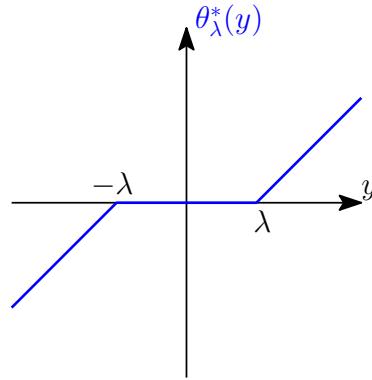
As shown above, where we represent the level set of a potential loss function, the solution of minimizing the loss subject to the ℓ_1 -constraint (in green) is obtained when level sets are “tangent” to the constraint set. In the right part, this is obtained at a point away from

the axes, but on the left part, this is achieved at one of the corners of the ℓ_1 -ball, which are points where one of the components of θ is equal to zero. Such corners are “attractive”, that is, minimizers tend to be precisely at these corners, and this exactly leads to sparse solutions.

One-dimensional problem. Another classical way to understand the sparsity-inducing effect is to consider the one-dimensional problem:

$$\min_{\theta \in \mathbb{R}} F(\theta) = \frac{1}{2}(y - \theta)^2 + \lambda|\theta|.$$

Since F is strongly-convex, it has a unique minimizer $\theta_\lambda^*(y)$. For $\lambda = 0$ (no regularization), we have $\theta_0^*(y) = y$, while for $\lambda > 0$, by computing left and right derivatives at zero (to be done as an exercise), one can check that $\theta_\lambda^*(y) = 0$ if $|y| \leq \lambda$, and $\theta_\lambda^*(y) = y - \lambda$ for $y > \lambda$, and $\theta_\lambda^*(y) = y + \lambda$ for $y < -\lambda$, which can be put all together as $\theta_\lambda^*(y) = \max\{|y| - \lambda, 0\} \text{sign}(y)$, which is depicted below. This is referred to as iterative soft thresholding (this will be useful for proximal methods below).



Note that the minimizer is either sent to zero or shrunk toward zero.

Optimization algorithms. We can adapt algorithms from Chapter 5 to the problem in Eq. (8.4).

- **Iterative soft-thresholding:** We can apply proximal methods to the objective function of the form $F(\theta) + \lambda\|\theta\|_1$ for $F(\theta) = \frac{1}{2n}\|y - \Phi\theta\|_2^2$, for which $F'(\theta) = -\frac{1}{n}\Phi^\top(y - \Phi\theta)$. The plain (non-accelerated) proximal method recursion is

$$\theta_t = \arg \min_{\theta \in \mathbb{R}^d} F(\theta_{t-1}) + F'(\theta_{t-1})^\top(\theta - \theta_{t-1}) + \frac{L}{2}\|\theta - \theta_{t-1}\|_2^2 + \lambda\|\theta\|_1,$$

with $L = \lambda_{\max}(\frac{1}{n}\Phi^\top\Phi)$. This leads to $(\theta_t)_j = \max\{|(\eta_t)_j| - \lambda, 0\} \text{sign}((\eta_t)_j)$, for $\eta_t = \theta_{t-1} - \frac{1}{L}F'(\theta_{t-1})$. This simple algorithm can also be accelerated. The convergence

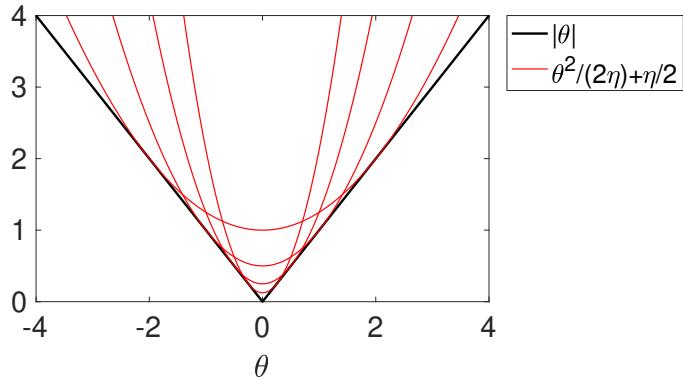
rate then depends on the invertibility of $\frac{1}{n}\Phi^\top\Phi$ (if invertible, we get an exponential convergence rate in t , with only $O(1/t)$ otherwise).

- **Coordinate descent:** Although the ℓ_1 -norm is a non-differentiable function, coordinate descent can be applied (because the ℓ_1 -norm is “separable”). At each iteration, we select a coordinate to update (at random or by cycling) and optimize with respect to this coordinate, which is a one-dimensional problem that can be solved in closed form. The convergence properties are similar to proximal methods (Fercoq and Richtárik, 2015).

η -trick. The non-differentiability of the ℓ_1 -norm may also be treated through the simple identity:

$$|\theta_j| = \inf_{\eta_j > 0} \frac{\theta_j^2}{2\eta_j} + \frac{\eta_j}{2},$$

where the minimizer is attained at $\eta_j = |\theta_j|$. See below an example in one dimension, with $|\theta|$ and several quadratic upper bounds.



This leads to the reformulation of Eq. (8.4) as

$$\inf_{\theta \in \mathbb{R}^d} \frac{1}{2n} \|y - \Phi\theta\|_2^2 + \lambda \|\theta\|_1 = \inf_{\eta \in \mathbb{R}_+^d} \inf_{\theta \in \mathbb{R}^d} \frac{1}{2n} \|y - \Phi\theta\|_2^2 + \frac{\lambda}{2} \sum_{j=1}^d \frac{\theta_j^2}{2\eta_j} + \frac{\lambda}{2} \sum_{j=1}^d \eta_j,$$

and alternating optimization algorithms can be used: (a) minimizing with respect to η when θ is fixed can be done in closed form as $\eta_j = |\theta_j|$, while minimizing with respect to θ when η is fixed is a quadratic optimization problem which can be solved by a linear system.²

²See more details in <https://francisbach.com/the-%ce%b7-trick-or-the-effectiveness-of-reweighted-least-squares/>

Optimality conditions (♦). To study the estimator defined by Eq. (8.4), it is often necessary to characterize when a certain θ is optimal or not, that is, to derive optimality conditions.

Since the objective function $H(\theta) = F(\theta) + \lambda\|\theta\|_1$ is not differentiable, we need other tools than having the gradient equal to zero. The gradient looks only at d directions (along the coordinate axis), while, in the non-smooth context, we need to look at all directions, that is, for all $\Delta \in \mathbb{R}^d$, we require that the directional derivative,

$$\partial H(\theta, \Delta) = \lim_{\varepsilon \rightarrow 0} \frac{1}{\varepsilon} [H(\theta + \varepsilon\Delta) - H(\theta)],$$

is non-negative. That is, we need to go up in all directions. When H is differentiable at θ , then $\partial H(\theta, \Delta) = H'(\theta)^\top \Delta$, and the positivity for all Δ is equivalent to $H'(\theta) = 0$.

For $H(\theta) = F(\theta) + \lambda\|\theta\|_1$, we have:

$$\partial H(\theta, \Delta) = F'(\theta)^\top \Delta + \lambda \sum_{j, \theta_j \neq 0} \text{sign}(\theta_j)\Delta_j + \lambda \sum_{j, \theta_j=0} |\Delta_j|.$$

It is separable in Δ_j , $j = 1, \dots, d$, and it is non-negative for all j , if and only if all components that depend on Δ_j are non-negative.

When $\theta_j \neq 0$, then this requires $F'(\theta)_j + \lambda \text{sign}(\theta_j) = 0$, while when $\theta_j = 0$, then we need $F'(\theta)_j \Delta_j + \lambda |\Delta_j| \geq 0$ for all Δ_j , which is equivalent to $|F'(\theta)_j| \leq \lambda$. This leads to the set of conditions:

$$\begin{cases} F'(\theta)_j + \lambda \text{sign}(\theta_j) = 0, & \forall j \in \{1, \dots, d\} \text{ such that } \theta_j \neq 0, \\ |F'(\theta)_j| \leq \lambda, & \forall j \in \{1, \dots, d\} \text{ such that } \theta_j = 0. \end{cases}$$

See [Giraud \(2014\)](#) for more details. Note that we could have also used subgradients to derive these optimality conditions.

Homotopy method (♦♦). We assume for simplicity that $\Phi^\top \Phi$ is invertible so that the minimizer $\theta(\lambda)$ is unique. Given a certain sign pattern for θ , optimality conditions are all convex in λ and thus define an interval in λ where the sign is constant. Given the sign, then the solution $\theta(\lambda)$ is affine in λ , leading to a piecewise affine function in λ (see an example of a regularization path in Figure 8.1).

If we know the breakpoints in λ and the associated signs, we can compute all solutions for all λ . This is the source of the homotopy algorithm for Eq. (8.4), which starts with large λ and builds the path of solutions by computing break points one by one. See more details by [Osborne et al. \(2000\)](#); [Mairal and Yu \(2012\)](#).

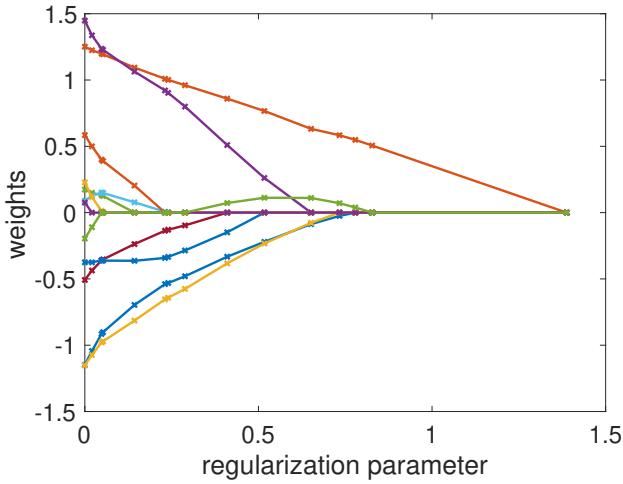


Figure 8.1: Regularization path for a Lasso problem in dimension $d = 32$ and $n = 32$ input observations sampled from a standard Gaussian distribution with 4 non-zero weights equal to -1 or $+1$, and outputs generated with additive Gaussian noise with unit variance. The random seed was chosen so that at least one weight comes in and out in the regularization path.

8.3.2 Slow rates

We first consider an analysis based on simple tools with no assumptions on the design matrix Φ . We will see that we can deal with high-dimensional inference problems where d can be large, but it will be with rates in $1/\sqrt{n}$ and not $1/n$, hence the denomination “slow”.

We study the penalization by a general norm $\Omega : \mathbb{R}^d \rightarrow \mathbb{R}$ with dual norm Ω^* defined as $\Omega^*(z) = \sup_{\Omega(\theta) \leq 1} z^\top \theta$ (see Exercise 8.2 below for classical examples). We thus denote by $\hat{\theta}$ a minimizer of

$$\frac{1}{2n} \|y - \Phi\theta\|_2^2 + \lambda\Omega(\theta). \quad (8.5)$$

We start with a lemma characterizing the excess risk in two situations: (a) where λ is large enough, and (b) in the general case.

Lemma 8.4 *Let $\hat{\theta}$ be a minimizer of Eq. (8.5).*

- (a) *If $\Omega^*(\Phi^\top \varepsilon) \leq \frac{n\lambda}{2}$, then we have $\Omega(\hat{\theta}) \leq 3\Omega(\theta_*)$ and $\frac{1}{n}\|\Phi(\hat{\theta} - \theta_*)\|_2^2 \leq 3\lambda\Omega(\theta_*)$.*
- (b) *In all cases, $\frac{1}{n}\|\Phi(\hat{\theta} - \theta_*)\|_2^2 \leq \frac{4}{n}\|\varepsilon\|_2^2 + 4\lambda\Omega(\theta_*)$.*

Proof We have, like in Section 8.1.1, by optimality of $\hat{\theta}$ for Eq. (8.5):

$$\|\Phi(\hat{\theta} - \theta_*)\|_2^2 \leq 2\varepsilon^\top \Phi(\hat{\theta} - \theta_*) + 2n\lambda\Omega(\theta_*) - 2n\lambda\Omega(\hat{\theta}).$$

Then, with the dual norm $\Omega^*(z) = \sup_{\Omega(\theta) \leq 1} z^\top \theta$, assuming that $\Omega^*(\Phi^\top \varepsilon) \leq \frac{n\lambda}{2}$, and using the triangle inequality:

$$\begin{aligned}\|\Phi(\hat{\theta} - \theta_*)\|_2^2 &\leq 2\Omega^*(\Phi^\top \varepsilon)\Omega(\hat{\theta} - \theta_*) + 2n\lambda\Omega(\theta_*) - 2n\lambda\Omega(\hat{\theta}) \\ &\leq n\lambda\Omega(\hat{\theta} - \theta_*) + 2n\lambda\Omega(\theta_*) - 2n\lambda\Omega(\hat{\theta}) \\ &\leq n\lambda\Omega(\hat{\theta}) + n\lambda\Omega(\theta_*) + 2n\lambda\Omega(\theta_*) - 2n\lambda\Omega(\hat{\theta}) \leq 3n\lambda\Omega(\theta_*) - n\lambda\Omega(\hat{\theta}).\end{aligned}$$

This implies that $\Omega(\hat{\theta}) \leq 3\Omega(\theta_*)$ and $\frac{1}{n}\|\Phi(\hat{\theta} - \theta_*)\|_2^2 \leq 3\lambda\Omega(\theta_*)$.

We also have a general bound through:

$$\|\Phi(\hat{\theta} - \theta_*)\|_2^2 \leq 2\|\varepsilon\|_2\|\Phi(\hat{\theta} - \theta_*)\|_2 + 2n\lambda\Omega(\theta_*),$$

which leads to, using the identity $2ab \leq \frac{1}{2}a^2 + 2b^2$,

$$\|\Phi(\hat{\theta} - \theta_*)\|_2^2 \leq \frac{1}{2}\|\Phi(\hat{\theta} - \theta_*)\|_2^2 + 2\|\varepsilon\|_2^2 + 2n\lambda\Omega(\theta_*),$$

which leads to the desired bound. ■

Exercise 8.2 For $p \in [1, \infty]$, show that the dual of the ℓ_p -norm is the ℓ_q -norm, for $\frac{1}{p} + \frac{1}{q} = 1$.

We can now use the lemma above to compute the excess risk of the Lasso, for which $\Omega = \|\cdot\|_1$ and $\Omega^*(\Phi^\top \varepsilon) = \|\Phi^\top \varepsilon\|_\infty$. The key is to note that since $\|\Phi^\top \varepsilon\|_\infty$ is a maximum of $2d$ zero-mean terms that scale as \sqrt{n} , according to Section 1.2.4, its maximum scales as $\sqrt{n \log(d)}$, and we will apply the lemma above when λ is larger than $\sqrt{\frac{\log d}{n}}$. We denote by $\|\widehat{\Sigma}\|_\infty$ the largest element of the matrix $\widehat{\Sigma}$ in absolute value.

Proposition 8.3 (Lasso - slow rate) Assume $y = \Phi\theta_* + \varepsilon$, with $\varepsilon \in \mathbb{R}^n$ a vector with independent Gaussian components of zero mean and variance σ^2 . Let $\hat{\theta}$ be the minimizer of Eq. (8.4). Then, for $\lambda = \frac{2\sigma}{\sqrt{n}}\sqrt{2\|\widehat{\Sigma}\|_\infty}\sqrt{\log(d) + \log\frac{1}{\delta}}$, we have, with probability greater than $1 - \delta$:

$$\frac{1}{n}\|\Phi(\hat{\theta} - \theta_*)\|_2^2 \leq 3\|\theta_*\|_1 \cdot \frac{2\sigma}{\sqrt{n}}\sqrt{2\|\widehat{\Sigma}\|_\infty}\sqrt{\log(d) + \log\frac{1}{\delta}}.$$

Proof For each j , the random variable $(\Phi^\top \varepsilon)_j$ is Gaussian with mean zero and variance $n\sigma^2\widehat{\Sigma}_{jj}$. Thus, we get from the union bound and from the fact that for a standard Gaussian variable z , $\mathbb{P}(|z| \geq t) \leq \exp(-t^2/2)$:³

$$\mathbb{P}\left(\|\Phi^\top \varepsilon\|_\infty > \frac{n\lambda}{2}\right) \leq \sum_{j=1}^d \mathbb{P}\left(|\Phi^\top \varepsilon|_j > \frac{n\lambda}{2}\right) \leq \sum_{j=1}^d \exp\left(\frac{-n\lambda^2}{8\sigma^2\widehat{\Sigma}_{jj}}\right) \leq d \exp\left(\frac{-n\lambda^2}{8\sigma^2\|\widehat{\Sigma}\|_\infty}\right) = \delta.$$

³We have for $t \geq 0$: $e^{t^2/2}\mathbb{P}(|z| \geq t) = \frac{2}{\sqrt{2\pi}} \int_t^{+\infty} e^{t^2/2-s^2/2} dt \leq \frac{2}{\sqrt{2\pi}} \int_t^{+\infty} e^{-(s-t)^2/2} dt = 1$.

Thus, with probability greater than $1 - \delta$, we can apply the first part of Lemma 8.4, and therefore the error is less than $3\lambda\|\theta^*\|_1$. For a result in expectation, see the exercise below. ■



Check homogeneity!

We already observe some high-dimensional phenomenon with the term $\sqrt{\frac{\log d}{n}}$, where n can be much larger than d (if, of course, we assume that the optimal predictor θ_* is sparse, so that $\|\theta_*\|_1$ does not grow with d). Note that the proposed regularization parameter depends on the unknown noise variance. A simple trick known as the “square root Lasso” allows to avoid that dependence on σ (see Giraud, 2014, Section 5.4), by minimizing $\frac{1}{\sqrt{n}}\|y - \Phi\theta\|_2 + \lambda\|\theta\|_1$.

The proposition above suggests a regularization parameter λ proportional to $1/\sqrt{n}$, which does enable estimation in high-dimensional situations, but can also add a significant bias because all non-zero components of $\hat{\theta}$ are shrunk towards zero. See Section 8.5 for methods to alleviate this effect.

Exercise 8.3 (♦) *With the same assumptions as Prop. 8.3, and with the choice of regularization parameter $\lambda = 4\sigma\sqrt{\frac{\log(dn)}{n}}\sqrt{\|\hat{\Sigma}\|_\infty}$, show the following bound in expectation:*

$$\mathbb{E}\left[\frac{1}{n}\|\Phi(\hat{\theta} - \theta_*)\|_2^2\right] \leq 32\sigma\sqrt{\frac{\log(dn)}{n}}\sqrt{\|\hat{\Sigma}\|_\infty}\|\theta_*\|_1 + \frac{32}{n}\sigma^2.$$

Exercise 8.4 (♦) *Using Rademacher complexities from Chapter 4, show a similar slow rate for ℓ_1 -constrained optimization with Lipschitz-continuous losses.*

Exercise 8.5 (♦) *We consider the Lasso (square loss) within the random design setting, with the assumption that $\|\varphi(x)\|_\infty \leq R$ almost surely, $y = \varphi(x)^\top\theta_* + \varepsilon$ with $|\varepsilon| \leq \sigma$ almost surely, for some $\theta_* \in \mathbb{R}^d$. Provide a result similar to Prop. 8.3 for the excess risk (using similar techniques based on Lemma 8.4). See also Section 4.5.5.*

8.3.3 Fast rates (♦)

We now consider conditions to obtain a fast rate with a leading term proportional to $\sigma^2\frac{k \log d}{n}$, which is the same as for ℓ_0 -penalty, but with tractable algorithms. This will come with extra (very) strong conditions on the design matrix Φ .

We start with a simple (but crucial) lemma, characterizing the solution of Eq. (8.4) in terms of the support A of θ_* .

Lemma 8.5 Let $\hat{\theta}$ be a minimizer of Eq. (8.5). Assume $\|\Phi^\top \varepsilon\|_\infty \leq \frac{n\lambda}{2}$. If $\Delta = \hat{\theta} - \theta_*$, then $\|\Delta_{A^c}\|_1 \leq 3\|\Delta_A\|_1$ and $\|\Phi\Delta\|_2^2 \leq 3n\lambda\|\Delta_A\|_1$.

Proof We have, like in previous proofs (e.g., Lemma 8.4), with $\Delta = \hat{\theta} - \theta_*$, and A the support of θ_* :

$$\|\Phi\Delta\|_2^2 \leq 2\varepsilon^\top \Phi\Delta + 2n\lambda\|\theta_*\|_1 - 2n\lambda\|\hat{\theta}\|_1.$$

Then, assuming that $\|\Phi^\top \varepsilon\|_\infty \leq \frac{n\lambda}{2}$,

$$\begin{aligned} \|\Phi\Delta\|_2^2 &\leq 2\|\Phi^\top \varepsilon\|_\infty\|\Delta\|_1 + 2n\lambda\|\theta_*\|_1 - 2n\lambda\|\hat{\theta}\|_1 \\ \|\Phi\Delta\|_2^2 &\leq n\lambda\|\Delta\|_1 + 2n\lambda\|\theta_*\|_1 - 2n\lambda\|\hat{\theta}\|_1. \end{aligned}$$

We then use, by using the decomposability of the ℓ_1 -norm and the triangle inequality:

$$\|\theta_*\|_1 - \|\hat{\theta}\|_1 = \|(\theta_*)_A\|_1 - \|\theta_* + \Delta\|_1 = \|(\theta_*)_A\|_1 - \|(\theta_* + \Delta)_A\|_1 - \|\Delta_{A^c}\|_1 \leq \|\Delta_A\|_1 - \|\Delta_{A^c}\|_1,$$

to get

$$\begin{aligned} \|\Phi\Delta\|_2^2 &\leq n\lambda\|\Delta\|_1 + 2n\lambda(\|\theta_*\|_1 - \|\hat{\theta}\|_1) \leq n\lambda\|\Delta\|_1 + 2n\lambda(\|\Delta_A\|_1 - \|\Delta_{A^c}\|_1) \\ &\leq n\lambda(\|\Delta_A\|_1 + \|\Delta_{A^c}\|_1) + 2n\lambda(\|\Delta_A\|_1 - \|\Delta_{A^c}\|_1) = 3n\lambda\|\Delta_A\|_1 - n\lambda\|\Delta_{A^c}\|_1. \end{aligned}$$

This leads to $\|\Delta_{A^c}\|_1 \leq 3\|\Delta_A\|_1$ and the other desired inequality. ■

We can now add an extra assumption that will make the proof go through, namely that there exists $\kappa > 0$ such that

$$\frac{1}{n}\|\Phi\Delta\|_2^2 \geq \kappa\|\Delta_A\|_2^2 \tag{8.6}$$

for all Δ that satisfies the condition $\|\Delta_{A^c}\|_1 \leq 3\|\Delta_A\|_1$. This is called the “restrictive eigenvalue property” because if the smallest eigenvalue of $\frac{1}{n}\Phi^\top \Phi$ is greater than κ , the condition is satisfied (but this is only possible if $n \geq d$). The relevance of this assumption is discussed in Section 8.3.4.

This leads to the following proposition.

Proposition 8.4 (Lasso - fast rate) Assume $y = \Phi\theta_* + \varepsilon$, with $\varepsilon \in \mathbb{R}^n$ a vector with independent Gaussian components of zero mean and variance σ^2 . Let $\hat{\theta}$ be the minimizer of Eq. (8.4). Then, for $\lambda = \frac{2\sigma}{\sqrt{n}}\sqrt{2\|\widehat{\Sigma}\|_\infty}\sqrt{\log(2d) + \log\frac{1}{\delta}}$, we have, if Eq. (8.6) is satisfied, and with probability greater than $1 - \delta$:

$$\mathbb{E}\left[\frac{1}{n}\|\Phi(\hat{\theta} - \theta_*)\|_2^2\right] \leq \frac{72|A|\sigma^2}{n}\frac{\|\widehat{\Sigma}\|_\infty}{\kappa}\left(\log(2d) + \log\frac{1}{\delta}\right).$$

Proof (♦) We have, when λ is large enough, and by application of Lemma 8.5, and using Eq. (8.6):

$$\|\Delta_A\|_1 \leq |A|^{1/2} \|\Delta_A\|_2 \leq \frac{|A|^{1/2}}{\sqrt{n\kappa}} \|\Phi\Delta\|_2 \leq \frac{|A|^{1/2}}{\sqrt{n\kappa}} \sqrt{3n\lambda \|\Delta_A\|_1},$$

which leads to $\|\Delta_A\|_1 \leq \frac{3|A|\lambda}{\kappa}$. We then get $\frac{1}{n} \|\Phi\Delta\|_2^2 \leq \frac{9|A|\lambda^2}{\kappa}$, which leads to the desired result. ■

The dominant part of the rate is proportional to $\sigma^2 k \frac{\log d}{n}$, which is a fast rate but depends crucially on a very strong assumption.

Exercise 8.6 (♦♦) With the same assumptions as Prop. 8.4, with the choice of regularization parameter $\lambda = 4\sigma \sqrt{\frac{\log(dn)}{n}} \sqrt{\|\widehat{\Sigma}\|_\infty}$, show that $\mathbb{E} \left[\frac{1}{n} \|\Phi(\hat{\theta} - \theta_*)\|_2^2 \right] \leq \frac{144|A|\sigma^2 \|\widehat{\Sigma}\|_\infty \log(dn)}{\kappa} + \frac{24}{n} \sigma^2 + \frac{32}{dn^2} \|\theta_*\|_1 \sigma \sqrt{\frac{\log(dn)}{n}} \sqrt{\|\widehat{\Sigma}\|_\infty}$.

8.3.4 Zoo of conditions (♦♦)

Conditions to obtain fast rates are plentiful: they all assume that there is low correlation among predictors, which is rarely the case in practice (in particular, if there are two equal features, they are never satisfied).

Restricted eigenvalue property (REP). The most direct condition is the so-called restricted eigenvalue property (REP), which is exactly Eq. (8.6), with the supremum taken over the unknown set A of cardinality less than k :

$$\inf_{|A| \leq k} \inf_{\|\Delta_{A^c}\|_1 \leq 3\|\Delta_A\|_1} \frac{\|\Phi\Delta\|_2^2}{n\|\Delta_A\|_2^2} \geq \kappa > 0. \quad (8.7)$$

Mutual incoherence condition. A simpler one to check, but stronger, is the mutual incoherence condition:

$$\sup_{i \neq j} |\widehat{\Sigma}_{ij}| \leq \frac{\min_{j \in \{1, \dots, d\}} \widehat{\Sigma}_{jj}}{14k}, \quad (8.8)$$

which states that all cross-correlation coefficients are small (pure decorrelation would set them to zero).

This is weaker than the REP condition above. Indeed, by expanding, we have:

$$\begin{aligned} \|\Phi\Delta\|_2^2 &= \|\Phi_A \Delta_A + \Phi_{A^c} \Delta_{A^c}\|_2^2 = \|\Phi_A \Delta_A\|_2^2 + 2\Delta_A^\top \Phi_A^\top \Phi_{A^c} \Delta_{A^c} + \|\Phi_{A^c} \Delta_{A^c}\|_2^2 \\ &\geq \|\Phi_A \Delta_A\|_2^2 + 2\Delta_A^\top \Phi_A^\top \Phi_{A^c} \Delta_{A^c}. \end{aligned}$$

Moreover, we have:

$$\begin{aligned}\Delta_A^\top \widehat{\Sigma}_{AA} \Delta_A &= \Delta_A^\top \text{Diag}(\text{diag}(\widehat{\Sigma}_{AA})) \Delta_A + \Delta_A^\top (\widehat{\Sigma}_{AA} - \text{Diag}(\text{diag}(\widehat{\Sigma}_{AA}))) \Delta_A \\ &\geq \min_{j \in \{1, \dots, d\}} \widehat{\Sigma}_{jj} (\|\Delta_A\|_2^2 - \frac{1}{14k} \|\Delta_A\|_1^2),\end{aligned}$$

and

$$|\Delta_A^\top \Phi_A^\top \Phi_{A^c} \Delta_{A^c}| \leq \frac{\min_{j \in \{1, \dots, d\}} \widehat{\Sigma}_{jj}}{14k} \|\Delta_{A^c}\|_1 \|\Delta_A\|_1 \leq \frac{3 \min_{j \in \{1, \dots, d\}} \widehat{\Sigma}_{jj}}{14k} \|\Delta_A\|_1^2.$$

This leads to $\frac{1}{n} \|\Phi \Delta\|_2^2 \geq \min_{j \in \{1, \dots, d\}} \widehat{\Sigma}_{jj} \left(\|\Delta_A\|_2^2 - \frac{7}{14k} \|\Delta_A\|_1^2 \right) \geq \min_{j \in \{1, \dots, d\}} \widehat{\Sigma}_{jj} \left(\|\Delta_A\|_2^2 - \frac{7k}{14k} \|\Delta_A\|_2^2 \right) = \kappa \|\Delta_A\|_2^2$, with $\kappa = \min_{j \in \{1, \dots, d\}} \widehat{\Sigma}_{jj}/2$, thus leading to the REP condition in Eq. (8.7).

Restricted isometry property. One of the earlier conditions was the restricted isometry property: all eigenvalues of submatrices of $\widehat{\Sigma}$ of size less than $2k$, are between $1 - \delta$ and $1 + \delta$ for δ small enough. See [Giraud \(2014\)](#); [Wainwright \(2019\)](#) for details.

Gaussian designs (♦). It is not obvious that the conditions above are non-trivial (that is, there may exist no matrix with good sizes d and n for k large enough). For our results to be non-trivial, we need that $k \frac{\log d}{n}$ to be small but not too small. We show without proof in this paragraph that when sampling from Gaussian distributions, the assumptions above are satisfied. This is a first step towards a random design assumption.

Theorem 8.1 (Wainwright, 2019, Theorem 7.16) *If sampling $\varphi(x)$ from a Gaussian with mean zero and covariance matrix Σ , then with probability greater than $1 - \frac{e^{-n/32}}{1-e^{-n/32}}$, the REP property is satisfied with $\kappa = \frac{1}{16} \lambda_{\min}(\Sigma)$ as soon as $k \frac{\log d}{n} \leq \frac{1}{3200} \frac{\lambda_{\min}(\Sigma)}{\|\Sigma\|_\infty}$.*

The theorem above is hard to prove; the following exercise proposes to prove a weaker result, showing that the guarantees for the maximal cardinality k of the support have to be smaller.

Exercise 8.7 (♦♦♦) *If sampling $\varphi(x)$ from a Gaussian with mean zero and covariance matrix identity, then with large probability, for n greater than a constant times $k \frac{2 \log d}{n}$, the mutual incoherence property in Eq. (8.8) is satisfied.*

Model selection and irrepresentable condition (♦). Given that the Lasso aims at performing variable selection, it is natural to study its capacity to find the support of θ_* , that is, the set of non-zero variables. It turns out that it also depends on some conditions on the design matrix, which are stronger than the REP conditions, and called the “irrepresentable condition”, and also valid for Gaussian random matrices with similar scalings between n , d , and k . See [Giraud \(2014\)](#); [Wainwright \(2019\)](#) for details.



Algorithmic and theoretical tools are similar to “compressed sensing”, where the design matrix represents a set of measurements, which the user/theoretician can choose. In this context, sampling from i.i.d. Gaussians makes sense. For machine learning and statistics, the design matrix is the data and comes **as it is**, often with strong correlations.

8.3.5 Random design (♦)

In this section, we study the Lasso in the random design setting instead of the fixed design setting. For slow rates in $1/\sqrt{n}$, we can directly use Section 4.5.5 to get the exact same slow rate as for fixed design. In this section, we will only consider fast rates.

We now consider the well-specified Lasso case, where the expected risk is equal to $\mathcal{R}(\theta) = \frac{\sigma^2}{2} + \frac{1}{2}(\theta - \theta^*)^\top \Sigma(\theta - \theta^*)$. We assume that $\lambda_{\min}(\Sigma) \geq \mu \geq 0$, that is, the *expected* risk is μ -strongly convex (and not the empirical risk).

We assume that $y_i = \varphi(x_i)^\top \theta^* + \varepsilon_i$, and denote $\Phi \in \mathbb{R}^{n \times d}$ the design matrix, as well as $\varepsilon \in \mathbb{R}^n$ the vector of noises, which we assume independent and sub-Gaussian. Therefore we have

$$\hat{\mathcal{R}}(\theta) = \frac{1}{2n} \|\Phi(\theta - \theta^*) - \varepsilon\|_2^2 = \frac{1}{2}(\theta - \theta^*)^\top \hat{\Sigma}(\theta - \theta^*) - (\theta - \theta^*)^\top \left(\frac{1}{n} \Phi^\top \varepsilon \right) + \frac{1}{2n} \|\varepsilon\|_2^2, \quad (8.9)$$

where $\hat{\Sigma} = \frac{1}{n} \sum_{i=1}^n \varphi(x_i) \varphi(x_i)^\top = \frac{1}{n} \Phi^\top \Phi \in \mathbb{R}^{d \times d}$ is the empirical non-centered covariance matrix.

We will need that $\left\| \frac{1}{n} \Phi^\top \varepsilon \right\|_\infty = \left\| \frac{1}{n} \sum_{i=1}^n \varepsilon_i \varphi(x_i) \right\|_\infty$ is small enough, as well as $\|\hat{\Sigma} - \Sigma\|_\infty$. Assuming that ε is sub-Gaussian with constant σ^2 , and that $\|\varphi(x)\|_\infty \leq R$ almost surely, we get that, using results from Section 1.2.1,

$$\mathbb{P}\left(\left\| \frac{1}{n} \Phi^\top \varepsilon \right\|_\infty \geq \frac{\sigma R t}{\sqrt{n}}\right) \leq 2d \exp(-t^2/2) \text{ and } \mathbb{P}\left(\|\hat{\Sigma} - \Sigma\|_\infty \geq \frac{R^2 t}{\sqrt{n}}\right) \leq 2d(d+1)/2 \exp(-t^2/2).$$

Thus, the probability that at least one is satisfied is less than $d(d+3) \exp(-t^2/2) \leq 4d^2 \exp(-t^2/2)$.

We now assume that $\left\| \frac{1}{n} \Phi^\top \varepsilon \right\|_\infty \leq \frac{\sigma R t}{\sqrt{n}}$ and $\left\| \hat{\Sigma} - \Sigma \right\|_\infty \leq \frac{R^2 t}{\sqrt{n}}$, which happens with probability at least $1 - 4d^2 \exp(-t^2/2)$. From Lemma 8.5, we know that if $\lambda \geq 2 \left\| \frac{1}{n} \Phi^\top \varepsilon \right\|_\infty$, then we have, with $\hat{\Delta} = \hat{\theta}_\lambda - \theta^*$, and A the support of θ^* :

$$\|\hat{\Delta}_{A^c}\|_1 \leq 3\|\hat{\Delta}_A\|_1 \text{ and } \|\hat{\theta}_\lambda\|_1 \leq 3\|\theta^*\|_1.$$

Let $v = \mathcal{R}(\hat{\theta}_\lambda) - \mathcal{R}(\theta^*)$. We have:

$$\begin{aligned} v &\leq \mathcal{R}(\hat{\theta}_\lambda) - \mathcal{R}(\theta^*) - \hat{\mathcal{R}}_\lambda(\hat{\theta}_\lambda) + \hat{\mathcal{R}}_\lambda(\theta^*) \text{ since } \hat{\theta}_\lambda \text{ minimizes } \hat{\mathcal{R}}_\lambda, \\ &= \mathcal{R}(\hat{\theta}_\lambda) - \mathcal{R}(\theta^*) - \hat{\mathcal{R}}(\hat{\theta}_\lambda) + \hat{\mathcal{R}}(\theta^*) + \lambda\|\theta^*\|_1 - \lambda\|\hat{\theta}_\lambda\|_1 \text{ by definition of } \hat{\mathcal{R}}_\lambda, \\ &= \frac{1}{2} \hat{\Delta}^\top (H - \hat{H}) \hat{\Delta} + \hat{\Delta}^\top \left(\frac{1}{n} \Phi^\top \varepsilon \right) + \lambda\|\theta^*\|_1 - \lambda\|\hat{\theta}_\lambda\|_1 \text{ using Eq. (8.9)}, \\ &\leq \frac{1}{2} \left\| \hat{\Sigma} - \Sigma \right\|_\infty \cdot \|\hat{\Delta}\|_1^2 + \left\| \frac{1}{n} \Phi^\top \varepsilon \right\|_\infty \cdot \|\hat{\Delta}\|_1 + \lambda\|\hat{\Delta}\|_1 \text{ using norm inequalities}, \\ &\leq \frac{\sigma R t}{\sqrt{n}} \cdot \|\hat{\Delta}\|_1 + \frac{R^2 t}{2\sqrt{n}} \cdot \|\hat{\Delta}\|_1^2 + \lambda\|\hat{\Delta}\|_1 \text{ using our assumptions}. \end{aligned}$$

Moreover, we have, since $\lambda_{\min}(\Sigma) \geq \mu$, $v = \mathcal{R}(\hat{\theta}_\lambda) - \mathcal{R}(\theta^*) \geq \frac{\mu}{2} \|\hat{\Delta}\|_2^2 \geq \frac{\mu}{2|A|} \|\hat{\Delta}_A\|_1^2$, leading to $\|\hat{\Delta}\|_1 \leq 4\|\hat{\Delta}_A\|_1 \leq 4\sqrt{\frac{2|A|v}{\mu}}$. We also have $\|\hat{\Delta}\|_1 \leq \|\theta^*\|_1 + \|\hat{\theta}_\lambda\|_1 \leq \|\theta^*\|_1 + 3\|\theta^*\|_1 \leq 4\|\theta^*\|_1$. We thus get, with $\lambda = \frac{2\sigma R t}{\sqrt{n}}$, two inequalities:

$$v \leq \frac{3\sigma R t}{\sqrt{n}} \cdot \|\hat{\Delta}\|_1 + \frac{R^2 t}{2\sqrt{n}} \cdot \|\hat{\Delta}\|_1^2 \text{ and } \|\hat{\Delta}\|_1 \leq 4\sqrt{\frac{2|A|v}{\mu}}. \quad (8.10)$$

If $1 \geq \frac{32R^2 t}{\sqrt{n}} \frac{|A|}{\mu}$, then the last term in the first inequality in Eq. (8.10) is less than $\frac{v}{2}$, and we get $\frac{v}{2} \leq \frac{3\sigma R t}{\sqrt{n}} 4\sqrt{\frac{2|A|v}{\mu}}$, that is, $\sqrt{v} \leq \frac{24\sigma R t}{\sqrt{n}} \sqrt{\frac{2|A|}{\mu}}$. This leads to, with $\lambda = \frac{2\sigma R}{\sqrt{n}} t = \frac{2\sigma R}{\sqrt{n}} \sqrt{2 \log \frac{4d^2}{\delta}}$, with probability greater than $1 - \delta$,

$$\mathcal{R}(\hat{\theta}_\lambda) - \mathcal{R}(\theta^*) \leq 2304 \cdot \frac{R^2}{\mu} \frac{\sigma^2 |A|}{n} \log \frac{4d^2}{\delta}.$$

Exercise 8.8 With the notations above, show that if $\mu = 0$, from Eq. (8.10) we can recover the slow rate $\mathcal{R}(\hat{\theta}_\lambda) - \mathcal{R}(\theta^*) \leq \frac{4R\|\theta^*\|_1}{\sqrt{n}} (3\sigma + 2R\|\theta^*\|_1) \sqrt{2 \log \frac{4d^2}{\delta}}$.

8.4 Experiments

In this section, we perform a simple experiment on Gaussian design matrices, where all entries in $\Phi \in \mathbb{R}^{n \times d}$ are sampled independently from a standard Gaussian distribution, with

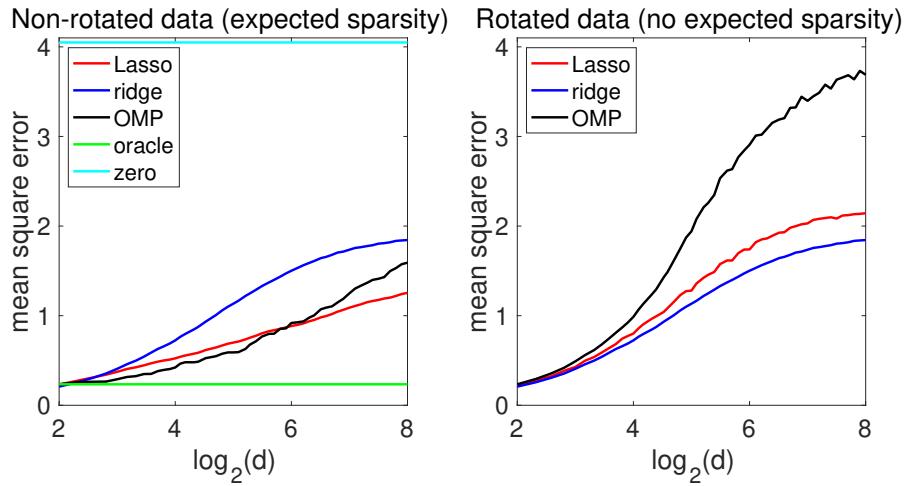


Figure 8.2: Comparison of estimators on least-squares regression: problem with sparse optimal predictor (left), and non-sparse optimal predictor (right).

$n = 64$, and varying d . Then θ_* is taken to be zero except on $k = 4$ components where it is randomly equal to -1 or 1 . We consider $\sigma = \sqrt{k}$ (to have a constant signal-to-noise ratio when k varies). We perform 128 replications. For each method and each value of its hyperparameter, we averaged the test risk over the 128 replications and reported the minimum value (with respect to the hyperparameter). We compare the following three methods in Figure 8.2:

- Ridge regression: penalty by $\lambda\|\theta\|_2^2$.
- Lasso regression: penalty by $\lambda\|\theta\|_1$.
- Orthogonal matching pursuit (greedy forward method), with hyperparameter k (the number of included variables).

We compare two situations: (1) non-rotated data (exactly the model above), and (2) rotated data, where we replace Φ by ΦR and θ_* by $R^\top \theta_*$, where R is a random rotation matrix. For the rotated data, we do not expect sparse solutions, and hence sparse methods are not expected to work better than ridge regression (and OMP performs significantly worse because once the support is chosen, there is no regularization). Note that the two curves for ridge regression are exactly the same (as expected from rotation invariance of the ℓ_2 -norm). The oracle performance corresponds to the estimator where the true support is given.



Sparse methods make assumptions regarding the best predictor. Like all assumptions, when this assumed prior knowledge is not correct, the method does not perform better.

8.5 Extensions

Sparse methods are more general than the ℓ_1 -norm and can be extended in several ways:

- **Group penalties:** in many cases, $\{1, \dots, d\}$ is partitioned into m subsets A_1, \dots, A_m , and the goal is to consider “group sparsity,” that is, if we select one variable within a group A_j , the entire group should be selected. Such behavior can be obtained using the penalty $\sum_{i=1}^m \|\theta_{A_i}\|_2$ or $\sum_{i=1}^m \|\theta_{A_i}\|_\infty$. This is particularly used when the output y is multi-dimensional (such as in multivariate regression or multi-category classification) to select variables relevant to all outputs. See, e.g., [Giraud \(2014\)](#) for details.

Exercise 8.9 Assuming that the design matrix Φ is orthogonal, compute the minimizer of $\frac{1}{2n}\|y - \Phi\theta\|_2^2 + \lambda \sum_{i=1}^m \|\theta_{A_i}\|_2$.

- **Structured sparsity:** it is also possible to favor other specific patterns for the selected variables, such as blocks, trees, etc., when such prior knowledge is needed. See [Bach et al. \(2012b\)](#) for details.

Exercise 8.10 We consider the d (overlapping) sets $A_i = \{1, \dots, i\}$, and the norm $\sum_{i=1}^d \|\theta_{A_i}\|_2$. Show that penalization with this norm will tend to select patterns of non-zeros of the form $\{i+1, \dots, d\}$.

- **Nuclear norm:** when learning on matrices, a natural form of sparsity is for a matrix to have a low rank. This can be achieved by penalizing by the sum of singular values of a matrix, which is a norm called the nuclear norm or the trace norm. See [Bach \(2008\)](#) and references therein.

Exercise 8.11 Compute the minimizer of $\frac{1}{2n}\|Y - \Theta\|_F^2 + \lambda\|\Theta\|_*$, where $\|M\|_F$ is the Frobenius norm and $\|M\|_*$ the nuclear norm.

- **Multiple kernel learning:** the group penalty can be extended when the groups have an infinite dimension and ℓ_2 -norms are replaced by RKHS norms defined in Chapter 7. This becomes a tool for learning the kernel matrix from data. See [Bach et al. \(2012a\)](#) for details.
- **Elastic net:** often, when both effects of the ℓ_1 -norm (sparsity) and the squared ℓ_2 -norm (strong-convexity) are desired, we can sum the two, which is referred to as the “elastic net” penalty. This leads to a strongly-convex optimization problem which is numerically better behaved.

- **Concave penalization and debiasing:** to obtain a sparsity-inducing effect, the penalty in the ℓ_1 -norm has to be quite large, such as in $1/\sqrt{n}$, which often creates a strong bias in the estimation once the support is selected. There are several ways of debiasing the Lasso, an elegant one being to use a “concave” penalty. That is, we use $\sum_{i=1}^d a(|\theta_i|)$ where a is a concave increasing function on \mathbb{R}^+ , such as $a(u) = u^\alpha$ for $\alpha \in (0, 1)$. This leads to a non-convex optimization problem, where iterative weighted ℓ_1 -minimization provides natural algorithms (see [Mairal et al., 2014](#), and references therein).

Chapter 9

Neural networks

Chapter summary

Neural networks are flexible models for non-linear predictions. They can be studied in terms of the three errors usually related to empirical risk minimization: optimization, estimation, and approximation errors. In this chapter, we focus on single hidden layer neural networks, which are linear combinations of simple affine functions with additional non-linearities.

- Optimization error: as the prediction functions are non-linearly dependent on their parameters, we obtain non-convex optimization problems, with only guaranteed convergence to stationary points.
- Estimation error: the number of parameters is not the driver of the estimation error, as the norms of the various weights play an important role, with explicit rates in $O(1/\sqrt{n})$ obtained from Rademacher complexity tools.
- Approximation error: for the “ReLU” activation function, the universal approximation properties can be characterized and are superior to kernel methods because they are adaptive to linear latent variables.

9.1 Introduction

In supervised learning, the main focus has been on methods to learn from n observations $(x_i, y_i), i = 1, \dots, n$, with $x_i \in \mathcal{X}$ (input space) and $y_i \in \mathcal{Y}$ (output/label space). As presented in Chapter 4, a large class of methods relies on minimizing a regularized empirical risk with

respect to a function $f : \mathcal{X} \rightarrow \mathbb{R}$ where the following cost function is minimized:

$$\frac{1}{n} \sum_{i=1}^n \ell(y_i, f(x_i)) + \Omega(f),$$

where $\ell : \mathcal{Y} \times \mathbb{R} \rightarrow \mathbb{R}$ is a loss function, and $\Omega(f)$ is a regularization term. Typical examples were:

- **Regression:** $\mathcal{Y} = \mathbb{R}$ and $\ell(y_i, f(x_i)) = \frac{1}{2}(y_i - f(x_i))^2$.
- **Classification:** $\mathcal{Y} = \{-1, 1\}$ and $\ell(y_i, f(x_i)) = \Phi(y_i f(x_i))$ where Φ is convex, e.g., $\Phi(u) = \max\{1 - u, 0\}$ (hinge loss leading to the support vector machine) or $\Phi(u) = \log(1 + \exp(-u))$ (leading to logistic regression). See more examples in Section 4.1.1.

The class of prediction functions we have considered so far were (with their “pros” and “cons”):

- **Linear functions in some explicit features:** given a feature map $\varphi : \mathcal{X} \rightarrow \mathbb{R}^d$, we consider $f(x) = \theta^\top \varphi(x)$, with parameters $\theta \in \mathbb{R}^d$, as analyzed in Chapter 3 (for least-squares) and Chapter 4.

() *Pros:* Simple to implement, as this leads to convex optimization with gradient descent algorithms, with running time complexity in $O(nd)$, as shown in Chapter 5, and theoretical guarantees which are not necessarily scaling badly with dimension d if regularizers are used (ℓ_2 or ℓ_1).

() *Cons:* Only applies to linear functions on explicit (and fixed feature spaces), so they can underfit the data.

- **Linear functions in some implicit features through kernel methods:** the feature map can have arbitrarily large dimension, that is, $\varphi(x) \in \mathcal{H}$ where \mathcal{H} is a Hilbert space, accessed through a kernel $k(x, x') = \langle \varphi(x), \varphi(x') \rangle_{\mathcal{H}}$, as presented in Chapter 7.

() *Pros:* Non-linear flexible predictions, simple to implement, as convex optimization algorithms with strong guarantees can be used. Provides adaptivity to the regularity of the target function, allowing higher-dimensional applications than local averaging methods from Chapter 6.

() *Cons:* Running-time complexity up to $O(n^2)$ with algorithms from Section 7.4 (but this scaling can be improved with appropriate techniques also discussed in the same section, such as column sampling). The method may still suffer from the curse of dimensionality for non-smooth enough target functions.

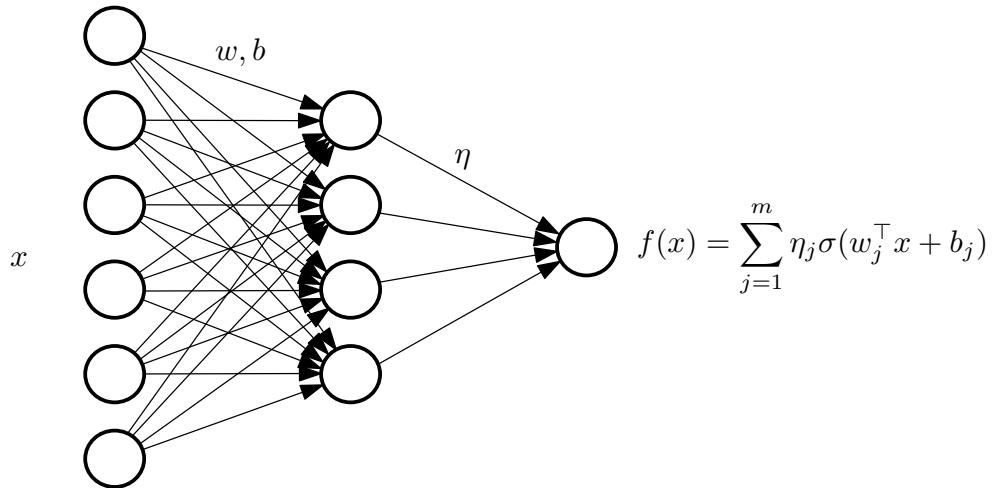
This chapter aims to explore another class of functions for non-linear predictions, namely neural networks, that come with additional benefits, such as more “adaptivity to linear latent variables”, but comes with some potential drawbacks, such as a harder optimization problem.

9.2 Single hidden layer neural network

We consider $\mathcal{X} = \mathbb{R}^d$ and the set of prediction functions that can be written as

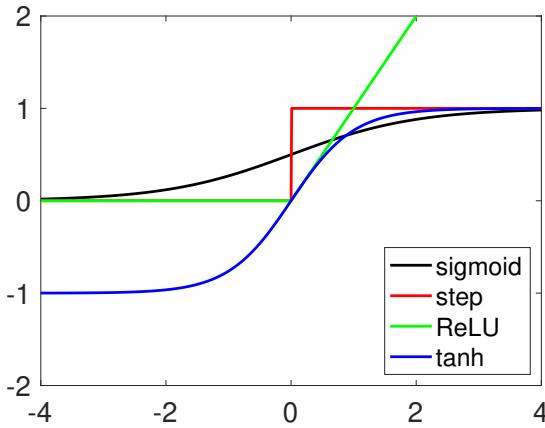
$$f(x) = \sum_{j=1}^m \eta_j \sigma(w_j^\top x + b_j), \quad (9.1)$$

where $w_j \in \mathbb{R}^d$, $b_j \in \mathbb{R}$ and $\eta_j \in \mathbb{R}$, $j = 1, \dots, m$, and σ is an “activation function”. This is often represented as a graph (see below). The same architecture can also be considered with $\eta_j \in \mathbb{R}^k$, for $k > 1$ to deal with multi-category classification.



The activation function is typically chosen from one of the following examples (see plot below):

- sigmoid $\sigma(u) = \frac{1}{1+e^{-u}}$,
- step function $\sigma(u) = 1_{u>0}$,
- “rectified linear unit” (ReLU) $\sigma(u) = (u)_+ = \max\{u, 0\}$, which will be the main focus of this chapter.
- hyperbolic tangent $\sigma(u) = \tanh(u) = \frac{e^u - e^{-u}}{e^u + e^{-u}}$.



The function f is defined as the linear combination of m functions $x \mapsto \sigma(w_j^\top x + b_j)$, which are the “hidden neurons”.

 The constant terms b_j are sometimes referred to as “biases”, which is unfortunate in a statistical context, as it already has a precise meaning within the bias/variance trade-off (see Chapter 3).

 Do not get confused by the name “neural network” and its biological inspiration. This inspiration is not a proper justification for its behavior on machine learning problems.

Cross-entropy loss and sigmoid activation function for the last layer. Following standard practice, we are not adding a non-linearity to the last layer; note that if we were to use an additional sigmoid activation and consider the cross-entropy loss for binary classification, we would exactly be using the logistic loss on the output without an extra activation function.

Indeed, if we consider $g(x) = \frac{1}{1+\exp(-f(x))} \in [0, 1]$, and given an output variable $y \in \{-1, 1\}$, the so-called “cross-entropy loss”, an instance of maximum likelihood (see more details in Chapter 14), is equal to $-\frac{1+y}{2} \log g(x) - \frac{1-y}{2} \log(1 - g(x))$. It can be rewritten as $\log(1 + \exp(-yf(x)))$, which is exactly the logistic loss defined in Section 4.1.1, applied to $f(x)$.

Theoretical analysis of neural networks. As with any method based on empirical risk minimization, we have to study the three classical aspects: (1) optimization (convergence properties of algorithms for minimizing the risk), (2) estimation error (effect of having a

finite amount of data on the prediction performance), and (3) approximation error (effect of having a finite number of parameters or a constraint on the norm of these parameters).

9.2.1 Optimization

To find parameters $\theta = \{(\eta_j), (w_j), (b_j)\} \in \mathbb{R}^{m(d+2)}$, empirical risk minimization can be applied, and the following optimization problem has to be solved:

$$\min_{\theta \in \mathbb{R}^{m(d+2)}} \frac{1}{n} \sum_{i=1}^n \ell\left(y_i, \sum_{j=1}^m \eta_j \sigma(w_j^\top x_i + b_j)\right),$$

with potentially additional regularization (often squared ℓ_2 -norm of all weights).

! Note that (as discussed in Chapter 5) the true objective is to perform well on unseen data, and the optimization problem above is just a mean to an end.

This is a non-convex optimization problem where the gradient descent algorithms from Chapter 5 can be applied without guarantees (see below for recent results on providing some qualitative global convergence guarantees when m is large).

While stochastic gradient descent remains an algorithm of choice (with also a good generalization behavior as discussed in Section 5.4), several algorithmic improvements have been observed to lead to better stability and performance: specific step-size decay schedules, preconditioning (Duchi et al., 2011), momentum (Kingma and Ba, 2014), batch-normalization (Ioffe and Szegedy, 2015), etc. But overall, the objective function is non-convex, and it remains challenging to understand precisely why gradient-based methods perform well in practice, particularly for deeper networks (some elements are presented below). See also boosting procedures in Section 10.3 and Chapter 11.

See <https://playground.tensorflow.org/> for a nice interactive illustration.

Global convergence of gradient descent for infinite widths (\blacklozenge). It turns out that global convergence can be shown for this non-convex optimization problem (Chizat and Bach, 2018; Bach and Chizat, 2022), with tools that go beyond the scope of this book and which are partially described in Chapter 11.¹

We simply show some experimental evidence below for a simple one-dimensional set-up, where we compare several runs of stochastic gradient descent (SGD) where observations are only seen once (so no overfitting is possible) and with random initializations, on a regression problem with deterministic outputs, thus with the optimal testing error (the Bayes rate)

¹See also <https://francisbach.com/gradient-descent-neural-networks-global-convergence/> for more details.

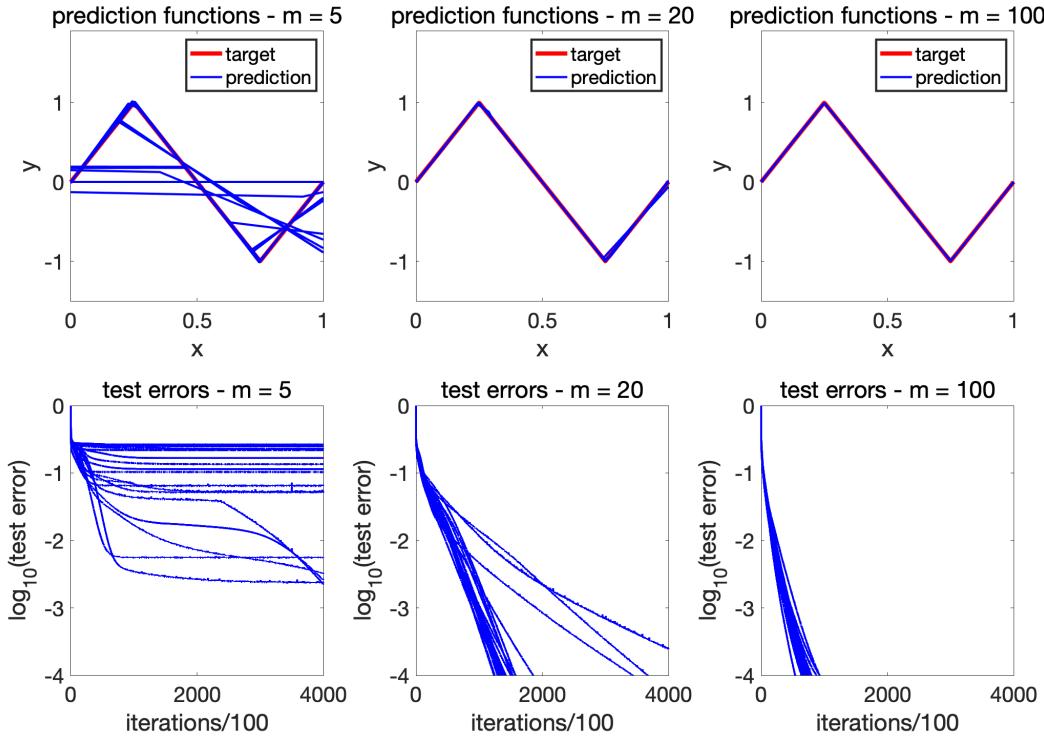


Figure 9.1: Comparison of optimization behavior for different numbers m of neurons, for ReLU activations (left: $m = 5$, middle: $m = 20$, and right: $m = 100$). Top: examples of final prediction functions at convergence, bottom: plot of test errors vs. number of iterations.

being equal to zero. We show in Figure 9.1 the estimated predictors and the corresponding testing errors with 20 different initializations. We see that when $m = 5$ (which is sufficient to attain zero testing errors), small errors are never achieved. With $m = 20$ neurons, SGD finds the optimal predictor for most restarts. When $m = 100$, all restarts have the desired behaviors, highlighting the benefits of over-parameterization.

9.2.2 Rectified linear units and homogeneity

From now on, we will mostly focus on the rectified linear unit $\sigma(u) = u_+$. The main property we will leverage is its “homogeneity”, that is, for $\alpha > 0$, $(\alpha u)_+ = \alpha u_+$. This implies that in the definition of the prediction function as the sum of terms $\eta_j(w_j^\top x + b_j)_+$, we can freely multiply η_j by a positive scalar α_j and divide (w_j, b_j) by the same α_j , without changing the prediction function.

This has a particular effect when using a squared ℓ_2 -regularizer on all weights, which is standard, either explicitly (by adding a penalty to the cost function) or implicitly (see

Section 11.1). Indeed, we consider penalizing $\eta_j^2 + \|w_j\|_2^2 + b_j^2/R^2$ for each $j \in \{1, \dots, m\}$, where we have added the factor R^2 on the constant term for homogeneity reasons (R will be a bound on the ℓ_2 -norm of input data). Thus, optimizing with respect to the scaling factor α_j above (which impacts only the regularizer), we have to minimize $\alpha_j^2 \eta_j^2 + \frac{\|w_j\|_2^2 + b_j^2/R^2}{\alpha_j^2}$, with $\alpha_j^2 = \frac{(\|w_j\|_2^2 + b_j^2/R^2)^{1/2}}{|\eta_j|}$ as a minimizer, and with the optimal value of the penalty equal to $2|\eta_j|(\|w_j\|_2^2 + b_j^2/R^2)^{1/2}$.

For the theoretical analysis, we can thus choose to normalize each (w_j, b_j) to have unit norm $\|w_j\|_2^2 + b_j^2/R^2 = 1$, and use the penalty $|\eta_j|$ for each $j \in \{1, \dots, m\}$, and thus use an overall ℓ_1 -norm penalty on η , that is, $\|\eta\|_1$. We now focus on this choice of regularization in the following sections.

9.2.3 Estimation error

To study the estimation error, we will consider that the parameters of the network are constrained, that is, $\|w_j\|_2^2 + b_j^2/R^2 \leq 1$ for each $j \in \{1, \dots, m\}$, and $\|\eta\|_1 \leq D$. This defines a set Θ of allowed parameters. Note that we use $\|w_j\|_2^2 + b_j^2/R^2 \leq 1$ instead of $\|w_j\|_2^2 + b_j^2/R^2 = 1$ (as suggested above) as it does not impact the bound on estimation error.

We can then compute the Rademacher complexity of the associated class \mathcal{F} of functions we just defined, using tools from Chapter 4 (Section 4.5). We assume that almost surely, $\|x\|_2 \leq R$, that is, the input data are bounded in ℓ_2 -norm by R .

Following the developments of Section 4.5, we denote $\mathcal{G} = \{(x, y) \mapsto \ell(y, f(x)), f \in \mathcal{F}\}$, the set of loss functions for a prediction function $f \in \mathcal{F}$ (which is here the set of neural network models f_θ with parameters θ such that $\theta \in \Theta$). Note that following Section 4.5.3, we consider a constraint on $\|\eta\|_1$, but that we could also penalize, which is closer to practice and can be tackled with tools from Section 4.5.5.

We have, by definition of the Rademacher complexity $R_n(\mathcal{G})$ of \mathcal{G} , and taking expectations with respect to the data (x_i, y_i) , $i = 1, \dots, n$ (which are assumed i.i.d.) and the independent Rademacher random variables $\varepsilon_i \in \{-1, 1\}$, $i = 1, \dots, n$:

$$R_n(\mathcal{G}) = \mathbb{E} \left[\sup_{\theta \in \Theta} \frac{1}{n} \sum_{i=1}^n \varepsilon_i \ell(y_i, f_\theta(x_i)) \right].$$

This quantity is known to provide an upper-bound on the expected risk (e.g., testing error) $\mathcal{R}(\hat{f})$ of the minimizer $\hat{f} \in \mathcal{F}$ of the empirical risk, through the estimation error, as (using symmetrization from Prop. 4.2 and Eq. (4.8) from Section 4.4):

$$\mathbb{E} \left[\mathcal{R}(\hat{f}) - \inf_{f \in \mathcal{F}} \mathcal{R}(f) \right] \leq 4R_n(\mathcal{G}).$$

We can now use properties of Rademacher complexities presented in Section 4.5, particularly their nice handling of non-linearities. Assuming the loss is almost surely G -Lipschitz-continuous with respect to the second variable, using Proposition 4.3 from Chapter 4 that allows getting rid of the loss, we get the bound:

$$R_n(\mathcal{G}) \leq G \mathbb{E} \left[\sup_{\theta \in \Theta} \frac{1}{n} \sum_{i=1}^n \varepsilon_i f_\theta(x_i) \right] = G \mathbb{E} \left[\sup_{\theta \in \Theta} \frac{1}{n} \sum_{i=1}^n \sum_{j=1}^m \eta_j \varepsilon_i \sigma(w_j^\top x_i + b_j) \right].$$

Using the ℓ_1 -constraint on η and using $\sup_{\|\eta\|_1 \leq D} z^\top \eta = D \|z\|_\infty$, we can directly maximize with respect to η , leading to (note that another ℓ_p -constraint on η , with $p \neq 1$, would be harder to deal with):

$$R_n(\mathcal{G}) \leq G \mathbb{E} \left[\sup_{j \in \{1, \dots, m\}} \sup_{\|w_j\|_2^2 + b_j^2 / R^2 \leq 1} D \left| \frac{1}{n} \sum_{i=1}^n \varepsilon_i \sigma(w_j^\top x_i + b_j) \right| \right].$$

Since the ReLU activation function σ is 1-Lipschitz continuous and satisfies $\sigma(0) = 0$, we get, this time using the extension of Proposition 4.3 from Chapter 4 to Rademacher complexities defined with an absolute value (that is, Prop. 4.4):

$$R_n(\mathcal{G}) \leq 2GD \mathbb{E} \left[\sup_{j \in \{1, \dots, m\}} \sup_{\|w_j\|_2^2 + b_j^2 / R^2 \leq 1} \left| w_j^\top \left(\frac{1}{n} \sum_{i=1}^n \varepsilon_i x_i \right) + b_j \left(\frac{1}{n} \sum_{i=1}^n \varepsilon_i \right) \right| \right].$$

We can now perform the optimization with respect to (w_j, b_j) in closed form, with the same value for all $j \in \{1, \dots, m\}$, leading to:

$$R_n(\mathcal{G}) \leq 2GD \mathbb{E} \left[\left(\left(\frac{1}{n} \sum_{i=1}^n \varepsilon_i x_i \right)^2 + R^2 \left(\frac{1}{n} \sum_{i=1}^n \varepsilon_i \right)^2 \right)^{1/2} \right].$$

We thus get, using Jensen's inequality (here of the form $\mathbb{E}[Z] \leq \sqrt{\mathbb{E}[Z^2]}$), as well as the independence, zero mean, and unit variance of $\varepsilon_1, \dots, \varepsilon_n$:

$$\begin{aligned} R_n(\mathcal{G}) &\leq 2GD \left(\mathbb{E} \left[\left(\frac{1}{n} \sum_{i=1}^n \varepsilon_i x_i \right)^2 + R^2 \left(\frac{1}{n} \sum_{i=1}^n \varepsilon_i \right)^2 \right] \right)^{1/2} \\ &= 2GD \left(\frac{1}{n} \mathbb{E}[\|x\|_2^2] + \frac{R^2}{n} \right)^{1/2} \leq \frac{2GDR\sqrt{2}}{\sqrt{n}}. \end{aligned}$$

Thus, we get the following proposition, with a bound proportional to $1/\sqrt{n}$ with no explicit dependence in the number of parameters.

Proposition 9.1 *Let \mathcal{F} be the class of functions $(y, x) \mapsto \ell(y, f(x))$ where f is a neural network defined in Eq. (9.1), with the constraint that $\|\eta\|_1 \leq D$, $\|w_j\|_2^2 + b_j^2 / R^2 \leq 1$ for all*

$j \in \{1, \dots, m\}$. If the loss function is G -Lipschitz-continuous and the activation function σ is the ReLU, the Rademacher complexity is upper bounded as

$$R_n(\mathcal{G}) \leq \frac{4GDR}{\sqrt{n}}.$$

The proposition above allows bounding the estimation error for neural networks, as the maximal deviation between expected risk and empirical risk over all potential networks with bounded parameters is bounded in expectation by four times the Rademacher complexity above.

This will be combined with a study of the approximation properties in Section 9.3, with a summary in Section 9.3.7.



The number of parameters is irrelevant!!!!!!
What counts is the overall norm of the weights.

We will see in Chapter 11 some recent results showing how optimization algorithms add an implicit regularization that leads to provable generalization in over-parameterized neural networks (that is, networks with many hidden units).

Exercise 9.1 (♦) Provide the bound for the constraint $\|w_j\|_1 + |b_j|/R \leq 1$, where R denotes the supremum of $\|x\|_\infty$ over all x in the support of its distribution.

Before moving on to approximation properties of neural networks, we note that the reasoning above to compute the Rademacher complexity can be extended by recursion to deeper networks, as the following exercise shows (see, e.g., Neyshabur et al., 2015, for further results).

Exercise 9.2 (♦) We consider a 1-Lipschitz-continuous activation function σ such that $\sigma(0) = 0$, and the classes of functions defined recursively as $\mathcal{F}_0 = \{x \mapsto \theta^\top x, \|\theta\|_2 \leq D_0\}$, and, for $i = 1, \dots, M$, $\mathcal{F}_i = \{x \mapsto \sum_{j=1}^{m_i} \theta_j \sigma(f_j(x)), f_j \in \mathcal{F}_{i-1}, \|\theta\|_1 \leq D_i\}$, corresponding to a neural network with M layers. Assuming that $\|x\|_2 \leq R$ almost surely, show by recursion that the Rademacher complexity satisfies $R_n(\mathcal{F}_M) \leq 2^M \frac{R}{\sqrt{n}} \prod_{i=0}^M D_i$.

9.3 Approximation properties

As seen above, the estimation error for constrained output weights grows as $\frac{\|\eta\|_1}{\sqrt{n}}$ where η is the vector of output weights and is independent of the number m of neurons. Three important questions will be tackled in the following sections:

- Can we approximate any prediction function with a sufficiently large number of neurons?
- What is the associated approximation error so that we can derive generalization bounds? How can we use the control of the ℓ_1 -norm $\|\eta\|_1$, particularly when the number of neurons m is allowed to tend to infinity?
- What is the number of neurons required to reach such a behavior?

For this, we need to understand the space of functions that neural networks span and how they relate to the smoothness properties of the function (like we did for kernel methods in Chapter 7).

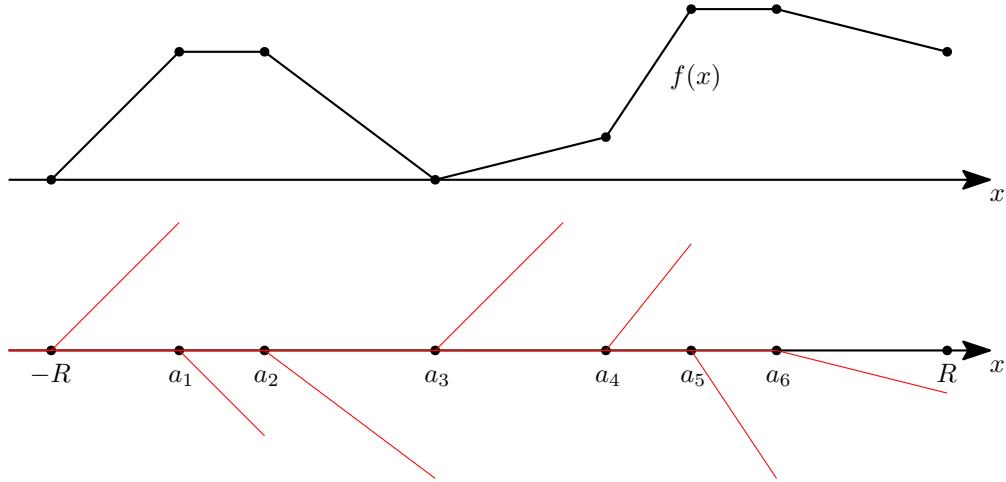
In this section, like in the previous section, we focus primarily on the ReLU activation function, noting that universal approximation results exist as soon as σ is not a polynomial (Leshno et al., 1993). We start with a simple non-quantitative argument to show universality in one dimension (and then in all dimensions) before formalizing the function space obtained by letting the number of neurons go to infinity.

9.3.1 Universal approximation property in one dimension

We start with simple non-quantitative arguments.

Approximation of piecewise affine functions. Since each function $x \mapsto \eta_j(w_j x + b_j)_+$ is piecewise affine, the output of a neural network has to be piecewise affine. It turns out that all piecewise affine functions with $m - 2$ kinks in the open interval $(-R, R)$ can be represented by m neurons on $[-R, R]$.

Indeed, as illustrated below with $m = 8$, if we assume that the function f is such that $f(-R) = 0$, with kinks $a_1 < \dots < a_{m-2}$ on $(-R, R)$, we can approximate it on $[-R, a_1]$ by the function $v_1(x + R)_+$ where v_1 is the slope of f on $[-R, a_1]$. The approximation is tight on $[-R, a_1]$. To have a tight approximation on $[a_1, a_2]$ without perturbing the approximation on $[-R, a_1]$, we can add to the approximation $v_2(x - a_1)_+$ where v_2 is exactly what is needed to compensate the change in slope of f . By pursuing the reasoning, we can represent the function on $[-R, R]$ exactly with $m - 1$ neurons.



To remove the constraint that $f(-R) = 0$, we can simply notice that $\frac{1}{2R}(x + R)_+$ + $\frac{1}{2R}(-x + R)_+$ is equal to 1 on $[-R, R]$. Thus with one additional neuron (only one since $(x + R)_+$ has already been used), we can represent any piecewise-affine function with $m - 2$ kinks with m neurons.

Universal approximation properties. Now that we can represent exactly all piecewise affine functions on $[-R, R]$, we can use classical approximation theorems for functions on $[-R, R]$. They come in different flavors depending on the norm we use to characterize the approximation. For example, continuous functions can be approximated by piecewise affine functions with arbitrary precision in L_∞ -norm (defined as the maximal value of $|f(x)|$ for $x \in [-R, R]$) by simply taking the piecewise interpolant from a grid (see quantitative arguments in Section 9.3.3). With a weaker criterion such as the L_2 -norm (with respect to the Lebesgue measure), we can approximate any function in L_2 (see, e.g., Rudin, 1987). This can be extended to any dimension d by using the Fourier transform representation as $f(x) = \frac{1}{(2\pi)^d} \int_{\mathbb{R}^d} \hat{f}(\omega) e^{i\omega^\top x} d\omega$ and approximating the one-dimensional functions sine and cosine as linear superpositions of ReLU's. See a more formal quantitative argument in Section 9.3.4.

To obtain precise bounds in all dimensions, in terms of the number of kinks or the ℓ_1 -norm of output weights, we first need to define the limit when the number of neurons is allowed to be unbounded.

9.3.2 Infinitely many neurons and variation norm

In this section, we consider neural networks of the form $f(x) = \sum_{j=1}^m \eta_j \sigma(w_j^\top x + b_j)$, where the input weights are constrained, that is, $(w_j, b_j/R) \in K$, for K a compact subset of \mathbb{R}^{d+1} , such as the unit ℓ_2 -sphere. We will primarily consider the ReLU activation σ in subsequent

sections, but this is not needed in this section (where boundedness or Lipschitz-continuity are sufficient).

In this section, for a function $f : \mathcal{X} \rightarrow \mathbb{R}$, where \mathcal{X} is the ℓ_2 -ball of radius R and center 0 in \mathbb{R}^d , we want to study the limit when $m \rightarrow \infty$, of the smallest ℓ_1 -norm of η for f representable with m neurons and output weights η , that is,

$$\gamma_1^{(m)}(f) = \inf_{\eta_j, (w_j, b_j) \in K, \forall j \in \{1, \dots, m\}} \|\eta\|_1 \text{ such that } \forall x \in \mathcal{X}, f(x) = \sum_{j=1}^m \eta_j \sigma(w_j^\top x + b_j).$$

The index 1 in $\gamma_1^{(m)}$ will become natural when we compare with kernels in Section 9.4. When f is not representable by m neurons, we let $\gamma_1^{(m)}(f) = +\infty$. By construction the sequence $\gamma_1^{(m)}(f)$ is non-increasing in m , and non-negative. Thus it has a limit when m tends to ∞ , which we denote $\gamma_1(f)$, which is infinite when f cannot be represented by a neural network with finitely many neurons. The function γ_1 is positively homogeneous, that is $\gamma_1(\lambda f) = \lambda \gamma_1(f)$ when $\lambda > 0$ and sub-additive, that is, $\gamma_1(f+g) \leq \gamma_1(f) + \gamma_1(g)$. Moreover, one can show that $\gamma_1(f) = 0$ implies that $f = 0$ (proofs left as an exercise). Thus, γ_1 is a norm on the set of functions $f : \mathcal{X} \rightarrow \mathbb{R}$ such that $\gamma_1(f) < +\infty$. It is possible to “complete” this space by adding limits of functions such that their γ_1 -norm remains bounded. We obtain a Banach space \mathcal{F}_1 of functions, with a norm γ_1 , which is often referred to as the “variation norm” (Kurková and Sanguineti, 2001). This characterizes the set of functions that can be represented by neural networks with bounded ℓ_1 -norm of output weights, regardless of the number of neurons.

Formulation through measures. We can write $f(x) = \sum_{j=1}^m \eta_j \sigma(w_j^\top x + b_j)$, as $f(x) = \int_K (w^\top x + b)_+ d\nu(w, b)$, for ν the measure $\nu = \sum_{j=1}^m \eta_j \delta_{(w_j, b_j)}$ where $\delta_{(w_j, b_j)}$ is the Dirac measure at (w_j, b_j) . Then, the penalty can be written as $\|\eta\|_1 = \int_K |d\nu(w, b)|$, which is the “total variation” of ν . We can therefore see $\gamma_1(f)$ as the infimum of all $\int_K |d\nu(w, b)|$ such that $\forall x \in \mathcal{X}, f(x) = \int_K (w^\top x + b)_+ d\nu(w, b)$, and ν is supported on a countable set. By a density argument (every measure is the “weak” limit of empirical measures), we can remove the constraint on the support and get that

$$\gamma_1(f) = \inf_{\nu \in \mathcal{M}(K)} \int_K |d\nu(w, b)| \text{ such that } \forall x \in \mathcal{X}, f(x) = \int_K \sigma(w^\top x + b) d\nu(w, b), \quad (9.2)$$

where $\mathcal{M}(K)$ is the set of measures on K with finite total variation (see Bach, 2017, and references therein for more details and formal definitions). This formulation is typically easier to deal with for sufficiently smooth functions, as the optimal measure ν is typically not a finite sum of Diracs.

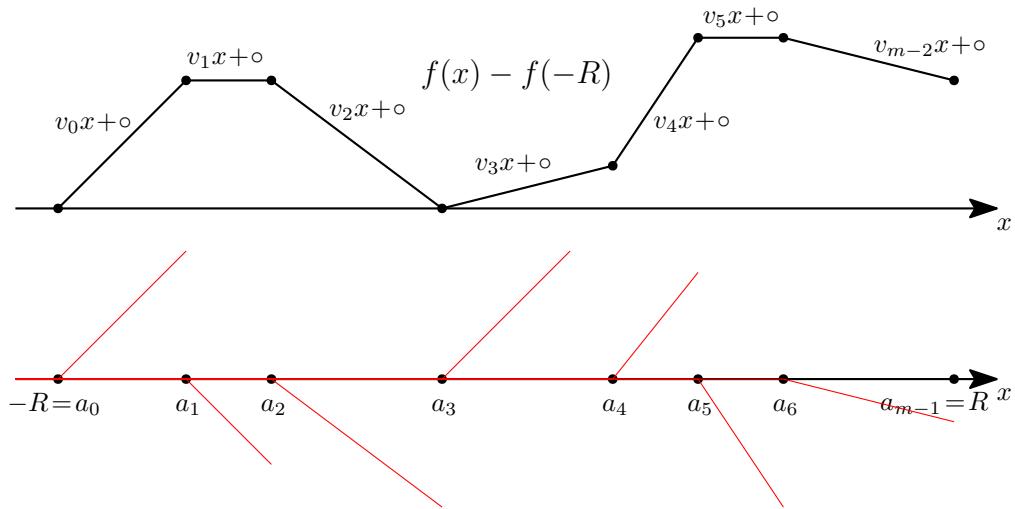
Studying the approximation properties of \mathcal{F}_1 . Now that we have defined the function space through Eq. (9.2), we need to describe the set of functions with finite norm and relate

this norm to classical smoothness properties. To do so, we consider a smaller set than the unit ℓ_2 -sphere, that is, the set of $(w, b/R)$ such that $\|w\|_2 = \frac{1}{\sqrt{2}}$ and $|b| \leq \frac{R}{\sqrt{2}}$, which is enough to obtain upper-bounds on the approximation errors. For simplicity, and losing a factor $\sqrt{2}$, we consider the normalization $K = \{(w, b) \in \mathbb{R}^{d+1}, \|w\|_2 = 1, |b| \leq R\}$, and consider the norm γ_1 defined in Eq. (9.2) with this set K . Note that for $d = 1$, we have $K = \{(w, b) \in \mathbb{R}^2, w \in \{-1, 1\}, |b| \leq R\}$. We could stick to the ℓ_2 -sphere, but our particular choice of K leads to simpler formulas.

9.3.3 Variation norm in one dimension

The ReLU activation function is specific and leads to simple approximation properties in the interval $[-R, R]$. As already qualitatively described in Section 9.3.1, we start with piecewise affine functions, which, given the shape of the ReLU activation, should be easy to approximate (and immediately leads to universal approximation results as all “reasonable” functions can be approximated by piecewise affine functions). See more details by Breiman (1993); Barron and Klusowski (2018).

Piecewise affine functions. We can make the reasoning in Section 9.3.1 quantitative. We consider a continuous piecewise affine function on $[-R, R]$ with specific knots at each $R = a_0 < a_1 < \dots < a_{m-2} < a_{m-1} = R$, so that on $[a_j, a_{j+1}]$, f is affine with slope v_j , for $j \in \{0, \dots, m-2\}$.



We can first start to fit the function $x \mapsto f(x) - f(-R)$ on $[a_0, a_1]$, as $g_0(x) = v_0(x - a_0)_+$. For $x > a_0$, this approximation has slope v_0 . In order for the approximation to be exact on $[a_1, a_2]$ (while not modifying the function on $[a_0, a_1]$), we consider $g_1(x) = g_0(x) + (v_1 -$

$v_0)(x - a_1)_+$, which is now exact on $[a_0, a_2]$; we can pursue recursively by considering, for $j \in \{1, \dots, m-2\}$

$$g_j(x) = g_{j-1}(x) + (v_j - v_{j-1})(x - a_j)_+,$$

which is equal to $f(x) - f(-R)$ for $x \in [a_0, a_{j+1}]$. We can thus represent $f(x) - f(-R)$ on $[a_0, a_{m-1}]$ on $[0, R]$ exactly with $g_{m-2}(x)$. We have:

$$g_{m-2}(x) = v_0(x - a_0)_+ + \sum_{j=1}^{m-2} (v_j - v_{j-1})(x - a_j)_+.$$

In other words, we can represent any piecewise affine function as (using that on $[-R, R]$, $(x - a_0)_+ = (x + R)_+ = x + R$):

$$f(x) = f(-R) + v_0(x + R) + \sum_{j=1}^{m-2} (v_j - v_{j-1})(x - a_j)_+. \quad (9.3)$$

To obtain a representation that is invariant by a sign change, we also consider the same representation starting from the right (which can, for example, be obtained by applying the one above to $x \mapsto f(-x)$):

$$f(x) = f(R) + v_{m-1}(R - x) + \sum_{j=1}^{m-2} (v_{j-1} - v_j)(a_j - x)_+. \quad (9.4)$$

Note that this also shows that such representations are not unique. By averaging Eq. (9.3) and Eq. (9.4), and using that $\frac{1}{2R}(x + R)_+ + \frac{1}{2R}(-x + R)_+$ is equal to 1 on $[-R, R]$, we get:

$$\begin{aligned} f(x) &= \frac{1}{2} [f(R) + f(-R)] \left[\frac{1}{2R}(x + R)_+ + \frac{1}{2R}(-x + R)_+ \right] \\ &\quad + \frac{1}{2} f'_+(-R)(x + R)_+ - \frac{1}{2} f'_-(R)(-x + R)_+ + \frac{1}{2} \sum_{j=1}^{m-2} (v_j - v_{j-1}) [(x - a_j)_+ + (a_j - x)_+], \end{aligned}$$

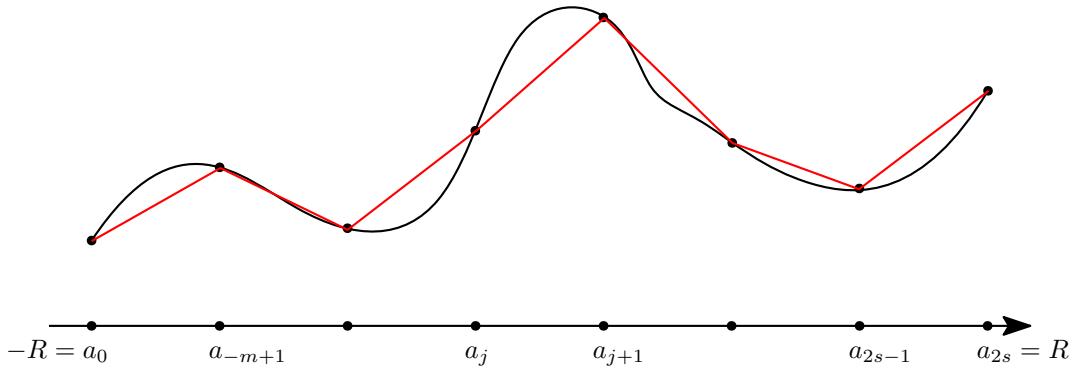
and thus, by construction of the norm γ_1 , we have

$$\gamma_1(f) \leq \frac{1}{2} \left| \frac{1}{2R} [f(-R) + f(R)] + f'_+(-R) + \left(\frac{1}{2} \left| \frac{1}{2R} [f(-R) + f(R)] - f'_-(R) \right| + \sum_{j=1}^{m-2} |v_j - v_{j-1}| \right) \right|.$$

The norm is thus upper-bounded by the values of f and its derivatives at the boundaries of the interval and the sums of the changes in slope.

Twice continuously differentiable functions. We consider a twice continuously differentiable function f on $[-R, R]$, and we would like to express it as a continuous linear combination of functions $x \mapsto (\pm x + b)_+$. We will consider two arguments: one through approximation by piecewise affine functions and one through the Taylor formula with integral remainder.

Piecewise-affine approximation. We consider equally-spaced knots $a_j = -R + \frac{j}{s}$, for $j \in \{0, \dots, 2s\}$, and the piecewise affine interpolation from values $a_j, f(a_j)$, $j \in \{0, \dots, 2s\}$, for s that will tend to infinity (see illustration below).



For the approximant \hat{f} , the value $f'_+(-R)$ is equal to $s[f(-R + 1/s) - f(-R)] \sim f'(-R)$, and $f'_-(R) = s[f(R) - f(R - 1/s)] \sim f'(R)$ when s tends to infinity, while the differences in slopes $|v_j - v_{j-1}|$ are equal to

$$\left| \frac{s}{R} \left(f\left(\frac{j+1}{s}R\right) - f\left(\frac{j}{s}R\right) \right) - \frac{s}{R} \left(f\left(\frac{j}{s}R\right) - f\left(\frac{j-1}{s}R\right) \right) \right| = \frac{s}{R} \left| f\left(\frac{j+1}{s}R\right) - 2f\left(\frac{j}{s}R\right) + f\left(\frac{j-1}{s}R\right) \right|,$$

which is equivalent to $\frac{R}{s} |f''(\frac{j}{s}R)|$ when $s \rightarrow +\infty$.

Thus, the approximant \hat{f} has γ_1 -norm bounded asymptotically as

$$\gamma_1(\hat{f}) \leq \frac{1}{2} \left| \frac{1}{2R} [f(-R) + f(R)] + f'(-R) \right| + \frac{1}{2} \left| \frac{1}{2R} [f(-R) + f(R)] - f'(R) \right| + \frac{R}{s} \sum_{j=1}^{m-2} |f''(\frac{j}{s}R)|.$$

The last term $\frac{R}{s} \sum_{j=1}^{m-2} |f''(\frac{j}{s}R)|$ tends to $\int_{-R}^R |f''(x)| dx$. Thus, letting s tend to infinity, we get (informally here, as the reasoning below will make it more formal):

$$\gamma_1(f) \leq \frac{1}{2} \left| \frac{1}{2R} [f(-R) + f(R)] + f'(-R) \right| + \frac{1}{2} \left| \frac{1}{2R} [f(-R) + f(R)] - f'(R) \right| + \int_{-R}^R |f''(x)| dx. \quad (9.5)$$

This notably shows that if the number of neurons is allowed to grow, then the ℓ_1 -norm of the weights remain bounded by the quantity above to represent the function f exactly.

Direct proof through Taylor formula. Eq. (9.5) above can be extended to continuous functions, which are only twice differentiable almost everywhere with integrable second-order derivatives. In this section, we assume that the function f is twice continuously differentiable and can extend to only integrable second-derivatives by a density argument (see, e.g., [Rudin](#),

1987). For such a function, using the Taylor formula with integral remainder, we have, for $x \in [-R, R]$:

$$\begin{aligned} f(x) &= f(-R) + f'(-R)(x + R) + \int_{-R}^x f''(b)(x - b)db \\ &= f(-R) + f'(-R)(x + R) + \int_{-R}^{\textcolor{red}{R}} f''(b)(x - b)_{+}db. \end{aligned}$$

We also have the symmetric version (obtained by applying the one above to $x \mapsto f(-x)$, replacing x by $-x$, and by a change of variable $b \rightarrow -b$ in the integral):

$$f(x) = f(R) - f'(R)(R - x) + \int_{-R}^R f''(b)(-x - b)_{+}db.$$

By averaging the two equalities, we get:

$$\begin{aligned} f(x) &= \frac{1}{2} \left[\frac{f(-R) + f(R)}{2R} + f'(-R) \right] (x + R) + \frac{1}{2} \left[\frac{f(-R) + f(R)}{2R} - f'(-R) \right] (R - x) \\ &\quad + \frac{1}{2} \int_{-R}^R f''(b)(x - b)_{+}db - \frac{1}{2} \int_{-R}^R f''(b)(-x - b)_{+}db. \end{aligned}$$

This leads to the exact same upper-bound on $\gamma_1(f)$ as obtained from piecewise affine interpolation:

$$\gamma_1(f) \leq \frac{1}{2} \left| \frac{1}{2R} [f(-R) + f(R)] + f'(-R) \right| + \frac{1}{2} \left| \frac{1}{2R} [f(-R) + f(R)] - f'(R) \right| + \int_{-R}^R |f''(x)| dx. \quad (9.6)$$

One can check that the upper bound is indeed a norm (left as an exercise). Moreover, the upper bound happens to be tight (see the exercise below).

We will also use a simpler upper-bound

$$\gamma_1(f) \leq \frac{1}{2R} |f(-R) + f(R)| + \frac{1}{2} |f'(R) + f'(-R)| + \int_{-R}^R |f''(x)| dx. \quad (9.7)$$

Exercise 9.3 (♦) Show that the upper-bound in Eq. (9.6) is in fact an equality.

Exercise 9.4 (♦) Show that the minimum norm interpolant from data $-R < x_1 < \dots < x_n < R$, $y_1, \dots, y_n \in \mathbb{R}$, is equal to the piecewise-affine interpolant on $[x_1, x_n]$.

9.3.4 Variation norm in arbitrary dimension

If we assume that f is continuous on the ball of center zero and radius R , then the Fourier transform $\hat{f}(\omega) = \int_{\mathbb{R}^d} f(x)e^{-i\omega^\top x} dx$ is defined everywhere, and we can write

$$f(x) = \frac{1}{(2\pi)^d} \int_{\mathbb{R}^d} \hat{f}(\omega) e^{i\omega^\top x} d\omega.$$

To compute an upper-bound on $\gamma_1(f)$, it suffices to upper-bound for each $\omega \in \mathbb{R}^d$, $\gamma_1(x \mapsto e^{i\omega^\top x})$ (using complex-valued functions, for which the developments of the previous section still apply), which is easy because we have the representation from Section 9.3.3 and Eq. (9.7) applied to $g : u \mapsto e^{iu\|\omega\|_2}$, for $u \in [-R, R]$,

$$e^{iu\|\omega\|_2} = \int_{-R}^R \eta_+(b, \|\omega\|_2)(u - b)_+ db + \int_{-R}^R \eta_-(b, \|\omega\|_2)(-u - b)_+ db,$$

$$\text{with } \int_{-R}^R |\eta_+(b, \|\omega\|_2)| db + \int_{-R}^R |\eta_-(b, \|\omega\|_2)| db \leq \frac{1}{R} + \|\omega\|_2 + 2R\|\omega\|_2^2 \leq \frac{2}{R}(1 + 2R^2\|\omega\|_2^2).$$

We can therefore decompose

$$\begin{aligned} e^{i\omega^\top x} &= e^{i(x^\top \omega / \|\omega\|_2)\|\omega\|_2} \\ &= \int_{-R}^R \eta_+(b, \|\omega\|_2)(x^\top (\omega / \|\omega\|_2) - b)_+ db + \int_{-R}^R \eta_-(b, \|\omega\|_2)(x^\top (-\omega / \|\omega\|_2) - b)_+ db, \end{aligned}$$

with weights being in the correct constraint set (unit norm for w 's and $|b| \leq R$), leading to

$$\gamma_1(x \mapsto e^{i\omega^\top x}) \leq \frac{2}{R}(1 + 2R^2\|\omega\|_2^2).$$

Thus, we obtain

$$\gamma_1(f) \leq \frac{1}{(2\pi)^d} \int_{\mathbb{R}^d} |\hat{f}(\omega)| \gamma_1(x \mapsto e^{i\omega^\top x}) d\omega \leq \frac{1}{(2\pi)^d} \frac{2}{R} \int_{\mathbb{R}^d} |\hat{f}(\omega)| (1 + 2R^2\|\omega\|_2^2) d\omega. \quad (9.8)$$

Given a function $g : \mathbb{R}^d \rightarrow \mathbb{R}$, $\int_{\mathbb{R}^d} |\hat{g}(\omega)| d\omega$ is a measure of smoothness of g , and so $\gamma_1(f)$ being finite imposes that f and all second-order derivatives of f have this form of smoothness. See [Klusowski and Barron \(2018\)](#) for more details.

To relate the norm γ_1 to other function spaces such as Sobolev spaces, we will consider further upper bounds (and relate them to another norm γ_2 in Section 9.4).

9.3.5 Precise approximation properties

Precise rates of approximation. In this section, we will relate the space \mathcal{F}_1 to Sobolev spaces, bounding, using Cauchy-Schwarz inequality, the norm γ_1 as:

$$\begin{aligned}\gamma_1(f) &\leq \frac{1}{(2\pi)^d} \frac{2}{R} \int_{\mathbb{R}^d} |\hat{f}(\omega)| (1 + 2R^2 \|\omega\|_2^2)^{d/2+1/2} d\omega \quad \text{from Eq. (9.8),} \\ &= \frac{1}{(2\pi)^d} \frac{2}{R} \int_{\mathbb{R}^d} |\hat{f}(\omega)| (1 + 2R^2 \|\omega\|_2^2)^{d/4+5/4} \frac{d\omega}{(1 + 2R^2 \|\omega\|_2^2)^{d/4+1/4}} \\ &\leq \frac{1}{(2\pi)^d} \frac{2}{R} \sqrt{\int_{\mathbb{R}^d} |\hat{f}(\omega)|^2 (1 + 2R^2 \|\omega\|_2^2)^{d/2+5/2} d\omega} \sqrt{\int_{\mathbb{R}^d} \frac{d\omega}{(1 + 2R^2 \|\omega\|_2^2)^{d/2+1/2}}}, \quad (9.9)\end{aligned}$$

which is a constant times $\sqrt{\int_{\mathbb{R}^d} |\hat{f}(\omega)|^2 (1 + 2R^2 \|\omega\|_2^2)^s d\omega}$, which is exactly the Sobolev norm from Chapter 7, with $s = \frac{d}{2} + \frac{5}{2}$ derivatives, which is a reproducing kernel Hilbert space (RKHS) since $s > d/2$.

Thus, all approximation properties from Chapter 7 apply. See Chapter 7 for precise rates. Note, however, that, *using this reasoning*, if we start from a Lipschitz-continuous function, then to approximate it up to $L_2(\mathbb{R}^d)$ -norm ε requires a γ_1 -norm growing as $\varepsilon^{-(s-1)} \geq \varepsilon^{-(d/2+3/2)}$ (as obtained at the end of Section 7.5.2 of Chapter 7). Thus, in the generic situation where no particular directions are preferred, using \mathcal{F}_1 (neural networks) is not really more advantageous than using kernel methods (see also more details in Section 9.3.7 and Section 9.4). This changes drastically when such linear structures are present, as shown below.

Adaptivity to linear latent variables. We consider a target function f^* that depends only on a r -dimensional projection of the data, that is, f^* is of the form $f^*(x) = g(V^\top x)$, where $V \in \mathbb{R}^{d \times r}$ is full rank and has all singular values less than 1, and $g : \mathbb{R}^r \rightarrow \mathbb{R}$. Without loss of generality, we can assume that V has orthonormal columns. Then if $\gamma_1(g)$ is finite (as a function defined on \mathbb{R}^r), it can be written as

$$g(z) = \int_{\mathbb{R}^{r+1}} (w^\top z + b)_+ d\mu(w, b),$$

with μ supported on $\{(w, b) \in \mathbb{R}^{r+1}, \|w\|_2 = 1, |b| \leq R\}$, and $\gamma_1(g) = \int_{\mathbb{R}^{r+1}} |d\mu(w, b)|$. We then have:

$$f^*(x) = g(V^\top x) = \int_{\mathbb{R}^{r+1}} ((Vw)^\top x + b)_+ d\mu(w, b),$$

leading to $\gamma_1(f^*) \leq \int_{\mathbb{R}^{r+1}} |d\mu(w, b)| = \gamma_1(g)$ (because $\|Vw\|_2 \leq 1$). Thus the approximation properties of g translate to f^* , and thus we pay only the price of these r dimensions and not

of all d variables, *without* the need to know V in advance. For example, (a) if g has more than $r/2 + 5/2$ squared integrable derivatives, then $\gamma_1(g)$ and thus $\gamma_1(f^*)$ is finite, or (b) if g is Lipschitz-continuous, then both g and f can be approached in $L_2(\mathbb{R}^d)$ with error ε with a function with γ_1 -norm of order $\varepsilon^{-(r/2+5/2)}$, thus escaping the curse of dimensionality. See [Bach \(2017\)](#) for more details and precise learning rates in Section 9.3.7.



Kernel methods do not have such adaptivity. In other words, as shown in Section 9.4, using the ℓ_2 -norm instead of the ℓ_1 -norm on the output weights leads to worse performance.

9.3.6 From the variation norm to a finite number of neurons

Given a measure μ on \mathbb{R}^d , and a function $g : \mathbb{R}^d \rightarrow \mathbb{R}$ such that $\gamma_1(g)$ is finite, we would like to find a set of m neurons $(w_j, b_j) \in K \subset \mathbb{R}^{d+1}$ (which is the compact support of all measures that we consider), such that the associated function defined through

$$g(x) = \sum_{j=1}^m \eta_j \sigma(w_j^\top x + b_j)$$

is close to g for the norm $L_2(\mu)$.

Since input weights are fixed in K , the bound on $\gamma_1(g)$ should translate to a bound $\|\eta\|_1 \leq \gamma_1(g)$. The set of such functions f is the convex hull of functions $s_j \gamma_1(g) \sigma(w_j^\top x + b_j)$, for $s_j \in \{-1, 1\}$. Thus, we are faced with the problem of approximating elements of a convex hull as an explicit linear combination of extreme points, if possible, with as few extreme points as possible.

In finite dimension, Carathéodory's theorem tells that the number of such extreme points can be taken equal to the dimension to get an exact representation. In our case of infinite dimensions, we need an approximate version of Carathéodory's theorem. It turns out that we can create a “fake” optimization problem of minimizing $\min_{f \in \mathcal{F}_1} \|f - g\|_{L_2(\mu)}^2$ such that $\gamma_1(f) \leq \gamma_1(g)$, whose solution is $f = g$, with an algorithm that constructs an approximate solution from extreme points. This will be achieved by the Frank-Wolfe algorithm (a.k.a. conditional gradient algorithm). This algorithm is applicable more generally; for more details, see [Jaggi \(2013\); Bach \(2015\)](#).

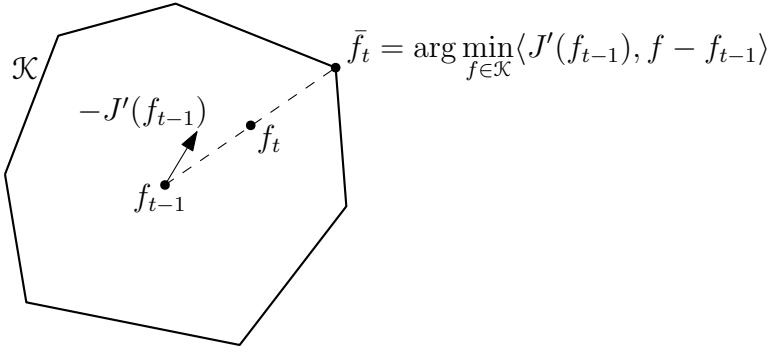
Frank-Wolfe algorithm. We thus make a detour by considering an algorithm defined in a Hilbert space \mathcal{H} , such that \mathcal{K} is a bounded convex set and J a convex, smooth function from \mathcal{H} to \mathbb{R} , that is such that there exists a gradient function $J' : \mathcal{H} \rightarrow \mathcal{H}$ such that for all elements f, g of \mathcal{H} :

$$J(g) + \langle J'(g), f - g \rangle_{\mathcal{H}} \leq J(f) \leq J(g) + \langle J'(g), f - g \rangle_{\mathcal{H}} + \frac{L}{2} \|f - g\|_{\mathcal{H}}^2.$$

The goal is to minimize J on the bounded convex set \mathcal{K} , with an algorithm that only requires access to the set \mathcal{K} through a “linear minimization” oracle (i.e., through minimizing linear functions), as opposed to the projection oracle that we required in Chapter 5.

We consider the following recursive algorithm, started from a vector $f_0 \in \mathcal{K}$:

$$\begin{aligned}\bar{f}_t &\in \arg \min_{f \in \mathcal{K}} \langle J'(f_{t-1}), f - f_{t-1} \rangle_{\mathcal{H}}, \\ f_t &= \frac{t-1}{t+1} f_{t-1} + \frac{2}{t+1} \bar{f}_t = f_{t-1} + \frac{2}{t+1} (\bar{f}_t - f_{t-1}).\end{aligned}$$



Because \bar{f}_t is obtained by minimizing a linear function on a bounded convex set, we can restrict the minimizer \bar{f}_t to be extreme points of \mathcal{K} , so that, f_t is the convex combination of t such extreme points $\bar{f}_1, \dots, \bar{f}_t$ (note that the first point f_0 disappears). We now show that

$$J(f_t) - \inf_{f \in \mathcal{K}} J(f) \leq \frac{2L}{t+1} \text{diam}_{\mathcal{H}}(\mathcal{K})^2.$$

Proof of convergence rate (♦). This is obtained by using smoothness:

$$\begin{aligned}J(f_t) &\leq J(f_{t-1}) + \langle J'(f_{t-1}), f_t - f_{t-1} \rangle_{\mathcal{H}} + \frac{L}{2} \|f_t - f_{t-1}\|_{\mathcal{H}}^2 \\ &= J(f_{t-1}) + \frac{2}{t+1} \langle J'(f_{t-1}), \bar{f}_t - f_{t-1} \rangle_{\mathcal{H}} + \frac{4}{(t+1)^2} \frac{L}{2} \|\bar{f}_t - f_{t-1}\|_{\mathcal{H}}^2 \\ &\leq J(f_{t-1}) + \frac{2}{t+1} \min_{f \in \mathcal{K}} \langle J'(f_{t-1}), f - f_{t-1} \rangle_{\mathcal{H}} + \frac{4}{(t+1)^2} \frac{L}{2} \text{diam}_{\mathcal{H}}(\mathcal{K})^2.\end{aligned}$$

By convexity of J , we have for all $f \in \mathcal{K}$, $J(f) \geq J(f_{t-1}) + \langle J'(f_{t-1}), f - f_{t-1} \rangle_{\mathcal{H}}$, leading to $\inf_{f \in \mathcal{K}} J(f) \geq J(f_{t-1}) + \inf_{f \in \mathcal{K}} \langle J'(f_{t-1}), f - f_{t-1} \rangle_{\mathcal{H}}$. Thus, we get

$$\begin{aligned}J(f_t) - \inf_{f \in \mathcal{K}} J(f) &\leq [J(f_{t-1}) - \inf_{f \in \mathcal{K}} J(f)] \frac{t-1}{t+1} + \frac{4}{(t+1)^2} \frac{L}{2} \text{diam}_{\mathcal{H}}(\mathcal{K})^2, \text{ leading to} \\ t(t+1)[J(f_t) - \inf_{f \in \mathcal{K}} J(f)] &\leq (t-1)t[J(f_{t-1}) - \inf_{f \in \mathcal{K}} J(f)] + 2L \text{diam}_{\mathcal{H}}(\mathcal{K})^2 \\ &\leq 2Lt \text{diam}_{\mathcal{H}}(\mathcal{K})^2 \text{ by using a telescoping sum,}\end{aligned}$$

and thus $J(f_t) - \inf_{f \in \mathcal{K}} J(f) \leq \frac{2L}{t+1} \text{diam}_{\mathcal{H}}(\mathcal{K})^2$, as claimed earlier.

Application to approximate representations with a finite number of neurons. We can apply this to $\mathcal{H} = L_2(\mathbb{R}^d)$ and $J(f) = \|f - g\|_{L_2(p)}^2$, leading to $L = 2$, with $\mathcal{K} = \{f \in L_2(\mathbb{R}^d), \gamma_1(f) \leq \gamma_1(g)\}$ for which the set of extreme points are exactly single neurons $s\sigma(w^\top \cdot + b)$ scaled by $\gamma_1(g)$ and with an extra sign $s \in \{-1, 1\}$.

We thus obtain after t steps a representation of f with t neurons for which

$$\|f - g\|_{L_2(p)}^2 \leq \frac{4\gamma_1(g)^2}{t+1} \sup_{(w,b) \in \mathcal{K}} \|\sigma(w^\top \cdot + b)\|_{L_2(p)}^2.$$

Thus, it is sufficient to have t of order $O(\gamma_1(g)^2/\varepsilon^2)$ to achieve $\|f - g\|_{L_2(p)} \leq \varepsilon$. Therefore the norm $\gamma_1(g)$ directly controls the approximability of the function g by a finite number of neurons and tells us how many neurons should be used for a given target function. For the ReLU activation, the bound above becomes: $\|f - g\|_{L_2(p)}^2 \leq \frac{16R^2\gamma_1(g)^2}{t+1}$; note that the dependence of the number of neurons in ε as ε^{-2} is not optimal, as it can be improved to $\varepsilon^{-2d/(d+3)}$ (see Bach, 2017, and references therein).

9.3.7 Putting things together

We can now consider putting both estimation and approximation errors together, using tools from Section 7.5.1, that give a rate for constrained optimization (this is done for simplicity, as using tools from Section 4.5.5, we could get similar results for penalized problems).

We thus minimized the empirical risk for a G -Lipschitz-continuous loss subject to $\gamma_1(f) \leq D$. From Section 9.2.3, we get an estimation error less than $\frac{16GDR}{\sqrt{n}}$, on which we need to add $G \inf_{\gamma_1(f) \leq D} \|f - f^*\|_{L_2(p)}$. Following the same reasoning as in Section 7.5.1, optimizing over D , leads to an upper-bound of the form:

$$\varepsilon_n = 2G \sqrt{\inf_{f \in \mathcal{F}_1} \left\{ \|f - f^*\|_{L_2(p)}^2 + \frac{256R^2}{n} \gamma_1(f)^2 \right\}}.$$

As shown in Section 7.5, given this bound, we can recover the bound D as $\frac{\sqrt{n}}{16RG}\varepsilon_n$, and thus, using Section 9.3.6, we will lose an extra factor ε_n with a number of neurons greater than $m \geq \frac{16D^2R^2G^2}{\varepsilon_n^2}$ which is exactly equal to a constant times n , that is, there is no need to have a number of neurons that greatly exceeds the number of observations.

We can now look at a series of structural assumptions on the target function f^* , for which we will see that neural networks provide adaptivity if the regularization parameter is well-chosen:

- No assumption: If we assume that f_* is Lipschitz-continuous, then we obtain a rate of $O(1/n^{1/(2s)}) = 1/n^{1/(d+5)}$, which exhibits the curse of dimensionality, which cannot anyway be much improved, as the optimal performance is of the order $1/n^{1/(d+2)}$ (see Chapter 12).
- Linear latent-variable: If we now assume that f_* depends on an r -dimensional *unknown* subspace, then we obtain a rate proportional $1/n^{1/(r+5)}$ (with constants independent from d). This is where neural networks have a strong advantage over kernel methods and sparse methods: they can perform variable selection with non-linear predictions.
- “Teacher network”: if we assume that f^* is the linear combination of k hidden neurons, then we obtain a convergence rate proportional to k/\sqrt{n} , as the norm $\gamma_1(f^*)$ is proportional to k .

Note that these rates are not as good as Bach (2017), since the exponent $s = \frac{d}{2} + \frac{5}{2}$ is not optimal, and in fact, a more careful analysis, as outlined in Section 9.4 would lead $s = \frac{d}{2} + \frac{3}{2}$.

9.4 Relationship with kernel methods (♦)

In this section, we relate our function space \mathcal{F}_1 to a simpler function space \mathcal{F}_2 that will, in the overparameterized regime when m tends to $+\infty$, correspond to only optimizing the output layer.

9.4.1 From a Banach space \mathcal{F}_1 to a Hilbert space \mathcal{F}_2 (♦)

Following the notations of Section 9.3.2, given a fixed probability measure τ on $K \subset \mathbb{R}^{d+1}$, we can define another norm as

$$\gamma_2^2(f) = \inf_{\nu \in \mathcal{M}(K)} \int_K \left| \frac{d\nu(w, b)}{d\tau(w, b)} \right|^2 d\tau(w, b) \text{ such that } \forall x \in \mathcal{X}, f(x) = \int_K \sigma(w^\top x + b) d\nu(w, b). \quad (9.10)$$

By construction (and by Jensen’s inequality), $\gamma_1(f) \leq \gamma_2(f)$, so the space \mathcal{F}_2 of functions f such that $\gamma_2(f) < +\infty$ is included in \mathcal{F}_1 .

Moreover, as shown in the proposition below, the space \mathcal{F}_2 is a reproducing kernel Hilbert space on $\mathcal{X} = \{x \in \mathbb{R}^d, \|x\|_2 \leq R\}$, as defined in Chapter 7.

Proposition 9.2 *The space \mathcal{F}_2 is the reproducing kernel Hilbert space associated with the positive definite kernel function*

$$k(x, x') = \int_K \sigma(w^\top x + b) \sigma(w^\top x' + b) d\tau(w, b). \quad (9.11)$$

Proof For a formal proof for all compact K , see [Bach \(2017, Appendix A\)](#). We only provide a proof for finite K and τ the uniform probability measure on K , we then have, $\gamma_2^2(f) = \inf_{\nu \in \mathbb{R}^K} \frac{1}{|K|} \sum_{(w,b) \in K} \nu_k^2$ such that $f(x) = \frac{1}{|K|} \sum_{(w,b) \in K} \nu_k \sigma(w^\top x + b)$, which corresponds to penalizing the ℓ_2 -norm of $\theta = \frac{1}{\sqrt{|K|}} \nu \in \mathbb{R}^K$ for $f(x) = \theta^\top \varphi(x)$, and $\varphi(x)_{(w,b)} = \frac{1}{|K|^{1/2}} \sigma(w^\top x + b)$. We thus get the desired kernel $k(x, x') = \frac{1}{|K|} \sum_{(w,b) \in K} \sigma(w^\top x + b) \sigma(w^\top x' + b)$. ■

Interpretation in terms of random features. As already mentioned in Section 7.4, the kernel defined in Eq. (9.11) can be approximated by sampling uniformly at random from τ , m points (w_j, b_j) , $j = 1, \dots, m$, and approximating $k(x, x')$ by

$$\hat{k}(x, x') = \frac{1}{m} \sum_{j=1}^m \sigma(w_j^\top x + b_j) \sigma(w_j^\top x' + b_j).$$

This corresponds to using $f(x) = \sum_{j=1}^m \eta_j \sigma(w_j^\top x + b_j)$, with a penalty proportional to $m \|\eta\|_2^2$. Thus random features correspond to only optimizing with respect to the output weights while keeping the input weights fixed (while for γ_1 , we optimize over all weights).

Therefore, infinite width networks where input weights are random and only output weights are learned are, in fact, kernel methods in disguise ([Neal, 1995; Rahimi and Recht, 2008](#)).

This kernel can be computed in closed form for simple activations and distributions of weights; see Section 9.4.2 and [Cho and Saul \(2009\); Bach \(2017\)](#). Thus, the same regularization properties may be achieved with algorithms from Chapter 7 (which are based on convex optimization and therefore come with guarantees). Note that as shown in Section 7.4, a common strategy for kernels defined as expectations is to use the *random feature* approximation $\hat{k}(x, x')$, that is, here, use the neural network representation explicitly.



The kernel approximation corresponds to input weights w_j, b_j sampled randomly and *held fixed*. Only the output weights η_j are optimized.



Because Dirac measures are not square integrable, the function $x \mapsto \sigma(w^\top x + b)$, that is, a single neuron, is typically not in the RKHS, which is typically composed of smooth functions. See the examples below.

Link between the two norms. To relate the two norms more precisely, we rewrite γ_1 using the fixed probability measure τ , as

$$\gamma_1(f) = \inf_{\eta: K \rightarrow \mathbb{R}} \int_K |\eta(w, b)| d\tau(w, b) \text{ such that } \forall x \in \mathcal{X}, f(x) = \int_K \sigma(w^\top x + b) \eta(w, b) d\tau(w, b).$$

| \mathcal{F}_2 | \mathcal{F}_1 |
|---|---|
| Hilbert space | Banach space |
| $\gamma_2(f)^2 = \inf \int_{\mathbb{R}^{d+1}} \eta(w, b) ^2 d\tau(w, b)$ s. t. $f(x) = \int_{\mathbb{R}^{d+1}} \eta(w, b) \sigma(w^\top x + b) d\tau(w, b)$ | $\gamma_1(f) = \inf \int_{\mathbb{R}^{d+1}} \eta(w, b) d\tau(w, b)$ s. t. $f(x) = \int_{\mathbb{R}^{d+1}} \eta(w, b) \sigma(w^\top x + b) d\tau(w, b)$ |
| Smooth functions Single neurons $\notin \mathcal{F}_2$ | Potentially non-smooth functions Single neurons $\in \mathcal{F}_1$ |

Table 9.1: Summary of properties of the norms γ_1 and γ_2 .

The only difference with the squared RKHS norm above is that we consider the L_1 -norm instead of the squared L_2 -norm of η (with respect to the probability measure τ). The minimum achievable norm is exactly $\gamma_1(f)$.

Note that typically, the infimum over all η is not achieved as the optimal measure in Eq. (9.2) may not have a density with respect to τ . Because we use an L_1 -norm penalty, the measures $\mu(w, b) = \eta(w, b)\tau(w, b)$ can span in the limit all measures $\mu(w, b)$ with finite total variation $\int_{\mathbb{R}^{d+1}} |d\mu(\eta, b)| = \int_{\mathbb{R}^{d+1}} |\eta(w, b)| d\tau(w, b)$.

Overall, we have the following properties (see Table 9.1 for a summary):

- Because of Jensen's inequality, we have $\gamma_1(f) \leq \gamma_2(f)$, and thus $\mathcal{F}_2 \subset \mathcal{F}_1$, that is the space \mathcal{F}_1 contains many more functions.
- ! A single neuron is in \mathcal{F}_1 with γ_1 -norm less than one, as the mass of a Dirac is equal to one.

9.4.2 Kernel function (♦♦)

We can compute in closed form the kernel function, which is only useful computationally if the number of random features m is larger than the number of observations (when using the kernel trick is advantageous, as outlined in Section 7.4).

In one dimension, with w uniform on the unit sphere, that is, $w \in \{-1, 1\}$, and with b uniform on $[-R, R]$, we have the following kernel

$$k(x, x') = \frac{1}{4R} \int_{-R}^R \left((x - b)_+ (x' - b)_+ + (-x - b)_+ (-x' - b)_+ \right) db.$$

After a short calculation left as an exercise, we can compute it in closed form as:

$$k(x, x') = \frac{R^2}{6} + \frac{xx'}{2} + \frac{1}{24R} |x - x'|^3.$$

In higher dimension, we have:

$$k(x, x') = \int_{\|w\|_2=1} \frac{1}{2R} \int_{-R}^R (w^\top x + b)_+ (w^\top x' + b)_+ db d\tau(w),$$

where τ is the uniform distribution on the sphere. After a longer calculation, also left as an exercise, we get:

$$k(x, x') = \frac{R^2}{6} + \frac{1}{2d} x^\top x' + \frac{1}{24R} \frac{\Gamma(2)\Gamma(\frac{d}{2})}{\Gamma(\frac{1}{2})\Gamma(\frac{d}{2} + \frac{3}{2})} \|x - x'\|_2^3. \quad (9.12)$$

See Figure 9.2 for comparing the RKHS (corresponding to $m = +\infty$ neurons) and the approximation with finite m .

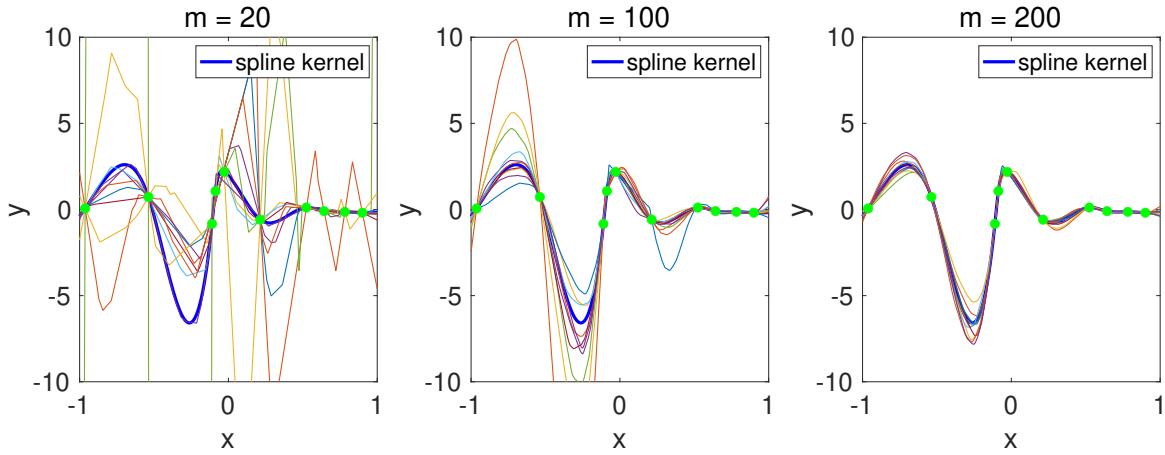


Figure 9.2: Examples of functions in the reproducing kernel Hilbert space \mathcal{F}_2 and its approximation based on random features, with $m = 20, 100, 200$. All functions are the minimum norm interpolators of the green points. This is to be contrasted with the Banach space \mathcal{F}_1 , where the minimum norm interpolator is the piecewise affine interpolator (see Exercise 9.4), and can be achieved with $m = n$ neurons, where n is the number of observed points.

9.4.3 Upper-bound on RKHS norm (♦♦)

We can now find upper bounds on the norm γ_2 . We can either use the kernel function from Eq. (9.12) or the random feature interpretation from Eq. (9.10). We first use the random feature interpretation in one dimension.

Upper-bound on RKHS norm γ_2 in one dimension. Using the same reasoning as the end of Section 9.4, we can get an upper-bound on $\gamma_2(f)$ by decomposing f as

$$f(x) = \int_{-R}^R \eta_+(b)(x - b)_+ \frac{db}{4R} + \int_{-R}^R \eta_-(b)(-x - b)_+ \frac{db}{4R},$$

with now $\gamma_2(f)^2 \leq \int_{-R}^R \eta_+(b)^2 \frac{db}{4R} + \int_{-R}^R \eta_-(b)^2 \frac{db}{4R}$.

By using as in Section 9.3.3 the Taylor expansion with integral remainder, we get, for any twice differentiable function f on $[-R, R]$:

$$\begin{aligned} f(x) &= \frac{1}{2}f(-R) + \frac{1}{2}f(R) + \frac{1}{2}f'(-R)(x+R) - \frac{1}{2}f'(R)(-x+R) \\ &\quad + \frac{1}{2} \int_{-R}^R f''(b)(x-b)_+ db - \frac{1}{2} \int_{-R}^R f''(b)(-x-b)_+ db \\ &= \frac{1}{2}[f'(R) + f'(-R)] + \frac{1}{2}[R(f'(-R) - f'(R)) + f(-R) + f(R)] \\ &\quad + \frac{1}{2} \int_{-R}^R f''(b)(x-b)_+ db - \frac{1}{2} \int_{-R}^R f''(b)(-x-b)_+ db. \end{aligned}$$

We can now use explicit representations of constants and linear functions, *without* Diracs, as we need finite L_2 -norms, as:

$$\begin{aligned} x &= \int_{-R}^R \frac{(x-b)_+ - (-x-b)_+}{2R} db = \int_{-R}^R \frac{x}{2R} db \\ -\frac{R^2}{6} &= \int_{-R}^R b(x-b)_+ \frac{db}{4R} + \int_{-R}^R b(-x-b)_+ \frac{db}{4R}. \end{aligned}$$

After a short calculation left as an exercise, this leads to

$$\gamma_2(f)^2 \leq 2R \int_{-R}^R f''(x)^2 dx + [f'(R) + f'(-R)]^2 + 3[R(f'(R) - f'(-R)) - f(-R) - f(R)]^2, \quad (9.13)$$

which happens to be an equality (which can be shown by showing that this defines a dot-product, for which $\langle f, k(\cdot, x) \rangle = f(x)$).

Exercise 9.5 Show that the upper bound on γ_2 from Eq. (9.13) is larger than the bound on γ_1 from Eq. (9.6).

The main difference with γ_1 is that the second-derivative is penalized by an L_2 -norm and not by an L_1 -norm, and that this L_2 -norm can be infinite when the L_1 -norm is finite, the classic example being for the hidden neuron functions $(x-b)_+$.

⚠ The RKHS is combining infinitely many hidden neuron functions $(x-b)_+$, none of them are inside the RKHS,

⚠ This smoothness penalty does not allow the ReLU to be part of the RKHS. However, this is still a universal penalty (as the set of functions with squared integrable second derivative is dense in L_2).

Upper-bound on RKHS norm γ_2 in all dimensions. We can first find a bound directly from the one on γ_1 in Eq. (9.8), which is exactly Eq. (9.9), ending up with the restriction on the ball of center 0 and radius R of the Sobolev space corresponding to square integrable $s = \frac{d}{2} + \frac{5}{2}$ derivatives on \mathbb{R}^d . It turns out that this provides a bound on γ_2 (as can be shown by reproducing the reasoning from Section 9.3.4).

However, this bound is not optimal, which can already be seen in dimension $d = 1$, where we obtain $s = 3$ instead of $s = 2$. It turns out that, in general, it is possible to show γ_2 is less than a Sobolev norm with index $s = \frac{d}{2} + \frac{3}{2}$. This can be done by drawing links with multivariate splines (Wahba, 1990).

9.5 Experiments

We consider the same experimental set-up as Section 7.7, that is, one-dimensional problems to highlight the adaptivity of neural network methods to the regularity of the target function, with smooth targets and non-smooth targets. We consider several values for the number m of hidden neurons, and we consider a neural network with ReLU activation functions and an additional global constant term. Training is done by stochastic gradient descent with a small constant step-size and random initialization.

Note that for small m , while a neural network with the same number of hidden neurons could fit the data better, optimization is not successful (that is, SGD gets trapped in a bad local minimum). Moreover, between $m = 32$ and $m = 100$, we do not see any overfitting, highlighting the potential underfitting behavior of neural networks. See also <https://francisbach.com/quest-for-adaptivity/>.

9.6 Extensions

Fully-connected single-hidden layer neural networks are far from what is being used in practice, particularly in computer vision and natural language processing. Indeed, state-of-the-art performance is typically achieved with the following extensions:

- **Going deep with multiple layers:** The most simple form of deep neural networks is a multilayer fully-connected neural network. Ignoring the constant terms for simplicity, it is of the form $f(x^{(0)}) = y^{(L)}$ with input $x^{(0)}$ and output $y^{(L)}$ given by:

$$\begin{aligned} y^{(k)} &= (W^{(k)})^\top x^{(k-1)} \\ x^{(k)} &= \sigma(y^{(k)}), \end{aligned}$$

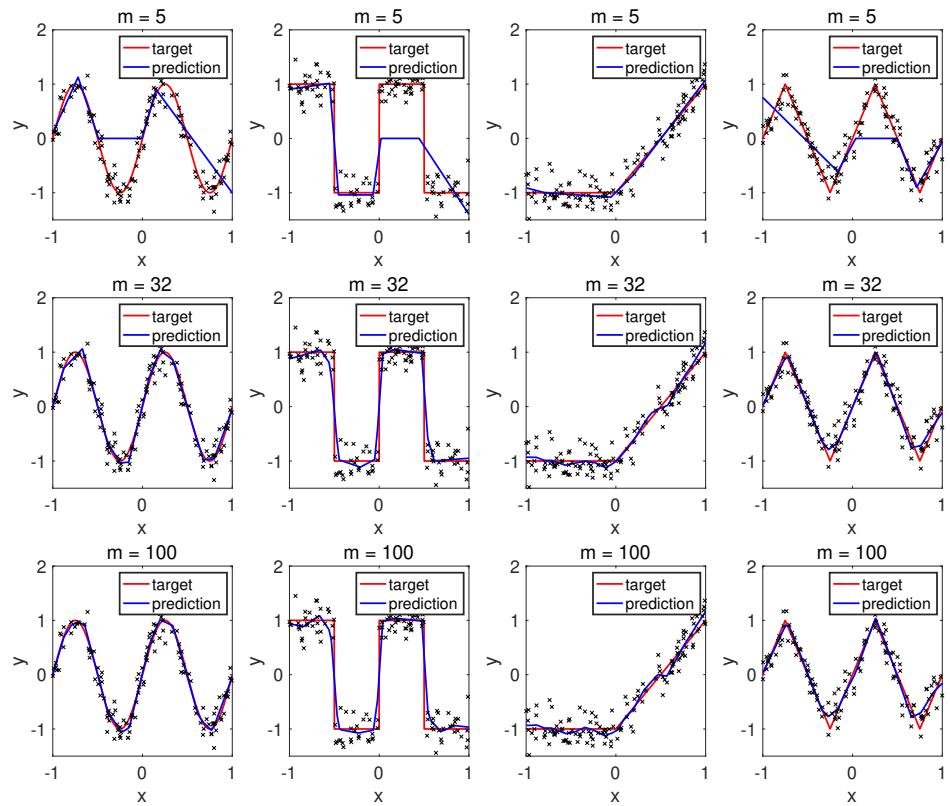


Figure 9.3: Fitting one-dimensional functions with various numbers of neurons m (top: $m = 5$, middle: $m = 32$, bottom: $m = 100$), with four different prediction problems (one per column).

where $W^{(\ell)}$ is the matrix of weights for layer ℓ . For these models, obtaining simple and powerful theoretical results is still an active area of research. See, e.g., [Lu et al. \(2020\)](#); [Ma et al. \(2020\)](#); [Yang and Hu \(2021\)](#).

- **Residual networks:** An alternative to stacking layers one after the other like above is to introduce a different architecture of the form:

$$\begin{aligned} y^{(k)} &= (W^{(k)})^\top x^{(k-1)} \\ x^{(k)} &= x^{(k-1)} + \sigma(y^{(k)}). \end{aligned}$$

The direct modeling of $x^{(k)} - x^{(k-1)}$ instead of $x^{(k)}$ through an extra non-linearity, originating from [He et al. \(2016\)](#), can be seen as a discretization of an ordinary differential equation ([Chen et al., 2018](#)).

- **Convolutional neural networks:** To tackle large data and improve performances, it is important to leverage prior knowledge about the typical data structure to process. For instance, for signals, images, or videos, it is important to take into account the translation invariance (up to boundary issues) of the domain. This is done by constraining the linear operators involved in the linear part of the neural networks to respect some form of translation invariance and thus to use convolutions. See [Goodfellow et al. \(2016\)](#) for details.

Part III

Special topics

Chapter 10

Ensemble learning

Chapter summary

- Combining several predictors learned on modified versions of the original dataset can have computational and/or statistical benefits.
- Averaging predictors on several reshuffled / resampled / uniformly projected data sets will typically lower the estimator's variance with a potentially limited increase in bias.
- Boosting: iteratively refining the prediction function by re-training on a reweighted dataset in a greedy fashion is an efficient way of building task-dependent features.

Given a supervised learning algorithm \mathcal{A} that goes from datasets \mathcal{D} to prediction rules $\mathcal{A}(\mathcal{D}) : \mathcal{X} \rightarrow \mathcal{Y}$, can we run it several times on different datasets constructed from the same original one, and combine the results to get a better overall predictor? The combination is typically a “linear” combination: like for local averaging methods which were combining labels from close-by inputs, we combine the predicted labels from the estimators learned on different datasets. For regression ($\mathcal{Y} = \mathbb{R}$), this is done by simply linearly combining predictions; for classification, this is done by a weighted majority vote, or by linearly combining real-valued predictions when convex surrogates are used (such as the logistic loss).

The construction of a new dataset given an old one $\mathcal{D} = \{(x_1, y_1), \dots, (x_n, y_n)\}$, is typically done by giving a different weight $v_i \in \mathbb{R}_+$ to each (x_i, y_i) . When the weights are integer-valued, this can be implemented by duplicating the corresponding observations several times (as many times as the integer weight) and then using an existing algorithm for (regularized) empirical risk minimization on the enlarged dataset. In particular, for stochastic gradient descent on the empirical risk, this can be implemented by sampling each observation (x_i, y_i) according to its weights v_i . Note, however, that most learning techniques, in particular the ones based on empirical risk minimization, can accommodate arbitrary weights directly.

In this chapter, we consider two classes of techniques:

- *Bagging / averaging techniques*: datasets are constructed in parallel, and the weights are typically random and “uniform” (for example, distributed uniformly or constant). A similar effect can be obtained by modifying the original dataset using random projections. This is studied in Section 10.1 and in Section 10.2.
- *Boosting techniques*: datasets are constructed sequentially, and these weights are adapted from previous datasets and thus not uniformly distributed. This is studied in Section 10.3.

The benefits of each combination technique will depend strongly on the original predictor, with three classes that we have considered in earlier chapters:

- Local averaging methods: they will be well-adapted to all ensemble learning techniques.
- Empirical risk minimization with non-linear models: from a set of functions $\varphi(w, \cdot)$, with $w \in \mathcal{W}$, then linear combinations increase the set of models to $\int_{\mathcal{W}} \varphi(w, x) d\nu(w)$, for $d\nu$ a signed measure on \mathcal{W} . These will be adapted to boosting techniques (we already saw some of them in Chapter 9 in the context of neural networks).
- Empirical risk minimization with linear models (linearity in the model’s parameters): the overall model class remains the same by taking linear combinations. Thus, these are typically not adapted to ensemble learning techniques (unless some variable/feature selection is added), as we do in Section 10.2.

10.1 Averaging / bagging

In this section, for simplicity, we consider the regression case with the square loss, noting that most results extend beyond that situation. See Exercise 10.1 below.

10.1.1 Independent datasets

The idea of bagging, and more generally of averaging methods, is to average predictions coming from estimators learned from datasets that are as independent as possible. In an idealized situation, we have m independent datasets of size n , composed of i.i.d. observations from the same distribution $p(x, y)$. We obtain for each of them an estimator $\hat{f}_\lambda^{(j)}$, where $j \in \{1, \dots, m\}$, and λ is an associated hyperparameter specific to the learning procedure. The new predictor is $\hat{f}_\lambda^{\text{bag}}$ is simply the average of all $\hat{f}_\lambda^{(j)}$.

If we denote $\text{bias}^{(j)}(x) = \mathbb{E}[\hat{f}_\lambda^{(j)}(x)] - f^*(x)$, and $\text{var}^{(j)}(x) = \text{var}[\hat{f}_\lambda^{(j)}(x)]$ (assuming x is fixed and only taking expectations with respect to the data), then they are the same for all $j \in \{1, \dots, m\}$, and the bias of $\hat{f}_\lambda^{\text{bag}}$ is the same as the base bias for a single dataset, while the variance is divided by m because the datasets are assumed independent.

Thus in the bias/variance trade-off, the selected hyperparameter will typically select a higher variance (or equivalently lower bias) estimator than for $m = 1$. We now give a few examples.

k -nearest neighbor regression. We consider the analysis from Section 6.3.2 on prediction problems over $\mathcal{X} \subset \mathbb{R}^d$, where we showed in Prop. 6.2 that the (squared) bias was upper-bounded by $8B^2 \text{diam}(\mathcal{X})^2 \left(\frac{2k}{n}\right)^{2/d}$ (for $d \geq 2$). At the same time, the variance was bounded by $\frac{\sigma^2}{k}$, where σ^2 is a bound on the noise variance on top of the target function f^* , while B is the Lipschitz-constant of the target function. Thus, with m replications, we get an excess risk upper-bounded by

$$\frac{\sigma^2}{km} + 8B^2 \text{diam}(\mathcal{X})^2 \left(\frac{2k}{n}\right)^{2/d}.$$

When optimizing the bound above with respect to k , we get that $k^{2/d+1} \propto \frac{n^{2/d}}{m}$, leading to $k \propto \frac{1}{m^{d/(2+d)}} n^{2/(2+d)}$. Compared to Section 6.3.2, we obtain a smaller number of neighbors (which is consistent with favoring higher variance estimators). The overall excess risk ends up being proportional to $\frac{1}{(mn)^{2/(d+2)}}$, which is exactly the rate for a dataset of $N = mn$ observations.

Thus, dividing a dataset of N observations in m chunks of $n = N/m$ observations, estimating independently, and combining linearly does not lead to an overall improved statistical behavior compared to learning all at once. Still, it can have significant computational advantages when the m estimators can be computed in parallel (and totally independently). We thus obtain a distributed algorithm with the same worst-case predictive performance as for a single machine.

Note here that there is an upper bound on the number of replications to get the same (optimal rate), as we need k to be larger than one, and thus, m cannot grow larger than $n^{2/d}$.

Exercise 10.1 *We consider k -nearest neighbor multi-category classification with a majority vote rule. What is the optimal choice of m when using independent datasets?*

Ridge regression. Following the analysis from Section 7.6.6, the variance of the ridge regression estimator was proportional to $\frac{\sigma^2}{n} \lambda^{-1/\alpha}$ and the bias proportional to $\lambda^{t/s}$ (see precise definitions in Section 7.6.6). With m replications, we thus get an excess risk proportional to $\frac{\sigma^2}{nm} \lambda^{-1/\alpha} + \lambda^{t/s}$, and the averaged estimator behaves like having $N = nm$ observations.

Again, with the proper choice of regularization parameter (lower λ than for the full dataset), there is no statistical advantage. Still, there may be a computational one, not only for parallel processing but also with a single machine, as the training time for ridge regression is super-linear in the number of observations (see the exercise below).

Exercise 10.2 Assuming that obtaining an estimator for ridge regression has running-time complexity $O(n^\beta)$ for $\beta \geq 1$ for n observations, what is the complexity of using a split of the data into m chunks? What is the optimal value of m ?

Beyond independent datasets. Having independent datasets may not be possible, and one typically needs to artificially “create” such replicated datasets from a single one, which is precisely what bagging methods will do in the next section, with still a reduced variance, but this time potentially higher bias.

10.1.2 Bagging

We consider data sets $\mathcal{D}^{(b)}$, obtained with random weights $v_i^{(b)} \in \mathbb{R}_+$, $i = 1, \dots, n$. For the bootstrap, we consider m samples from the original n data points with replacement, which corresponds to $v_i^{(b)} \in \mathbb{N}$, $i = 1, \dots, n$, that sum to n . We study $m = \infty$ for simplicity, that is, infinitely many replications (in practice, the infinite m behavior can be achieved with moderate m 's).

Infinitely many bootstrap replications lead to a form of stabilization, which is important for highly variable predictors (which usually imply a large estimation variance).

For linear estimators (in the definition of Section 6.2.1) with the square loss, such as kernel ridge regression or local averaging, this leads to another linear estimator. Therefore, this provides alternative ways of regularizing, which typically may not provide a strong statistical gain over existing methods, but provide a computational gain, in particular when each estimator is very efficient to compute. Overall, as shown below for 1-nearest-neighbor, bagging will lower variance while increasing the bias, thus leading to trade-offs that are common in regularizing methods.

For simplicity, we will consider averaging estimators obtained by randomly selecting s observations from the n available ones, doing this many times (infinitely many for the analysis), and averaging the predictions.

Exercise 10.3 Show that when sampling n elements with replacement from n items, the expected fraction of distinct items is $1 - (1 - 1/n)^n$, and that it tends to $1 - 1/e$.

One-nearest neighbor regression. We focus on the 1-nearest neighbor estimator where the strong effect of bagging is striking. The analysis below follows from [Biau et al. \(2010\)](#). The key observation is that if we denote $(x_{(i)}(x), y_{(i)}(x))$ the pair of observations, which is the i -th nearest neighbor of x from the dataset x_1, \dots, x_n (ignoring ties), then we can write the bagged estimate as

$$\hat{f}(x) = \sum_{i=1}^n V_i y_{(i)}(x),$$

where the non-negative weights V_i sum to one, and *do not depend on x* . The weight V_i is the probability that the i -th nearest neighbor of x is the 1-nearest-neighbor of x in a uniform subsample of size s . We consider sampling without replacement and leave sampling with replacement as an exercise (see [Biau et al., 2010](#), for more details). We assume $s \geq 2$.

To select the i -th nearest neighbor as the 1-nearest-neighbor in a subsample, we need that the i -th nearest neighbor is selected but none of the closer neighbors, which leaves $s - 1$ elements to choose among $n - i$ possibilities. This shows, that if $i > n - s + 1$, then $V_i = 0$, while otherwise $V_i = \binom{n}{s}^{-1} \binom{n-i}{s-1}$, as the total number of subsets of size s is $\binom{n}{s}$ and there are $\binom{n-i}{s-1}$ relevant ones.

We can now use the reasoning from Section 6.3.2. Since for any x , the weights given to each observation (once they are ordered in the distance to x) are V_1, \dots, V_n , the variance term is equal to $\sum_{i=1}^n V_i^2$. To obtain a bound, we note that for $i \leq n - s + 1$,

$$V_i = \frac{s}{n-s+1} \frac{\prod_{j=0}^{s-2} (n-i-j)}{\prod_{j=0}^{s-2} (n-j)} = \frac{s}{n-s+1} \prod_{j=0}^{s-2} \left(1 - \frac{i}{n-j}\right) \leq \frac{s}{n-s+1} \prod_{j=0}^{s-2} \left(1 - \frac{i}{n}\right),$$

leading to, upper-bounding the sum by an integral:

$$\begin{aligned} \sum_{i=1}^n V_i^2 &\leq \frac{s^2}{(n-s+1)^2} \sum_{i=1}^n \left(1 - \frac{i}{n}\right)^{2(s-1)} \leq \frac{ns^2}{(n-s+1)^2} \int_0^1 (1-t)^{2(s-1)} dt \\ &\leq \frac{ns^2}{(n-s+1)^2} \frac{1}{2s-1} \leq \frac{ns}{(n-s+1)^2} = \frac{s}{n} \frac{1}{(1+1/n-s/n)^2}. \end{aligned}$$

For the bias term, we need to bound $\sum_{i=1}^n V_i \cdot \mathbb{E}[\|x - x_{(i)}(x)\|^2]$, where the expectation is with respect to the data and the test point x . We note here that by definition of V_i , and conditioning on the data and x , this is the expectation of the distance to the first nearest neighbor from a random sample of size s , and thus, by Lemma 6.1, less than $4\text{diam}(\mathcal{X})^2 \frac{1}{s^{2/d}}$ if $d \geq 2$ (which we now assume).

Thus, the overall excess risk is less than

$$4B^2 \text{diam}(\mathcal{X})^2 \frac{1}{s^{2/d}} + \frac{s}{n} \frac{1}{(1+1/n-s/n)^2},$$

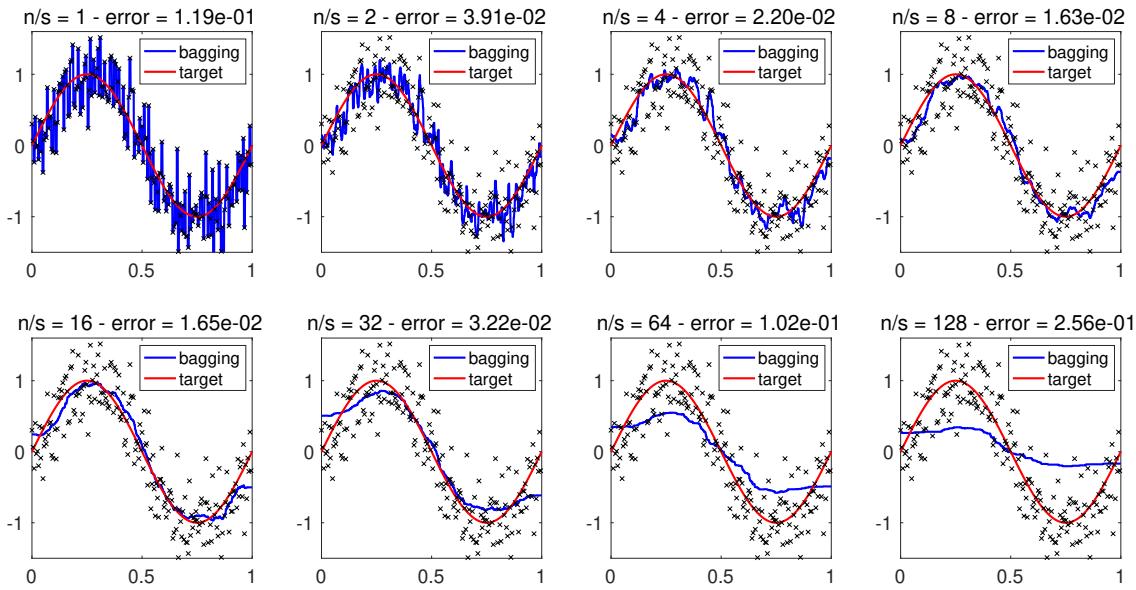


Figure 10.1: Subsampling estimates with $m = 20$ subsampled datasets, for varying subsampling ratios n/s , with an estimation of the testing error. When n/s is equal to one, we recover the 1-nearest neighbor classifier (which overfits), and when n/s grows, we get better fits until underfitting kicks in.

which we can balance by choosing $s^{1+2/d} \propto n$, leading to the same performance as k -nearest neighbor for a well chosen k , but now with a bagged estimate.

In Figure 10.1, simulations in one dimension are plotted, showing the regularizing effects of bagging; we see that when $s = n$ (no subsampling), we recover the 1-nearest neighbor estimate, and when s decreases, the variance indeed decreases, while the bias increases.

10.2 Random projections and averaging

In the previous section, we reweighted observations to be able to re-run the original algorithm. This can also be done through random projections of all observations. Such random projections can be performed in several ways: (a) for data in \mathbb{R}^d by selecting s of the d variables, (b) still for data in \mathbb{R}^d , by projecting the data in a more general s -dimensional subspace, (c) for kernel methods, using random features such as presented in Section 7.4. Such random projections can also be done to reduce the number of samples while keeping the dimension fixed.

In this section, we consider random projections for ordinary least-squares (with the same notation as in Chapter 3, with $y \in \mathbb{R}^n$ the response vector and $\Phi \in \mathbb{R}^{n \times d}$ the design matrix), in two settings:

- (a) *Sketching*: replacing $\min_{\theta \in \mathbb{R}^d} \|y - \Phi\theta\|_2^2$ by $\min_{\theta \in \mathbb{R}^d} \|Sy - S\Phi\theta\|_2^2$, where $S \in \mathbb{R}^{s \times n}$ is an i.i.d. Gaussian matrix (with independent zero mean and unit variance elements). This is an idealization of subsampling, as done in the previous section. Here we typically have $n > s > d$ (more observations than the feature dimension), and one of the benefits of sketching is to be able to store a reduced representation of the data ($\mathbb{R}^{s \times d}$ instead of $\mathbb{R}^{n \times d}$).
- (b) *Random projection*: replacing $\min_{\theta \in \mathbb{R}^d} \|y - \Phi\theta\|_2^2$ by $\min_{\eta \in \mathbb{R}^s} \|y - \Phi S\eta\|_2^2$ where $S \in \mathbb{R}^{d \times s}$ is a more general sketching matrix. Here we typically have $d > n > s$ (high-dimensional situation). The benefits of random projection are two-fold: reduction in computation time and regularization. This corresponds to replacing the corresponding feature vectors $\varphi(x) \in \mathbb{R}^d$ by $S^\top \varphi(x) \in \mathbb{R}^s$. We will consider Gaussian matrices, but also subsampling, and draw connections with kernel methods.

In the next sections, we study these precisely for the ordinary least-squares framework (it could also be done for ridge regression). We first briefly mention a commonly used related approach.

Random forests. A popular algorithm called random forests (Breiman, 2001) mixes both dimension reduction by projection and bagging: decision trees are learned on a bootstrapped sample of the data, with selecting a random subset of features at every splitting decision. This algorithm has nice properties (invariance to rescaling of the variables, robustness in high dimension due to the random feature selection, and can be extended in many ways. See Biau and Scornet (2016) for details.

10.2.1 Gaussian sketching

Following Section 3.3 on ordinary least-squares, we consider a design matrix $\Phi \in \mathbb{R}^{n \times d}$ with rank d (that is, $\Phi^\top \Phi \in \mathbb{R}^{d \times d}$ invertible), which implies $n \geq d$. We consider $s > d$ Gaussian random projections, with typically $s \leq n$, but this is not necessary in the analysis below.

The estimator $\hat{\theta}^{(j)}$ is obtained by using $S^{(j)} \in \mathbb{R}^{s \times n}$, with $j = 1, \dots, m$, where m denotes the number of replications. We then consider $\hat{\theta} = \frac{1}{m} \sum_{j=1}^m \hat{\theta}^{(j)}$. When $m = 1$, this is a single sketch.

We will consider the same assumptions as in Section 3.5, that is, $y = \Phi\theta_* + \varepsilon$, where $\varepsilon \in \mathbb{R}^n$ has independent zero-mean components with variance σ^2 , and $\theta_* \in \mathbb{R}^d$. Our goal is to compute the fixed design error $\frac{1}{n} \mathbb{E}_{\varepsilon, S} \|\Phi\hat{\theta} - \Phi\theta_*\|_2^2$, where we take both expectations, with respect to the learning problem (the noise vector ε) and the added randomization (the sketching matrices $S^{(j)}$, $j = 1, \dots, m$).

In order to compute this error, we first need to compute expectations and variances with respect to the random projections, assuming that ε is fixed.

Since the Gaussian matrices $S^{(j)}$ are invariant by left and right multiplication by an orthogonal matrix, we can assume that the singular value decomposition of $\Phi = UDV^\top$, where $V \in \mathbb{R}^{d \times d}$ is orthogonal (i.e., $V^\top V = VV^\top = I$), $D \in \mathbb{R}^{d \times d}$ is an invertible diagonal matrix, and $U \in \mathbb{R}^{n \times d}$ has orthonormal columns (i.e., $U^\top U = I$), is such that $U = \begin{pmatrix} I \\ 0 \end{pmatrix}$, and that we can write $S^{(j)} = (S_1^{(j)} \ S_2^{(j)})$ with $S_1^{(j)} \in \mathbb{R}^{s \times d}$ and $S_2^{(j)} \in \mathbb{R}^{s \times (n-d)}$. We can also split y as $y = \begin{pmatrix} y_1 \\ y_2 \end{pmatrix}$ for $y_1 \in \mathbb{R}^d$ and $y_2 \in \mathbb{R}^{n-d}$.

We can write down the normal equations that define $\hat{\theta}^{(j)}$, for each $j \in \{1, \dots, m\}$, that is, $(\Phi^\top (S^{(j)})^\top S^{(j)} \Phi) \hat{\theta}^{(j)} = \Phi^\top (S^{(j)})^\top S^{(j)} y$, leading to $\hat{\theta}^{(j)} = (\Phi^\top (S^{(j)})^\top S^{(j)} \Phi)^{-1} \Phi^\top (S^{(j)})^\top S^{(j)} y$.¹ Using the assumptions above regarding the SVD of Φ , we have: $S^{(j)} \Phi = S_1^{(j)} D V^\top$. We can then expand the prediction vector in \mathbb{R}^n as:

$$\begin{aligned}\Phi \hat{\theta}^{(j)} &= \Phi (\Phi^\top (S^{(j)})^\top S^{(j)} \Phi)^{-1} \Phi^\top (S^{(j)})^\top S^{(j)} y \\ &= \begin{pmatrix} I \\ 0 \end{pmatrix} D V^\top (V D (S_1^{(j)})^\top S_1^{(j)} D V^\top)^{-1} V D (S_1^{(j)})^\top S^{(j)} y = \begin{pmatrix} I \\ 0 \end{pmatrix} ((S_1^{(j)})^\top S_1^{(j)})^{-1} (S_1^{(j)})^\top S^{(j)} y \\ &= \begin{pmatrix} I \\ 0 \end{pmatrix} ((S_1^{(j)})^\top S_1^{(j)})^{-1} (S_1^{(j)})^\top (S_1^{(j)} y_1 + S_2^{(j)} y_2) = \begin{pmatrix} y_1 + ((S_1^{(j)})^\top S_1^{(j)})^{-1} (S_1^{(j)})^\top S_2^{(j)} y_2 \\ 0 \end{pmatrix}.\end{aligned}$$

Thus, since $\mathbb{E}[S_2^{(j)}] = 0$ and $S_2^{(j)}$ is independent of $S_1^{(j)}$, we get $\mathbb{E}_{S^{(j)}}[\Phi \hat{\theta}^{(j)}] = \begin{pmatrix} y_1 \\ 0 \end{pmatrix}$, which happens to be exactly the OLS estimator $\hat{\theta}_{\text{OLS}} = \Phi (\Phi^\top \Phi)^{-1} \Phi^\top y = \begin{pmatrix} I & 0 \\ 0 & 0 \end{pmatrix} y$. Moreover, we have the model $y = \Phi \theta_* + \varepsilon$ and, if we split ε as $\varepsilon = \begin{pmatrix} \varepsilon_1 \\ \varepsilon_2 \end{pmatrix}$, we have $y = \begin{pmatrix} I \\ 0 \end{pmatrix} D V^\top \theta_* + \varepsilon$, and thus $y_2 = \varepsilon_2$. We thus get:

$$\mathbb{E}_{S^{(j)}} \left[\|\Phi \hat{\theta}^{(j)} - \mathbb{E}_{S^{(j)}} \Phi \hat{\theta}^{(j)}\|^2 \right] = \mathbb{E}_{S^{(j)}} \left[\|((S_1^{(j)})^\top S_1^{(j)})^{-1} (S_1^{(j)})^\top S_2^{(j)} \varepsilon_2\|_2^2 \right].$$

Taking the expectation with respect to ε , and using expectations for the (inverse) Wishart distribution,² this leads to

$$\begin{aligned}\mathbb{E}_{\varepsilon, S^{(j)}} \left[\|\Phi \hat{\theta}^{(j)} - \mathbb{E}_{S^{(j)}} \Phi \hat{\theta}^{(j)}\|^2 \right] &= \sigma^2 \mathbb{E}_{S^{(j)}} \left[\text{tr} \left((S_2^{(j)})^\top (S_1^{(j)}) ((S_1^{(j)})^\top S_1^{(j)})^{-2} (S_1^{(j)})^\top S_2^{(j)} \right) \right] \\ &= (n-d)\sigma^2 \mathbb{E}_{S_1^{(j)}} \left[\text{tr} \left(((S_1^{(j)})^\top S_1^{(j)})^{-1} \right) \right] = \frac{d}{s-d-1} (n-d)\sigma^2.\end{aligned}$$

¹If $s \geq d$, then $S^{(j)} \Phi$ has almost surely rank d , and thus $\hat{\theta}^{(j)}$ is uniquely defined.

²If $S \in \mathbb{R}^{a \times b}$ has independent standard Gaussian components, then $\mathbb{E}[(S^\top S)^{-1}] = \frac{1}{a-b-1} I$ if $a > b+1$, and $\mathbb{E}[SS^\top] = bI$; see https://en.wikipedia.org/wiki/Inverse-Wishart_distribution.

We can now compute the overall expected generalization error:

$$\begin{aligned}
\frac{1}{n} \mathbb{E}_{\varepsilon, S^{(j)}} \left[\left\| \frac{1}{m} \sum_{j=1}^m \Phi \hat{\theta}^{(j)} - \Phi \theta_* \right\|_2^2 \right] &= \frac{1}{n} \mathbb{E}_\varepsilon \left[\left\| \frac{1}{m} \sum_{j=1}^m \mathbb{E}_{S^{(j)}} [\Phi \hat{\theta}^{(j)}] - \Phi \theta_* \right\|_2^2 \right] \\
&\quad + \frac{1}{nm} \mathbb{E}_{\varepsilon, S^{(1)}} \left[\left\| \Phi \hat{\theta}^{(1)} - \mathbb{E}_{S^{(1)}} \Phi \hat{\theta}^{(1)} \right\|^2 \right] \\
&= \frac{1}{n} \mathbb{E}_\varepsilon \left[\left\| \Phi \hat{\theta}_{\text{OLS}} - \Phi \theta_* \right\|_2^2 \right] + \sigma^2 \frac{d}{nm} \frac{n-d}{s-d-1} \\
&= \sigma^2 \frac{d}{n} + \sigma^2 \frac{d}{nm} \frac{n-d}{s-d-1}.
\end{aligned}$$

Thus, when m or s tends to infinity, we recover the traditional OLS behavior, while for m and s finite, the performance degrades gracefully. Moreover, when $s = n$, even for $m = 1$, we get essentially twice the performance of the OLS estimator. We note that in order to get the same performance as OLS (up to a factor of 2), we need $m = \frac{n-d}{s-d-1} \sim \frac{n}{s}$ replications.

As in the previous section, there is no statistical gain (here compared to OLS), but only potentially a computational one. See, e.g., [Dobriban and Liu \(2019\)](#) for other criteria and sketching matrices.

Beyond Gaussian sketching. In this section, we have chosen a Gaussian sketching matrix S . This made the analysis simple because of the properties of the Gaussian distribution (invariance by rotation and availability of exact expectations for inverse Wishart distributions). The analysis can be extended with more complex tools to other random sketching matrices with more attractive computational properties, such as with many zeros, leading to subsampling observations or dimensions. See [Wang et al. \(2018\)](#); [Dobriban and Liu \(2019\)](#) and references therein. For random projections below, our analysis will be applicable to more general sketches.

10.2.2 Random projections

We also consider the fixed design set-up, with a design matrix $\Phi \in \mathbb{R}^{n \times d}$ and a response vector of the form $y = \Phi \theta_* + \varepsilon$. We now assume that $n > d$ (high-dimensional set-up) and that the rank of Φ is n . For each $j \in \{1, \dots, n\}$, we consider a sketching matrix $S^{(j)} \in \mathbb{R}^{d \times s}$, for $s \leq n$ sampled independently from a distribution to be determined (we only assume that almost surely, its rank is equal to s). We then consider $\hat{\eta}^{(j)}$ as a minimizer of $\min_{\eta \in \mathbb{R}^s} \|y - \Phi S^{(j)} \eta\|_2^2$,

which is unique almost surely if $s \leq n$ (because our assumption on the rank of $S^{(j)}$), and then consider $\hat{\theta} = \frac{1}{m} \sum_{j=1}^m S^{(j)} \hat{\eta}^{(j)}$.

We thus consider the estimator $\hat{\eta}^{(j)} = ((S^{(j)})^\top \Phi^\top \Phi S^{(j)})^{-1} (S^{(j)})^\top \Phi^\top y \in \mathbb{R}^s$, obtained from the normal equation $(S^{(j)})^\top \Phi^\top \Phi S^{(j)} \hat{\eta}^{(j)} = (S^{(j)})^\top \Phi^\top y$, with denoised response vector

$$\hat{y}^{(j)} = \Phi S^{(j)} \hat{\eta}^{(j)} = \Phi S^{(j)} ((S^{(j)})^\top \Phi^\top \Phi S^{(j)})^{-1} (S^{(j)})^\top \Phi^\top y \in \mathbb{R}^n.$$

Denoting $\Pi^{(j)} = \Phi S^{(j)} ((S^{(j)})^\top \Phi^\top \Phi S^{(j)})^{-1} (S^{(j)})^\top \Phi^\top$, it is of the form $\hat{y}^{(j)} = \Pi^{(j)} y$. The matrix $\Pi^{(j)}$ is almost surely a projection matrix into an s -dimensional vector space, and its expectation is denoted $\Delta \in \mathbb{R}^{n \times n}$, and is such that $\text{tr}(\Delta) = s$. We have moreover $0 \preceq \Delta \preceq I$.

We can then compute expectations and variances:

$$\begin{aligned} \mathbb{E}_{S^{(j)}} [\hat{y}^{(j)}] &= \mathbb{E}_{S^{(j)}} [\Pi^{(j)} y] = \Delta y = \Delta [\Phi \theta_* + \varepsilon] = \Delta \varepsilon + \Delta \Phi \theta_* \\ \mathbb{E}_{S^{(j)}} [\hat{y}^{(j)}] - \Phi \theta_* &= \Delta \varepsilon + [\Delta - I] \Phi \theta_* \\ \mathbb{E}_{S^{(j)}} \|\hat{y}^{(j)} - \mathbb{E}_{S^{(j)}} [\hat{y}^{(j)}]\|_2^2 &= \mathbb{E}_{S^{(j)}} \|(\Pi^{(j)} - \Delta)y\|_2^2 = y^\top \mathbb{E}_{S^{(j)}} [(\Pi^{(j)} - \Delta)^2] y \\ &= y^\top \mathbb{E}_{S^{(j)}} [\Pi^{(j)} - \Delta \Pi^{(j)} - \Pi^{(j)} \Delta + \Delta^2] y \text{ since } \Pi^{(j)} \Pi^{(j)} = \Pi^{(j)}, \\ &= y^\top (\Delta - \Delta^2) y. \end{aligned}$$

Thus, the overall (fixed design) expected generalization error is equal to:

$$\begin{aligned} &\frac{1}{n} \mathbb{E}_{\varepsilon, S} \left\| \frac{1}{m} \sum_{j=1}^m \hat{y}^{(j)} - \Phi \theta_* \right\|_2^2 \\ &= \frac{1}{n} \mathbb{E}_\varepsilon \left[\left\| \mathbb{E}_{S^{(1)}} [\hat{y}^{(1)}] - \Phi \theta_* \right\|_2^2 + \frac{1}{m} \mathbb{E}_{S^{(1)}} \|\hat{y}^{(1)} - \mathbb{E}_{S^{(1)}} [\hat{y}^{(1)}]\|_2^2 \right] \\ &\quad \text{by taking expectations with respect to all } S^{(j)}, \\ &= \frac{1}{n} \mathbb{E}_\varepsilon \left[\|\Delta \varepsilon + [\Delta - I] \Phi \theta_*\|_2^2 + \frac{1}{m} y^\top (\Delta - \Delta^2) y \right] \text{ using the expressions above,} \\ &= \frac{\sigma^2}{n} \text{tr}(\Delta^2) + \frac{1}{n} \theta_*^\top \Phi^\top [I - \Delta]^2 \Phi \theta_* + \frac{1}{nm} [\sigma^2 (\text{tr}(\Delta) - \text{tr}(\Delta^2)) + \theta_*^\top \Phi^\top (\Delta - \Delta^2) \Phi \theta_*] \\ &\quad \text{using the model } y = \Phi \theta_* + \varepsilon \text{ and the fact that } \mathbb{E}[\varepsilon] = 0 \text{ and } \mathbb{E}[\varepsilon \varepsilon^\top] = \sigma^2 I, \\ &= \frac{\sigma^2}{n} \left(1 - \frac{1}{m}\right) \text{tr}(\Delta^2) + \frac{\sigma^2 s}{nm} + \frac{1}{n} \theta_*^\top \Phi^\top [\Delta - I]^2 \Phi \theta_* + \frac{1}{nm} \theta_*^\top \Phi^\top (\Delta - \Delta^2) \Phi \theta_* \\ &= \frac{\sigma^2}{n} \left(1 - \frac{1}{m}\right) \text{tr}(\Delta^2) + \frac{\sigma^2 s}{nm} + \frac{1}{n} \theta_*^\top \Phi^\top [I - \Delta + (\frac{1}{m} - 1)(\Delta - \Delta^2)] \Phi \theta_* \\ &\leq \frac{\sigma^2 s}{n} + \frac{1}{n} \theta_*^\top \Phi^\top [I - \Delta] \Phi \theta_*, \text{ since } \Delta^2 \preceq \Delta, \end{aligned}$$

which is the value for $m = 1$ (single replication). Note that the expectation (before taking the bound) is decreasing in m . We now follow [Kabán \(2014\)](#); [Thanei et al. \(2017\)](#) to bound the matrix $I - \Delta$.

Since Δ is the expectation of a projection matrix, we already know that $0 \preceq \Delta \preceq I$. We omit the superscript (j) for clarity, and consider $\Pi = \Phi S (S^\top \Phi^\top \Phi S)^{-1} S^\top \Phi$. For any vector $z \in \mathbb{R}^n$, we consider:

$$\begin{aligned} z^\top (I - \Delta) z &= \mathbb{E}_S [z^\top (I - \Pi) z] = \mathbb{E}_S [z^\top z - z^\top \Phi S (S^\top \Phi^\top \Phi S)^{-1} S^\top \Phi^\top z] \\ &= \mathbb{E}_S \left[\min_{u \in \mathbb{R}^s} \|z - \Phi S u\|_2^2 \right] \text{ by definition of projections,} \\ &\leq \mathbb{E}_S \left[\min_{v \in \mathbb{R}^d} \|z - \Phi S S^\top v\|_2^2 \right] \text{ by minimizing over a smaller subspace,} \\ &\leq \min_{v \in \mathbb{R}^d} \mathbb{E}_S [\|z - \Phi S S^\top v\|_2^2] \text{ by properties of the expectation.} \end{aligned}$$

We can expand to get:

$$\mathbb{E}_S [\|z - \Phi S S^\top v\|_2^2] = \|z\|_2^2 - 2z^\top \Phi \mathbb{E}_S [S S^\top] v + v^\top \mathbb{E}_S [S S^\top \Phi^\top \Phi S S^\top] v,$$

leading to, after selecting the optimal v as $v = (\mathbb{E}_S [S S^\top \Phi^\top \Phi S S^\top])^{-1} \mathbb{E}_S [S S^\top] \Phi^\top z$,

$$z^\top (I - \Delta) z \leq z^\top \left(I - \Phi \mathbb{E}_S [S S^\top] (\mathbb{E}_S [S S^\top \Phi^\top \Phi S S^\top])^{-1} \mathbb{E}_S [S S^\top] \Phi^\top \right) z.$$

We then need to apply to $z = \Phi \theta_*$, and get:

$$\theta_*^\top \Phi^\top [I - \Delta] \Phi \theta_* \leq \theta_*^\top \Phi^\top \left(I - \Phi \mathbb{E}_S [S S^\top] (\mathbb{E}_S [S S^\top \Phi^\top \Phi S S^\top])^{-1} \mathbb{E}_S [S S^\top] \Phi^\top \right) \Phi \theta_*.$$

Thus, we get an overall upper bound of

$$\frac{\sigma^2 s}{n} + \frac{1}{n} \theta_*^\top \Phi^\top \left(I - \Phi \mathbb{E}_S [S S^\top] (\mathbb{E}_S [S S^\top \Phi^\top \Phi S S^\top])^{-1} \mathbb{E}_S [S S^\top] \Phi^\top \right) \Phi \theta_*.$$

As shown below for special cases, we obtain a bias-variance trade-off similar to Eq. (3.6) for ridge regression in Section 3.6, but now with random projections. Note that in the fixed design setting, there is no explosion of the testing performance when $s = n$ (as opposed to the random design setting studied in Section 11.2 in the context of “double descent”).

Gaussian projections. If we assume Gaussian random projections, with $S \in \mathbb{R}^{d \times s}$ with independent standard Gaussian components, we get, from properties of the Wishart distribution:³

$$\mathbb{E}_S [S S^\top] = sI \text{ and } \mathbb{E}_S [S S^\top \Phi^\top \Phi S S^\top] = s(s+1)\Phi^\top \Phi + s \text{tr}(\Phi^\top \Phi)I.$$

³If $W = S_1 S_1^\top$ for $S_1 \in \mathbb{R}^{n \times s}$ with independent standard Gaussian components, then $\mathbb{E}[W] = sI$ and for an $n \times n$ diagonal matrix D we have $\mathbb{E}[WD^2W] = s(s+1)D^2 + s \text{tr}(D^2)I$.

We then get:

$$\begin{aligned}
\theta_*^\top \Phi^\top [I - \Delta] \Phi \theta_* &\leq \theta_*^\top \Phi^\top \left(I - \Phi \mathbb{E}_S [SS^\top] (\mathbb{E}_S [SS^\top \Phi^\top \Phi SS^\top])^{-1} \mathbb{E}_S [SS^\top] \Phi^\top \right) \Phi \theta_* \\
&= \theta_*^\top \Phi^\top \left(I - s^2 \Phi (s(s+1) \Phi^\top \Phi + s \text{tr}(\Phi^\top \Phi) I)^{-1} \Phi^\top \right) \Phi \theta_* \\
&= \theta_*^\top \Phi^\top \Phi (\Phi^\top \Phi + \text{tr}(\Phi^\top \Phi) I) ((s+1) \Phi^\top \Phi + \text{tr}(\Phi^\top \Phi) I)^{-1} \theta_* \\
&\leq 2 \text{tr}(\Phi^\top \Phi) \cdot \theta_*^\top \Phi^\top \Phi ((s+1) \Phi^\top \Phi + \text{tr}(\Phi^\top \Phi) I)^{-1} \theta_* \\
&\leq 2 \text{tr}(\Phi^\top \Phi) \frac{\|\theta_*\|_2^2}{s+1}.
\end{aligned}$$

The overall excess risk is then less than

$$\frac{\sigma^2 s}{n} + \frac{2}{n} \text{tr}(\Phi^\top \Phi) \frac{\|\theta_*\|_2^2}{s+1}, \quad (10.1)$$

which is exactly of the form in Eq. (3.6) with $s \sim \frac{\text{tr}(\Phi^\top \Phi)}{\lambda}$. We can consider other sketching matrices, with additional properties, such as sparsity (see the exercise below).

Exercise 10.4 We consider a sketching matrix $S \in \mathbb{R}^{d \times s}$, where each column is equal to one of the d canonical basis vectors of \mathbb{R}^d , selected uniformly at random and independently. Compute $\mathbb{E}[SS^\top]$, as well as, $\mathbb{E}_S [SS^\top \Phi^\top \Phi SS^\top]$, as well as a bound similar to Eq. (10.1).

Kernel methods. (♦) The random projection idea can be extended to kernel methods from Chapter 7. We consider the kernel matrix $K = \Phi \Phi^\top \in \mathbb{R}^{n \times n}$, and the assumption $y = \Phi \theta_* + \varepsilon$ with $\|\theta_*\|_2$ bounded, is turned into $y = y_* + \varepsilon$ with $y_*^\top K^{-1} y_*$ bounded. This corresponds to $y_* = K \alpha$, with an RKHS norm $\alpha^\top K \alpha$. We then consider a random “sketch” $\hat{\Phi} \in \mathbb{R}^{n \times s}$ and an approximate kernel matrix \hat{K} . We then learn with $\hat{y} = \hat{\Phi} (\hat{\Phi}^\top \hat{\Phi})^{-1} \hat{\Phi}^\top y$. The matrix Π above is then $\Pi = \hat{\Phi} (\hat{\Phi}^\top \hat{\Phi})^{-1} \hat{\Phi}^\top$, and for the analysis, we need to compute its expectation Δ . We have, following the same reasoning as above:

$$\begin{aligned}
z^\top (I - \Delta) z &= \mathbb{E}_{\hat{\Phi}} [z^\top (I - \Pi) z] = \mathbb{E}_{\hat{\Phi}} [z^\top z - z^\top \hat{\Phi} (\hat{\Phi}^\top \hat{\Phi})^{-1} \hat{\Phi}^\top z] \\
&= \mathbb{E}_{\hat{\Phi}} \left[\min_{u \in \mathbb{R}^s} \|z - \hat{\Phi} u\|_2^2 \right] \text{ by definition of projections,} \\
&\leq \mathbb{E}_{\hat{\Phi}} \left[\min_{v \in \mathbb{R}^n} \|z - \hat{\Phi} \hat{\Phi}^\top v\|_2^2 \right] \text{ by minimizing over a smaller subspace,} \\
&\leq \min_{v \in \mathbb{R}^n} \mathbb{E}_{\hat{\Phi}} \left[\|z - \hat{\Phi} \hat{\Phi}^\top v\|_2^2 \right] \text{ by properties of the expectation.}
\end{aligned}$$

We can expand to get:

$$\mathbb{E}_{\hat{\Phi}} \left[\|z - \hat{\Phi} \hat{\Phi}^\top v\|_2^2 \right] = \|z\|_2^2 - 2z^\top \mathbb{E}_{\hat{\Phi}} [\hat{\Phi} \hat{\Phi}^\top] v + v^\top \mathbb{E}_{\hat{\Phi}} [\hat{\Phi} \hat{\Phi}^\top \hat{\Phi} \hat{\Phi}^\top] v,$$

leading to, after selecting the optimal v as $v = (\mathbb{E}_{\hat{\Phi}}[\hat{\Phi}\hat{\Phi}^\top \hat{\Phi}\hat{\Phi}^\top])^{-1}\mathbb{E}_{\hat{\Phi}}[\hat{\Phi}\hat{\Phi}^\top]z$,

$$z^\top(I - \Delta)z \leq z^\top \left(I - \mathbb{E}_{\hat{\Phi}}[\hat{\Phi}\hat{\Phi}^\top](\mathbb{E}_{\hat{\Phi}}[\hat{\Phi}\hat{\Phi}^\top \hat{\Phi}\hat{\Phi}^\top])^{-1}\mathbb{E}_{\hat{\Phi}}[\hat{\Phi}\hat{\Phi}^\top] \right) z.$$

We then need to apply to $z = y_*$, we get that

$$\theta_*^\top \Phi^\top [I - \Delta] \Phi \theta_* \leq y_*^\top \left(I - \mathbb{E}_{\hat{\Phi}}[\hat{\Phi}\hat{\Phi}^\top](\mathbb{E}_{\hat{\Phi}}[\hat{\Phi}\hat{\Phi}^\top \hat{\Phi}\hat{\Phi}^\top])^{-1}\mathbb{E}_{\hat{\Phi}}[\hat{\Phi}\hat{\Phi}^\top] \right) y_*.$$

We can for example consider each column of $\hat{\Phi}$ to be sampled from a normal distribution with mean zero and covariance matrix K , for which we have:

$$\mathbb{E}_{\hat{\Phi}}[\hat{\Phi}\hat{\Phi}^\top] = sK \quad \text{and} \quad \mathbb{E}_{\hat{\Phi}}[\hat{\Phi}\hat{\Phi}^\top \hat{\Phi}\hat{\Phi}^\top] = s(s+1)K^2 + s \text{tr}(K) \cdot K.$$

This leads to the bound $\frac{\sigma^2 s}{n} + \frac{2}{n} \text{tr}(K) \frac{y_*^\top K^{-1} y_*}{s+1}$, which is exactly the bound in Eq. (10.1) in the kernel context. However, it is not interesting in practice as it requires to compute K and typically a square root to sample from the multivariate Gaussian distribution.

In practice, many kernels come with a random feature expansion of the form $k(x, x') = \mathbb{E}_v[\varphi(x, v)\varphi(x', v)]$, such that $|\varphi(x, v)| \leq R$ almost surely (as presented in Section 7.4). we can then take for each column of $\hat{\Phi}$ the vector $(\varphi(x_1, v), \dots, \varphi(x_n, v))^\top \in \mathbb{R}^n$, for a random independent v . We have then $\mathbb{E}[\hat{\Phi}\hat{\Phi}^\top] = sK$ by construction, while a short calculation lest as an exercise shows that the second-order moment can be bounded as

$$\mathbb{E}_{\hat{\Phi}}[\hat{\Phi}\hat{\Phi}^\top \hat{\Phi}\hat{\Phi}^\top] \leq s(s-1)K + nsR^2K.$$

This leads to the bound $\frac{\sigma^2 s}{n} + \frac{2}{n} R^2 \frac{y_*^\top K^{-1} y_*}{s+1}$, which is almost the same as above, but with now an efficient practical algorithm.

Experiments. In Figure 10.2, we consider a polynomial regression problem in dimension $d_x = 20$, with polynomials of degree at most 2, and thus a feature space of dimension $d = 1 + d_x + d_x(d_x + 1)/2 = 231$, and compare ridge regression with Gaussian random projections. We see a better performance as m grows, which is consistent with our bounds.

10.3 Boosting

In the previous section, we have focused on uniformly combining the outputs (e.g., plain averaging) of estimators obtained by randomly reweighted versions of the original datasets. Reweighting was performed independently of the performance of the resulting prediction functions, and the training procedures for all predictors could be done in parallel. In this

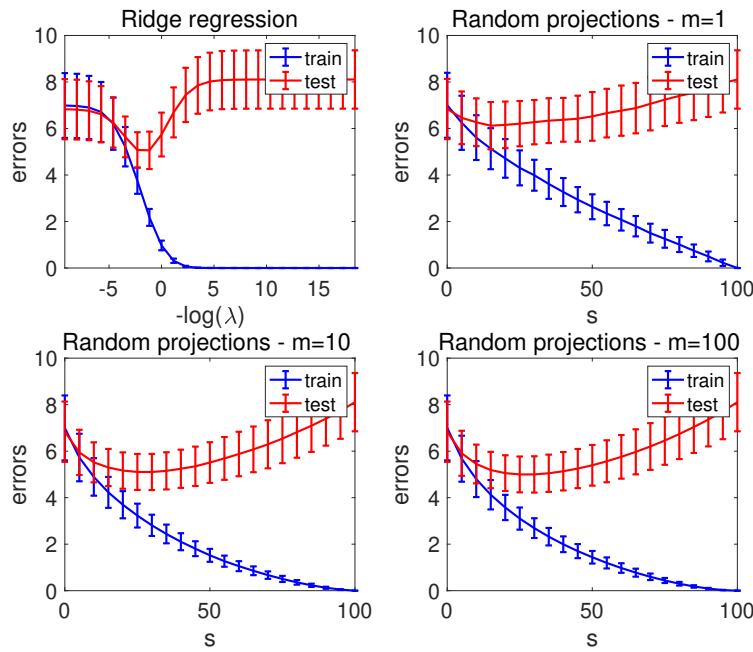


Figure 10.2: Polynomial regression in dimension 20, with polynomials of degree at most 2, with $n = 100$. Top left: training and testing errors for ridge regression in the fixed design setting (the input data are fixed and only the noise variables are resampled for computing the test error). All other plots: training and testing errors for Gaussian random projections, with different numbers of random projections, $m = 1$ (top right), $m = 10$ (bottom left), and $m = 100$ (bottom right). All curves are averaged over 100 replications (of the noise variables and the random projections).

section, we explore *sequential* reweightings of the training datasets that depend on the current mistakes made by the current prediction functions.

In the early boosting procedures adapted to binary classification, the original learning procedure was used directly on a reweighted version, e.g., Adaboost (see, e.g., [Freund et al., 1999](#)). We present a version of boosting procedures often referred to as “gradient boosting”, which is adapted to real-valued outputs, as done in the rest of the book (noting that for classification, we can use convex surrogates).

10.3.1 Problem set-up

Given an input space \mathcal{X} , and n observations $(x_i, y_i) \in \mathcal{X} \times \mathbb{R}$, $i = 1, \dots, n$, we are given a set of predictors $\varphi(w, \cdot) : \mathcal{X} \rightarrow \mathbb{R}$, for $w \in \mathcal{W}$, with \mathcal{W} typically a compact subset of \mathbb{R}^d .

The main assumption is that given weights $\alpha \in \mathbb{R}^n$, one can “easily” find the function $\varphi(w, \cdot)$ that minimizes

$$\sum_{i=1}^n \alpha_i \varphi(w, x_i),$$

that is the correlation between α and the n outputs of $\varphi(w, \cdot)$ on the n observations. In this section, for simplicity, we assume that this minimization can be done exactly. This is often referred to as the “weak learner” assumption. Many examples are available, such as:

- Linear stumps for $\mathcal{X} = \mathbb{R}^d$: $\varphi(w, x) = \pm(w_0^\top x + w_1)_+$, with sometimes the restriction that w has only non-zero components along a single coordinate (where the weak learning tractability assumption is indeed verified). This will lead to a predictor, which is a one-hidden layer neural network, but learned in a sequential way (rather than by gradient descent on the empirical risk).
- Decision trees for $\mathcal{X} = \mathbb{R}^d$: we consider here the space of piecewise constant functions of x , where the pieces with constant values are obtained by recursively partitioning the input space into half-spaces with normals along one of the coordinate axes. In this situation, the set of functions is more easily characterized through the estimation algorithm. See [Chen and Guestrin \(2016\)](#) for an efficient implementation of a boosting algorithm based on decision trees (referred to as “XGBoost”).

Boosting procedures will make sequential calls to the weak learner oracle that outputs $w_1, \dots, w_t \in \mathcal{W}$ with t the number of iterations, and *linearly combine* the function $\varphi(w_1, \cdot), \dots, \varphi(w_t, \cdot)$ (often with non-negative weights). Therefore, the set of predictors that are explored are not only the functions $\varphi(w, \cdot)$, but all linear combinations, that is, functions of the form

$$f(x) = \int_{\mathcal{W}} \varphi(w, x) d\nu(w), \quad (10.2)$$

for ν a positive measure on \mathcal{W} , which we assume to be with finite mass.

To avoid overfitting, some norm that will be explicitly or implicitly controlled need to be defined. As done in Section 9.3.2 with neural networks, we will consider an L_1 -norm, namely, since we have assumed that the measure is positive, the total mass of ν , that is:

$$\int_{\mathcal{W}} d\nu(w).$$

For functions $f : \mathcal{X} \rightarrow \mathbb{R}$ that can be represented as integrals in Eq. (10.2), the minimal value of $\int_{\mathcal{W}} d\nu(w)$ is referred to as the “variation norm” (Kurková and Sanguineti, 2001), or the “atomic norm” (Chandrasekaran et al., 2012), of f , and the set of functions with finite norm will be denoted \mathcal{F}_1 , with a norm γ_1 . Like in Section 9.3.2, this is to distinguish it from the squared norm $\int_{\mathcal{W}} \left| \frac{d\nu(w)}{d\mu(w)} \right|^2 d\mu(w)$, which corresponds to a reproducing kernel Hilbert space (see Chapter 7).

Note that by definition, for any $w \in \mathcal{W}$, $\gamma_1(\varphi(w, \cdot)) \leq 1$. We assume bounded features, that is, for all $w \in \mathcal{W}$, and $x \in \mathcal{X}$, $|\varphi(x, w)| \leq R$.

Following our traditional empirical risk minimization framework presented in Chapter 4, we consider smooth loss functions $\ell_i : \mathbb{R} \rightarrow \mathbb{R}$ that depends on x_i and y_i , such as the logistic loss $\ell_i(u_i) = \log(1 + \exp(-y_i u_i))$ when $y_i \in \{-1, 1\}$, or the square loss $\ell_i(u_i) = \frac{1}{2}(y_i - u_i)^2$. The smoothness constant is assumed to be less than G (with G assumed known, e.g., $1/4$ for the logistic loss and 1 for the square loss). This leads to a loss function $F : \mathbb{R}^n \rightarrow \mathbb{R}$, defined as $F(u) = \frac{1}{n} \sum_{i=1}^n \ell_i(u_i)$, which is (G/n) -smooth.

Statistical performance through Rademacher complexities. In order to study the generalization performance of constraining or penalizing by the variation norm defined above, we can naturally use the general framework of Rademacher complexities presented in Section 4.5. The uniform deviations for the set of predictors $g : \mathcal{X} \rightarrow \mathbb{R}$ such that $\gamma_1(g) \leq D$ on i.i.d. data x_1, \dots, x_n are controlled by the quantity

$$\mathbb{E} \left[\sup_{\gamma_1(g) \leq D} \frac{1}{n} \sum_{i=1}^n \varepsilon_i g(x_i) \right] = D \cdot \mathbb{E} \left[\sup_{w \in \mathcal{W}} \frac{1}{n} \sum_{i=1}^n \varepsilon_i \varphi(x_i, w) \right], \quad (10.3)$$

where the expectation is taken both with respect to the data x_1, \dots, x_n and the independent Rademacher random variables $\varepsilon_1, \dots, \varepsilon_n \in \{-1, 1\}$. Moreover, using tools from Section 4.5.5, we can also analyze penalized versions.

In Section 9.2.3, we computed an upperbound proportional to D/\sqrt{n} for $\varphi(x, w)$ of the form $\sigma(x^\top w)$ (which corresponds to learning a one-hidden layer neural network), showing that although the set \mathcal{W} is infinite, we can bound the uniform deviations. See another example is the exercise below.

Exercise 10.5 Given a metric space \mathcal{X} with distance d and finite diameter, we consider $\varphi(w) = \sigma(d(x, w))$, for $w \in \mathcal{W} = \mathcal{X}$. Compute an upper-bound on the Rademacher complexity in Eq. (10.3).

10.3.2 Greedy algorithms

In this section, we describe a boosting algorithm that at each iteration performs a first-order Taylor expansion at the current point (which requires to compute derivatives of the loss functions) and find the weak learner $x \mapsto \varphi(w, x)$ that makes most progress for this approximation of the risk. We thus consider the following “greedy” algorithm, starting from the zero function $g_0 = 0$, and iterating over $t \geq 1$:

- Loss gradient computations: compute $\alpha_i = \ell'_i(g_{t-1}(x_i))$ for $i \in \{1, \dots, n\}$.
- Weak learner: compute $w_t \in \mathcal{W}$ that minimizes $\sum_{i=1}^n \alpha_i \varphi(w, x_i)$ with respect to $w \in \mathcal{W}$.
- Function update: take $g_t = (1 - \rho_t)g_{t-1} + \rho_t b_t \varphi(w_t, \cdot)$ for well-chosen coefficients $\rho_t \in [0, 1]$ and $b_t \in \mathbb{R}_+$.

After time t , the prediction function g_t will be a positive linear combination of the functions $\varphi(w_u, \cdot)$, for $u \in \{1, \dots, t\}$, with only t atoms, thus leading to sparse combinations (in other words, the estimated measure ν is a sum of Diracs). There are several versions for the choice of step-sizes ρ_t and b_t (see below and Barron et al., 2008).

To provide a convergence rate for this algorithm, we formalize it as minimizing the convex function $F : \mathbb{R}^n \rightarrow \mathbb{R}$, which is smooth with constant $L = \frac{G}{n}$, with arguments u being positive linear combinations of some atoms $\psi(w) \in \mathbb{R}^n$, for $w \in \mathcal{W}$. In our particular context, we consider $\psi(w)_i = \varphi(w, x_i)$. By assumption, we have $\|\psi(w)\|_2 \leq B = \sqrt{n}R$.

We can then define a convex function $\gamma : \mathbb{R}^n \rightarrow \mathbb{R}$ as the infimum of $\int_{\mathcal{W}} d\nu(w)$ over all positive measures such that $u = \int_{\mathcal{W}} \psi(w) d\nu(w)$. This function is usually referred to as a “gauge” function associated with the convex hull \mathcal{K} of all $\psi(w)$, $w \in \mathcal{W}$. The key benefit of introducing γ is that we can cast the minimization with respect to the positive measure ν of

$$F\left(\int_{\mathcal{W}} \psi(w) d\nu(w)\right) + \lambda \int_{\mathcal{W}} d\nu(w)$$

as the minimization with respect to $u \in \mathbb{R}^n$ of

$$F(u) + \lambda \gamma(u)$$

(here $\lambda \in \mathbb{R}_+$ is a regularization parameter).

The algorithm above is then exactly equivalent to the iteration:

- Compute $w_t \in \mathcal{W}$ that minimizes $F'(u_{t-1})^\top \psi(w)$ with respect to $w \in \mathcal{W}$.
- Take $u_t = (1 - \rho_t)u_{t-1} + \rho_t b_t \psi(w_t)$, $\rho_t \in [0, 1]$, $b_t \in \mathbb{R}_+$.

We now provide an explicit convergence proof in two situations, with an $O(1/t)$ convergence rate for any $\lambda \geq 0$, and an exponential rate for $\lambda = 0$ and a strongly convex function F . We will make the assumption that 0 is in the interior of \mathcal{K} , which can be ensured by projecting \mathcal{K} into its affine hull and translating it. This assumption is made for the convergence rate, but is not explicitly needed for the algorithm. This notably implies that \mathcal{K} is the set of u such that $\gamma(u) \leq 1$. Note that given u , we never need to compute $\gamma(u)$ explicitly, which can be a difficult task.

10.3.3 Generalized conditional gradient algorithm

We will study in this section a slightly more general framework. We consider a convex smooth function $F : \mathbb{R}^n \rightarrow \mathbb{R}$, as well as a convex function G that has compact support \mathcal{C} . Our goal is to maximize $F + G$, based on gradients of F and a particular oracle on the function G , namely a linear minimization oracle: we assume that for any $z \in \mathbb{R}^n$, we can compute a minimizer of

$$\min_{u \in \mathbb{R}^n} u^\top z + G(u) = \min_{u \in \mathcal{C}} u^\top z + G(u).$$

Two cases are of particular importance:

- $G(u) = 0$ if $u \in \mathcal{C}$ and $+\infty$ otherwise, and we aim at solving $\min_{u \in \mathcal{C}} F(u)$, given the access to gradients of F and a linear minimization oracle on \mathcal{C} , a situation we have already encountered in Section 9.3.6 with the Frank-Wolfe algorithm (also known as the conditional gradient algorithm).
- $G(u) = \lambda \gamma(u)$ is $\gamma(u) \leq D$, and $+\infty$ otherwise. Here \mathcal{C} is $D\mathcal{K}$. This corresponds to our boosting algorithm when D is selected large enough. The minimization of $u^\top z + G(u)$ can then be done as follows: let $\bar{u} \in \mathcal{K}$ a minimizer of $u^\top z$ with respect to $u \in \mathcal{K}$. If $\lambda + \bar{u}^\top z \geq 0$, then we take $u = 0$, and $u = D\bar{u}$ otherwise (this can be shown by writing the optimization problem as $\min_{c \in [0, D]} \min_{\gamma(u)=c} u^\top z + \lambda \gamma(u)$).

We denote by u_* a minimizer of $F + G$. We can now define the algorithm and then show an $O(1/t)$ convergence rate.

Generalized conditional gradient algorithm. Following Bach (2015), we consider the following algorithm:

- Initialization: $u_0 \in \mathcal{C}$
- Iteration for $t \geq 1$:

$$\begin{aligned}\bar{u}_t &\in \arg \min_{u \in \mathcal{C}} F'(u_{t-1})^\top (u - u_{t-1}) + G(u), \\ u_t &= (1 - \rho_t)u_{t-1} + \rho_t\bar{u}_t.\end{aligned}$$

In this section, we consider $\rho_t = \frac{2}{t+1}$, but line searches could be considered as well (see the exercise below).

We can prove a convergence rate for the algorithm above with a very similar proof as the one for the Frank-Wolfe algorithm in Section 9.3.6. We start by using smoothness of F and convexity of G , to get:

$$\begin{aligned}F(u_t) + G(u_t) &\\ \leqslant & F(u_{t-1}) + F'(u_{t-1})^\top (u_t - u_{t-1}) + \frac{L}{2} \|u_t - u_{t-1}\|_2^2 + (1 - \rho_t)G(u_{t-1}) + \rho_t G(\bar{u}_t) \\ = & F(u_{t-1}) + \rho_t F'(u_{t-1})^\top (\bar{u}_t - u_{t-1}) + \frac{\rho_t^2 L}{2} \|\bar{u}_t - u_{t-1}\|_2^2 + (1 - \rho_t)G(u_{t-1}) + \rho_t G(\bar{u}_t).\end{aligned}$$

We can then use that $F'(u_{t-1})^\top (\bar{u}_t - u_{t-1}) + G(\bar{u}_t) \leqslant F'(u_{t-1})^\top (u_* - u_{t-1}) + G(u_*)$ (by definition of \bar{u}_t), and $F(u_{t-1}) - F(u_*) \leqslant F'(u_{t-1})^\top (u_{t-1} - u_*)$ (by convexity of F), to obtain that $F(u_t) + G(u_t)$ is less than:

$$\begin{aligned}F(u_{t-1}) + G(u_{t-1}) - \rho_t [F'(u_{t-1})^\top (u_{t-1} - \bar{u}_t) - G(\bar{u}_t) + G(u_{t-1})] + \frac{\rho_t^2 L}{2} \text{diam}(\mathcal{C})^2 \\ \leqslant F(u_{t-1}) + G(u_{t-1}) - \rho_t [F'(u_{t-1})^\top (u_{t-1} - u_*) - G(u_*) + G(u_{t-1})] + \frac{\rho_t^2 L}{2} \text{diam}(\mathcal{C})^2 \\ \leqslant F(u_{t-1}) + G(u_{t-1}) - \rho_t [F(u_{t-1}) - F(u_*) - G(u_*) + G(u_{t-1})] + \frac{\rho_t^2 L}{2} \text{diam}(\mathcal{C})^2.\end{aligned}$$

This leads to

$$F(u_t) + G(u_t) - [F(u_*) + G(u_*)] \leqslant (1 - \rho_t) \left(F(u_t) + G(u_t) - [F(u_*) + G(u_*)] \right) + \frac{\rho_t^2 L}{2} \text{diam}(\mathcal{C})^2,$$

and thus, following the same reasoning as in Section 9.3.6, for $\rho_t = 2/(t+1)$:

$$F(u_t) + G(u_t) - [F(u_*) + G(u_*)] \leqslant \frac{2L}{t+1} \text{diam}(\mathcal{C})^2.$$

We thus obtain a convergence rate in $O(1/t)$ for the generalized conditional gradient algorithm, and thus for the boosting algorithm.

Exercise 10.6 (♦) In the generalized conditional gradient algorithm, we can select $\rho_t \in [0, 1]$ that minimizes $\rho_t F'(u_t)^\top (\bar{u}_t - u_{t-1}) + \frac{L\rho_t^2}{2} \|\bar{u}_t - u_{t-1}\|_2^2 + (1 - \rho_t)G(u_{t-1}) + \rho_t G(\bar{u}_t)$. Provide a convergence rate for this algorithm.

10.3.4 Linear convergence of matching pursuit (♦)

If we make the extra assumption that F is μ -strongly convex, for example, when using the square loss, we get a simplified analysis (no need for the upper-bound D), and a stronger result (linear convergence) if additional assumptions are made on the gauge function γ , and if we consider $G = 0$ (plain minimization of F). We denote by u_* a minimizer of F , which is assumed to exist.

We assume that the set \mathcal{K} is centrally symmetric and since we have assumed that 0 is in the interior of \mathcal{K} , the gauge function γ is a norm, and we denote its dual norm by γ^* (which is not its Fenchel conjugate). We now assume that $\|u\|_2 \leq \gamma(u)B$, since we can write $u = \int_{\mathcal{W}} \psi(w)d\nu(w)$, for a positive measure ν , with $\|\psi(w)\|_2 \leq B$ and $\int_{\mathcal{W}} d\nu(w) = \gamma(u)$. Moreover, we assume that $\gamma(u) \leq C\|u\|_2$, where C has to exist because of the equivalence of norms in finite dimension.

We consider the following algorithm:

- Initialization: $u_0 \in \mathcal{K}$
- Iteration for $t \geq 1$:

$$\begin{aligned} \bar{u}_t &\in \arg \min_{u \in \mathcal{K}} F'(u_{t-1})^\top (u - u_{t-1}) \\ u_t &= u_{t-1} + \alpha \bar{u}_t \text{ with } \alpha = -\frac{1}{LB^2} F'(u_{t-1})^\top \bar{u}_t = \frac{1}{LB^2} \gamma^*(F'(u_{t-1})). \end{aligned}$$

For quadratic functions, this algorithm is referred to as matching pursuit. We can now provide an exponential convergence rate. We have the upper-bound from the smoothness of F and the link between the γ -norm and the ℓ_2 -norm:

$$F(u) \leq F(u_{t-1}) + F'(u_{t-1})^\top (u - u_{t-1}) + \frac{LB^2}{2} \gamma(u - u_{t-1})^2,$$

which is minimized exactly at u_t , leading to:

$$F(u_t) \leq F(u_{t-1}) - \frac{1}{2LB^2} \gamma^*(F'(u_{t-1}))^2 \leq F(u_{t-1}) - \frac{C^2}{2LB^2} \|F'(u_{t-1})\|_2^2.$$

We can then use Łojasiewicz inequality in Lemma 5.1, to get:

$$F(u_t) - F(u_*) \leq \left(1 - \frac{\mu C^2}{LB^2}\right) [F(u_{t-1}) - F(u_*)].$$

By defining smoothness and strong-convexity with respect to the norm γ , we would get rid of the term $\frac{C^2}{B^2}$, with different values of μ and γ .

Moreover, in terms of algorithms, we can also minimize

$$F(u_{t-1}) + F'(u_{t-1})^\top \alpha \bar{u}_t + \frac{L\alpha^2}{2} \|\bar{u}_t\|_2^2,$$

which leads to the same bound but a faster algorithm, with $\alpha = -F'(u_{t-1})^\top \bar{u}_t / (L\|\bar{u}_t\|_2^2)$.

Finite \mathcal{W} . While matching pursuit can be applied for any compact set \mathcal{W} (as long as the minimization oracle is available), an interesting special case corresponds to finite sets \mathcal{W} . Given our assumptions regarding central symmetry, we can rewrite it as:

$$\min_{u \in \mathbb{R}^n} F(u) \text{ such that } \exists \alpha \in \mathbb{R}^d, u = \sum_{i=1}^d \alpha_i \psi(w_i) = \min_{\alpha \in \mathbb{R}^d} F\left(\sum_{i=1}^d \alpha_i \psi(w_i)\right).$$

For the square loss, where F is strongly-convex, the optimization problem in u is strongly-convex, and exhibits linear convergence, while the problem in α is not. However, we still see a linear convergence for gradient descent on the problem in α , but with an implicit ℓ_2 -norm prior (see next chapter for a more formal argument), while the implicit prior for matching pursuit is essentially the ℓ_1 -norm (see, e.g., Rosset et al., 2004).

10.3.5 Experiments

In this section, we compare the boosting / conditional gradient algorithm described earlier on a simple linear regression task with feature selection. This corresponds to using $F(u) = \frac{1}{2n}\|y - u\|_2^2$, which is $(1/n)$ -smooth and $(1/n)$ -strongly convex, and $\gamma(u) = \inf_{w \in \mathbb{R}^d} \|w\|_1$ such that $u = \Phi w$.

We consider $n = 100$ observations in dimension $d = 1000$, sampled from a standard Gaussian random vector. A predictor β_* with $k = 5$ non-zero values in $\{-1, 1\}$ and data are generated from a linear model with Gaussian noise. We then compare the iterates of the boosting algorithm in terms of prediction errors (left plots) and variations of weights across iterations (right plots).

We also consider a rotation of the data, so that this is not anymore a sparse problem (bottom plot). We observe linear convergence of the training errors, as proved above, but with overfitting at convergence, strong for the non-sparse case, and weak for the sparse case.

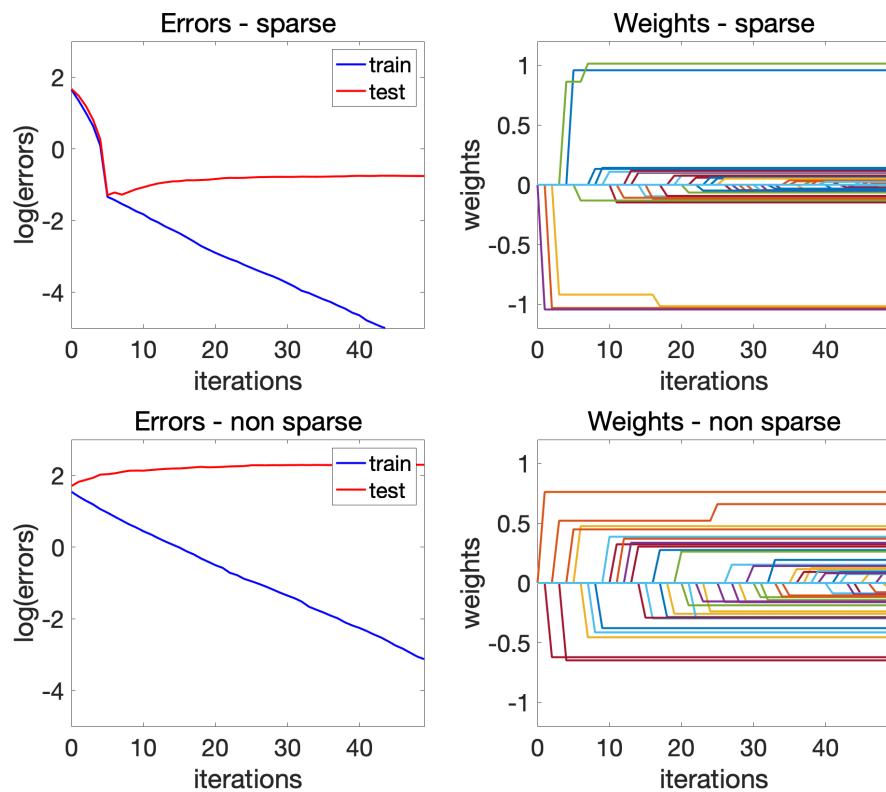


Figure 10.3: Matching pursuit algorithm on a problem with a sparse solution (top), and a non-sparse solution (bottom). Left: plots of training and testing errors. Right: plots of weights.

Chapter 11

Over-parameterized models

Chapter summary

- A model is said over-parameterized when it has sufficiently many parameters to perfectly fit the training data.
- Implicit regularization of gradient descent: for linear models, when there are several minimizers, gradient descent techniques tend to converge to the one with minimum Euclidean norm.
- Double descent: for unregularized models learned with gradient descent techniques, when the number of parameters grows and when gradient descent is used to fit the model; the performance can exhibit a second descent after the test error blows up when the number of parameters goes beyond the number of observations.
- Global convergence of gradient descent for two-layer neural networks: in the infinite width (and thus strongly over-parameterized) limit, gradient descent exhibits some globally convergent behavior for a non-convex problem, which can be analyzed for simple architectures.

In this chapter, we will cover three recent topics within learning theory, all related to high-dimensional models (such as neural networks) in the “over-parameterized” regime, where the number of parameters is larger than the number of observations. When regularization is added to the estimation procedures, we have seen in Chapter 7 and Chapter 8, that estimation can be numerically and statistically efficient by adding penalties to the empirical

risk. In this section, we consider mostly non-penalized problems, with a regularization coming from the choice of optimization algorithm (here gradient descent).



The number of parameters is not what generally characterizes the generalization capabilities of regularized learning methods. See Section 9.2.3.

11.1 Implicit bias of gradient descent

Given an optimization problem whose aim is to minimize some function $F(\theta)$ over some vector $\theta \in \mathbb{R}^d$, if there is a unique global minimizer θ_* , then the goal of optimization algorithms is to find this minimizer, that is, we want that the t -th iterate θ_t converges to θ_* . When there are multiple minimizers (thus for a function which cannot be strongly convex), we showed only that $F(\theta_t) - \inf_{\theta \in \mathbb{R}^d} F(\theta)$ is converging to zero for convex functions F (and only if a minimizer exists, see Chapter 5).

With some extra assumptions, it can be shown that the algorithm converges to one of the multiple minimizers of F (Bolte et al., 2010) (note that when F is convex, this set is also convex). But which one? This is referred to as the implicit regularization properties of optimization algorithms, and here gradient descent and its variants.

This is interesting in machine learning because, when $F(\theta)$ is the empirical loss on n observations, d is much larger than n , and no regularization is used, there are multiple minimizers. An arbitrary empirical risk minimizer is not expected to work well on unseen data, and a classical solution is to use explicit regularization (e.g., ℓ_2 -norms like in Chapter 3 and Chapter 7, or ℓ_1 -norms like in Chapter 8). In this section, we show that optimization algorithms have a similar regularizing effect. In a nutshell, gradient descent usually leads to minimum ℓ_2 -norm solutions. This shows that the chosen empirical risk minimizer is not arbitrary.

This will be explicitly shown for the quadratic loss and partially only for the logistic loss. These results will be used in subsequent sections.

11.1.1 Least-squares

We consider the least-squares objective function $F(\theta) = \frac{1}{2n} \|y - \Phi\theta\|_2^2$ from Chapter 3, with $\Phi \in \mathbb{R}^{n \times d}$ such that $d > n$ and (for simplicity) $\Phi\Phi^\top \in \mathbb{R}^{n \times n}$ invertible (this is the kernel matrix). There are thus infinitely many (a whole affine subspace) solutions such that $y = \Phi\theta$, since the column space of Φ is the entire space \mathbb{R}^n and θ has dimension $d > n$. We apply

gradient descent with step-size $\gamma \leq \frac{1}{\lambda_{\max}(\frac{1}{n}\Phi^\top\Phi)} = \frac{1}{\lambda_{\max}(\frac{1}{n}\Phi\Phi^\top)}$ starting from $\theta_0 = 0$, leading to $\theta_t = \theta_{t-1} - \frac{\gamma}{n}\Phi^\top(\Phi\theta_{t-1} - y)$, and thus

$$\begin{aligned}\Phi\theta_t - y &= \Phi\theta_{t-1} - y - \frac{\gamma}{n}\Phi\Phi^\top(\Phi\theta_{t-1} - y) = \left(I - \frac{\gamma}{n}\Phi\Phi^\top\right)(\Phi\theta_{t-1} - y) \\ &= \left(I - \frac{\gamma}{n}\Phi\Phi^\top\right)^t(\Phi\theta_0 - y) = \left(I - \frac{\gamma}{n}\Phi\Phi^\top\right)^t(-y).\end{aligned}\quad (11.1)$$

This leads to $\|\Phi\theta_t - y\|_2^2 \leq (1 - \frac{\gamma}{n}\lambda_{\max}(\Phi\Phi^\top))^{2t}\|y\|_2^2$; we thus get linear convergence of $\Phi\theta_t$ towards y .

Moreover, when started at $\theta_0 = 0$, gradient descent techniques (stochastic or not) will always have iterates θ_t that are linear combinations of rows of Φ , that is, of the form $\theta_t = \Phi^\top\alpha_t$ for some $\alpha_t \in \mathbb{R}^n$. This is an alternative algorithmic version of the representer theorem from Chapter 7.

Since $\Phi\theta_t$ converges to y , $\Phi\theta_t = \Phi\Phi^\top\alpha_t$ converges to y . Since $K = \Phi\Phi^\top$ is invertible, this means that α_t converges to $K^{-1}y$, and thus $\theta_t = \Phi^\top\alpha_t$ converges to $\Phi^\top K^{-1}y$. It turns out that this is exactly the minimum ℓ_2 -norm solution as by standard Lagrangian duality (Boyd and Vandenberghe, 2004):

$$\begin{aligned}\inf_{\theta \in \mathbb{R}^d} \frac{1}{2}\|\theta\|_2^2 \text{ such that } y = \Phi\theta &= \inf_{\theta \in \mathbb{R}^d} \sup_{\alpha \in \mathbb{R}^n} \frac{1}{2}\|\theta\|_2^2 + \alpha^\top(y - \Phi\theta) \\ &= \sup_{\alpha \in \mathbb{R}^n} \alpha^\top y - \frac{1}{2}\|\Phi^\top\alpha\|_2^2 \text{ with } \theta = \Phi^\top\alpha \text{ at optimum,} \\ &= \sup_{\alpha \in \mathbb{R}^n} \alpha^\top y - \frac{1}{2}\alpha^\top K\alpha.\end{aligned}$$

The last problem is exactly solved for $\alpha = K^{-1}y$, with at optimum $\theta = \Phi^\top\alpha$. Note that in Chapter 7, we used this formula for function interpolation to compare different RKHSs (see Prop. 7.1).

Łojasiewicz's inequality (\blacklozenge). It turns out that linear convergence shown below Eq. (11.1) can be obtained directly for any L -smooth function, for which we have the so-called Łojasiewicz's inequality:

$$\forall \theta \in \mathbb{R}^d, F(\theta) - F(\theta_*) \leq \frac{1}{2\mu}\|F'(\theta)\|_2^2, \quad (11.2)$$

for some $\mu > 0$.

We have seen in Chapter 5 that this is a consequence of μ -strong-convexity, but this can be satisfied without strong convexity. For example, for the least-squares example, we have, for any minimizer θ_* :

$$\|F'(\theta)\|_2^2 = \left\|\frac{1}{n}\Phi^\top\Phi(\theta - \theta_*)\right\|_2^2 = \frac{1}{n^2}(\theta - \theta_*)^\top\Phi^\top\Phi\Phi^\top\Phi(\theta - \theta_*) \geq \frac{\lambda_{\min}^+(\Phi\Phi^\top)}{n^2}(\theta - \theta_*)^\top\Phi^\top\Phi(\theta - \theta_*),$$

where $\lambda_{\min}^+(\Phi\Phi^\top) = \lambda_{\min}^+(\Phi^\top\Phi)$ is the smallest *non-zero* eigenvalue of $\Phi\Phi^\top$ (which is also the one of $\Phi^\top\Phi$). Thus, we have

$$\|F'(\theta)\|_2^2 \geq \frac{\lambda_{\min}^+(K)}{n^2} \|\Phi(\theta - \theta_*)\|_2^2 = \frac{2\lambda_{\min}^+(K)}{n} [F(\theta) - F(\theta_*)].$$

Thus, Eq. (11.2) is satisfied with $\mu = \frac{1}{n}\lambda_{\min}^+(K)$, where $K = \Phi\Phi^\top \in \mathbb{R}^{n \times n}$ is the kernel matrix. Note that this includes also the strongly-convex case since $\lambda_{\min}^+(\Phi^\top\Phi) \geq \lambda_{\min}(\Phi^\top\Phi)$.

When Eq. (11.2) is satisfied, we have for the t -th iterate of gradient descent with step-size $\gamma = 1/L$, following the analysis of Chapter 5 (Theorem 5.1):

$$F(\theta_t) - F(\theta_*) \leq F(\theta_{t-1}) - F(\theta_*) - \frac{1}{2L} \|F'(\theta_{t-1})\|_2^2 \leq \left(1 - \frac{\mu}{L}\right) [F(\theta_{t-1}) - F(\theta_*)].$$

Moreover, we can then show that the iterates x_t are also converging to a minimizer of F (see Bolte et al., 2010; Karimi et al., 2016, for more details).

11.1.2 Separable classification

We now consider logistic regression, that is, for $y_i \in \{-1, 1\}$, $i = 1, \dots, n$,

$$F(\theta) = \frac{1}{n} \sum_{i=1}^n \log(1 + \exp(-y_i \varphi(x_i)^\top \theta)), \quad (11.3)$$

with $\Phi \in \mathbb{R}^{n \times d}$ the design matrix such that $d > n$ and the kernel matrix $\Phi\Phi^\top \in \mathbb{R}^{n \times n}$ is invertible. In the regression setting, interpolation corresponds to $\Phi\theta = y$; in the classification setting, we predict perfectly if and only if $\text{sign}(\Phi\theta) = y$, which happens when $y \circ (\Phi\theta)$ has strictly positive components. Such an interpolator always exists (take for example the one for regression on y).

Maximum margin classifier. Since $\Phi\Phi^\top$ is invertible, there exists $\eta \in \mathbb{R}^d$ of unit norm such that $\forall i \in \{1, \dots, n\}$, $y_i \varphi(x_i)^\top \eta > 0$. We denote by η_* the one such that

$$\min_{i \in \{1, \dots, n\}} y_i \varphi(x_i)^\top \eta$$

is maximal (and thus strictly positive). We denote by $\frac{1}{\rho} > 0$ its value. This η_* solves the following problem, which can be rewritten as, using Lagrange duality:

$$\begin{aligned} \frac{1}{\rho} &= \sup_{\|\eta\|_2 \leq 1} \min_{i \in \{1, \dots, n\}} y_i \varphi(x_i)^\top \eta = \sup_{\|\eta\|_2 \leq 1, t \in \mathbb{R}} t \text{ such that } \forall i \in \{1, \dots, n\}, y_i \varphi(x_i)^\top \eta \geq t \\ &= \inf_{\alpha \in \mathbb{R}_+^n} \sup_{\|\eta\|_2 \leq 1, t \in \mathbb{R}} t + \sum_{i=1}^n \alpha_i (y_i \varphi(x_i)^\top \eta - t) \\ &= \inf_{\alpha \in \mathbb{R}_+^n} \left\| \sum_{i=1}^n \alpha_i y_i \varphi(x_i) \right\|_2 \text{ such that } \sum_{i=1}^n \alpha_i = 1, \end{aligned} \quad (11.4)$$

with $\eta \propto \sum_{i=1}^n \alpha_i y_i \varphi(x_i)$ at optimum. Moreover, by complementary slackness, a non-negative α_i is non zero only for i attaining the minimum in $\min_{i \in \{1, \dots, n\}} y_i \varphi(x_i)^\top \eta$.

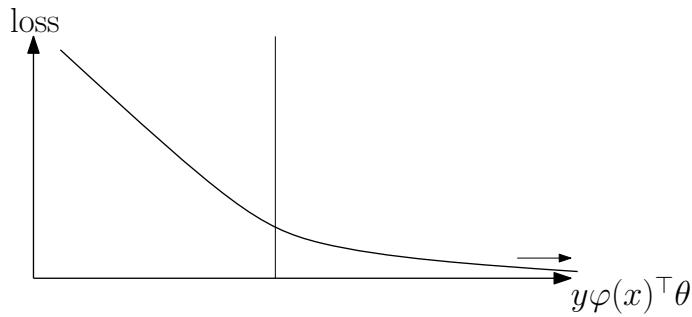
Reformulation as an SVM. Because of positive homogeneity, we want $\min_{i \in \{1, \dots, n\}} y_i \varphi(x_i)^\top \eta$ large and $\|\eta\|_2$ small, and we can decide to constrain the first and minimize the second one. In other words, we can see η_* as the unit-norm direction of the solution θ_* of:

$$\begin{aligned} \inf_{\theta \in \mathbb{R}^d} \frac{1}{2} \|\theta\|_2^2 \text{ such that } \text{Diag}(y) \Phi \theta \geq 1_n &= \inf_{\theta \in \mathbb{R}^d} \sup_{\alpha \in \mathbb{R}_+^n} \frac{1}{2} \|\theta\|_2^2 + \alpha^\top (1_n - \text{Diag}(y) \Phi \theta) \\ &= \sup_{\alpha \in \mathbb{R}_+^n} \alpha^\top 1_n - \frac{1}{2} \|\Phi^\top \text{Diag}(y) \alpha\|_2^2 \\ &\quad \text{with } \theta = \Phi^\top \text{Diag}(y) \alpha \text{ at optimum.} \end{aligned}$$

Note that above, $\text{Diag}(y) \Phi \theta \geq 1_n$ is the compact formulation of the constraint $\forall i \in \{1, \dots, n\}$, $y_i \varphi(x_i)^\top \theta \geq 1$. Given η , θ is equal to $\eta / \min_{i \in \{1, \dots, n\}} y_i \varphi(x_i)^\top \eta$, so that the optimal value of the problem above is $\frac{1}{2} \rho^2$.

The vector θ_* above is the solution of the separable SVM from Section 4.1.2 with vanishing regularization parameter, that is, of $\frac{1}{2} \|\theta\|_2^2 + C \sum_{i=1}^n (1 - y_i \varphi(x_i)^\top \theta)_+$ for C large enough. See Section 4.1.2 for an illustration.

Divergence and convergence of directions. Because the logistic loss plotted below is strictly positive and tends to zero at infinity, the function F in Eq. (11.3) has an infimum equal to zero, which is not attained. However, for any sequence θ_t such that all $y_i \varphi(x_i)^\top \theta_t$, $i = 1, \dots, n$, tend to $+\infty$, we have $F(\theta_t) \rightarrow \inf_{\theta \in \mathbb{R}^d} F(\theta) = 0$.



In such a situation, gradient descent cannot converge to a point, and, to achieve small values of F , it has to diverge. It turns out that it diverges along a direction, that is, $\|\theta_t\|_2 \rightarrow +\infty$, with $\frac{1}{\|\theta_t\|_2} \theta_t \rightarrow \eta$ for some $\eta \in \mathbb{R}^d$ of unit ℓ_2 -norm. That direction u has to lead to perfect classification (that is $y_i \varphi(x_i)^\top \eta > 0$ for all $i \in \{1, \dots, n\}$), and among all of them, the direction η is exactly the maximum margin one, that is, which maximizes

$\min_{i \in \{1, \dots, n\}} y_i \varphi(x_i)^\top \eta > 0$. See [Gunasekar et al. \(2018\)](#) for a detailed proof. Here, we just give a simple argument on a slightly modified problem.

Gradient flow on the exponential loss (\blacklozenge). We consider instead the exponential loss $G(\theta) = \frac{1}{n} \sum_{i=1}^n \exp(-y_i \varphi(x_i)^\top \theta)$, which is asymptotically equivalent to the logistic loss for $y_i \varphi(x_i)^\top \theta$ tending to infinity for all $i \in \{1, \dots, n\}$ (which is the case when gradient descent diverges). Moreover, we replace the gradient descent recursion $\theta_t = \theta_{t-1} - \gamma G'(\theta_{t-1})$ by the gradient flow $\xi'(\tau) = -G'(\xi(\tau))$. This ordinary differential equation provides an approximation of gradient descent for vanishing step-sizes, as $\xi(\gamma t) \approx \theta_t$ for γ tending to zero. The use of gradient flows instead of gradient descent is a standard theoretical simplification that allows using differential calculus (see, e.g., [Scieur et al., 2017](#), and references therein).

Once we have a gradient flow, we can freely change the speed at which we follow the flow, in other words, we can study any flow $\xi'(\tau) = -a(\xi(\tau))G'(\xi(\tau))$ instead for any positive function a . We consider $a(\xi(\tau)) = 1/G(\xi(\tau))$, and thus study the flow:

$$\xi'(\tau) = -\frac{G'(\xi(\tau))}{G(\xi(\tau))}.$$

We have, for all $\theta \in \mathbb{R}^d$:

$$\frac{G'(\theta)}{G(\theta)} = \frac{-\sum_{i=1}^n y_i \varphi(x_i) \exp(-y_i \varphi(x_i)^\top \theta)}{\sum_{i=1}^n \exp(-y_i \varphi(x_i)^\top \theta)} = -\sum_{i=1}^n \alpha_i y_i \varphi(x_i),$$

for α in the simplex (with non-negative components and summing to one). Thus, from Eq. (11.4) defining the maximum margin hyperplane, we get:

$$\frac{\|G'(\theta)\|}{G(\theta)} \geq \frac{1}{\rho}. \quad (11.5)$$

Moreover, comparing maxima and soft-maxima,¹

$$-\log(n) - \min_{i \in \{1, \dots, n\}} y_i \varphi(x_i)^\top \theta \leq \log G(\theta) \leq -\min_{i \in \{1, \dots, n\}} y_i \varphi(x_i)^\top \theta.$$

We thus have a flow $\tau \mapsto \xi(\tau)$ that cannot converge as $\|\xi'(\tau)\|_2 \geq 1/\rho$, and which is maximizing a function which is a constant away from the margin. It therefore has to diverge along a direction that maximizes this margin. We now make this precise.

¹We use $0 \geq \log\left(\frac{1}{n} \sum_{i=1}^n e^{z_i}\right) - \max_{i \in \{1, \dots, n\}} z_i = \log\left(\frac{1}{n} \sum_{i=1}^n e^{z_i - \max_{j \in \{1, \dots, n\}} z_j}\right) \geq \log(1/n)$.

Since the derivative of the function $\tau \mapsto \log G(\xi(\tau))$ is $\tau \mapsto \xi'(\tau)^\top G'(\xi(\tau))/G(\xi(\tau)) = -\|G'(\xi(\tau))\|_2^2/G(\xi(\tau))^2$, this implies by integration that, using Eq. (11.5) twice:

$$\begin{aligned} \min_{i \in \{1, \dots, n\}} y_i \varphi(x_i)^\top \xi(\tau) &\geq -\log G(\xi(\tau)) - \log(n) \\ &= -\log G(\xi(0)) + \int_0^\tau \frac{\|G'(\xi(u))\|_2^2}{G(\xi(u))^2} du - \log(n) \\ &\geq -\log G(\xi(0)) + \frac{1}{\rho} \int_0^\tau \frac{\|G'(\xi(u))\|_2}{G(\xi(u))} du - \log(n) \quad (11.6) \\ &\geq -\log G(\xi(0)) + \frac{1}{\rho^2} \tau - \log(n). \end{aligned}$$

Thus, from Eq. (11.7), for $\tau \geq \rho^2 [\log(n) + \log G(\xi(0))]$, we have a non-negative lower bound. Moreover the derivative of $\tau \mapsto \|\xi(\tau)\|_2$ is $\tau \mapsto -\left(\frac{G'(\xi(\tau))}{G(\xi(\tau))}\right)^\top \left(\frac{\xi(\tau)}{\|\xi(\tau)\|_2}\right)$, and its magnitude is less than $\left\|\frac{G'(\xi(\tau))}{G(\xi(\tau))}\right\|_2$. This implies by integration that

$$\|\xi(\tau)\|_2 \leq \|\xi(0)\|_2 + \int_0^\tau \frac{\|G'(\xi(u))\|_2}{G(\xi(u))} du.$$

We thus get from Eq. (11.6) and Eq. (11.5):

$$\begin{aligned} \min_{i \in \{1, \dots, n\}} y_i \varphi(x_i)^\top \left(\frac{\xi(\tau)}{\|\xi(\tau)\|_2}\right) &\geq \frac{-\log G(\xi(0)) + \frac{1}{\rho} \int_0^\tau \frac{\|G'(\xi(u))\|_2}{G(\xi(u))} du - \log(n)}{\|\xi(0)\|_2 + \int_0^\tau \frac{\|G'(\xi(u))\|_2}{G(\xi(u))} du} \\ &= \frac{-\log G(\xi(0)) + \frac{1}{\rho} \left(\|\xi(0)\|_2 + \int_0^\tau \frac{\|G'(\xi(u))\|_2}{G(\xi(u))} du \right) - \frac{1}{\rho} \|\xi(0)\|_2 - \log(n)}{\|\xi(0)\|_2 + \int_0^\tau \frac{\|G'(\xi(u))\|_2}{G(\xi(u))} du} \\ &= \frac{1}{\rho} + \frac{-\log G(\xi(0)) - \frac{1}{\rho} \|\xi(0)\|_2 - \log(n)}{\|\xi(0)\|_2 + \int_0^\tau \frac{\|G'(\xi(u))\|_2}{G(\xi(u))} du} \\ &\geq \frac{1}{\rho} - \frac{\log G(\xi(0)) + \frac{1}{\rho} \|\xi(0)\|_2 + \log(n)}{\|\xi(0)\|_2 + \tau/\rho}, \text{ since } \int_0^\tau \frac{\|G'(\xi(u))\|_2}{G(\xi(u))} du \geq \frac{\tau}{\rho}. \end{aligned}$$

The lower bound above tends to $\frac{1}{\rho}$ when τ tends to infinity, which is the maximal value. We thus get convergence to the maximum margin hyperplane.

Alternative proof (♦). We provide another informal derivation based on gradients. The gradient $F'(\theta)$ is equal to $F'(\theta) = -\frac{1}{n} \sum_{i=1}^n \frac{\exp(-y_i \varphi(x_i)^\top \theta)}{1 + \exp(-y_i \varphi(x_i)^\top \theta)} y_i \varphi(x_i)$.

Asymptotically, θ_t will behave as $\|\theta_t\| \eta$, with $\|\theta_t\|_2$ tending to infinity. Thus, because we have a sum of exponentials with arguments that go to infinity, the dominant term in $F'(\theta_t)$

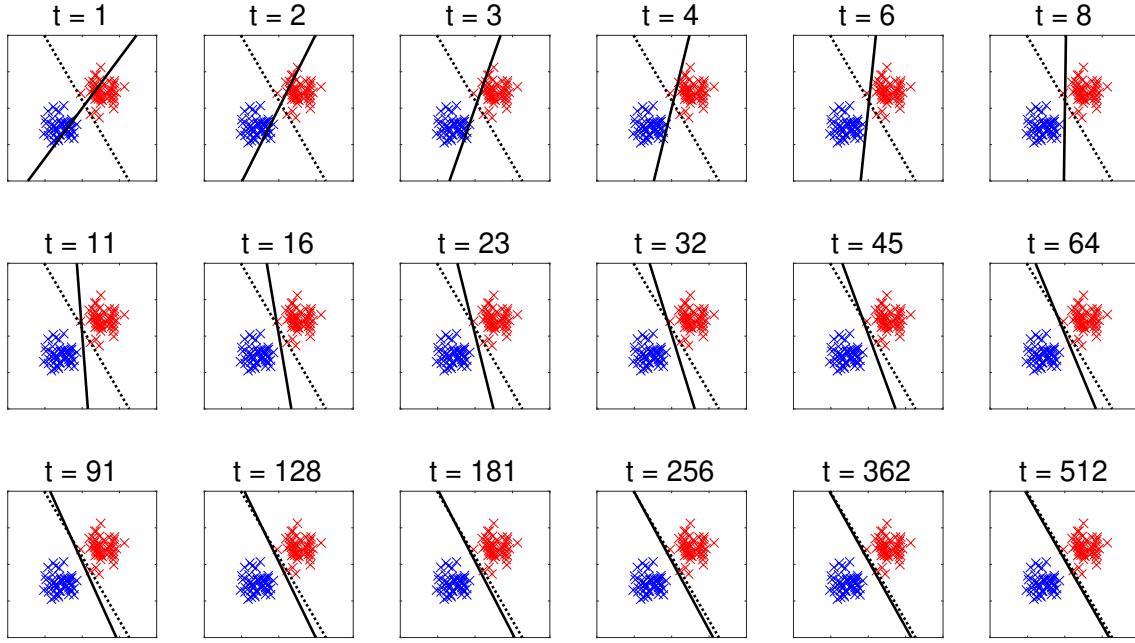


Figure 11.1: Logistic regression on separable data estimated with gradient descent on the unregularized empirical risk, at various numbers of iterations t . This is implemented by minimizing the logistic loss function with data $(x_i) \in \mathbb{R}^3$. The dotted line represents the maximum margin hyperplane.

corresponds to the indices i for which $-y_i\varphi(x_i)^\top \eta$ is largest. Moreover, all of these values have to be negative (indeed, we can only attain zero loss for well-classified training data). We denote by I this set. Thus, asymptotically,

$$F'(\theta_t) \sim -\frac{1}{n} \sum_{i \in I} y_i \exp(-\|\theta_t\|_2 y_i \varphi(x_i)^\top \eta) \varphi(x_i).$$

Moreover, if we admit for simplicity that $F'(\theta_t)$ diverges in the direction $-u$, thus u has to be proportional to a vector $\sum_{i \in I} \alpha_i y_i \varphi(x_i)$, where $\alpha \geq 0$, and $\alpha_i = 0$ as soon as i is not among the minimizers of $y_i \varphi(x_i)^\top \eta$. This is exactly the optimality condition for η_* in Eq. (11.4). Thus $\eta = \eta_*$.

Summary. Overall, we obtain a classifier corresponding to a minimum ℓ_2 -norm separating hyperplane. See examples in two dimensions in Figure 11.1. Note that gradient descent on the logistic regression problem may not be the most efficient way to obtain a maximum margin hyperplane. See convergence rates by Soudry et al. (2018); Ji and Telgarsky (2018), and a simpler subgradient algorithm below.

General result. The result above extends to more general situations beyond linear classification. See [Lyu and Li \(2019\)](#).

Subgradient method for the hinge loss (♦). Above, we considered linearly separable data, and we consider the “margin” $\rho > 0$ defined as

$$\rho^2 = \inf_{\theta \in \mathbb{R}^d} \|\theta\|_2^2 \text{ such that } \text{Diag}(y)\Phi\theta \geq 1_n. \quad (11.8)$$

To obtain a linear separator, one can use the subgradient method from Section 5.3 applied to the cost function

$$F(\theta) = \frac{1}{n} \sum_{i=1}^n (1 - y_i x_i^\top \theta)_+,$$

with iteration

$$\theta_t = \theta_{t-1} + \frac{\gamma}{n} \sum_{i=1}^n 1_{y_i x_i^\top \theta_{t-1} < 1} y_i x_i,$$

where γ is the step-size. With θ_* being the minimizer in Eq. (11.8), we have $F(\theta_*) = 0 = \min_{\theta \in \mathbb{R}^d} F(\theta)$, and after t steps, following the analysis of Theorem 5.3, we get:

$$\min_{u \leq t} F(\theta_u) \leq \frac{\gamma}{2R^2} + \frac{\rho^2}{2\gamma t}.$$

Since the classification error rate on the dataset made by the linear classifier defined by θ is upper bounded by F (see Section 4.1), the error rate is less than ε as soon as $\frac{\gamma}{2R^2} + \frac{\rho^2}{2\gamma t} \leq \varepsilon$, which can be achieved by $\gamma = R^2 \varepsilon$ and $t = \frac{\rho^2}{\gamma \varepsilon} = \frac{\rho^2}{R^2 \varepsilon^2}$, thus an error rate less than $\frac{\rho}{R\sqrt{t}}$. If $F(\theta) > 1/n$, then we have linearly separated the data, and this happens as soon as $t > (n\rho/R)^2$.

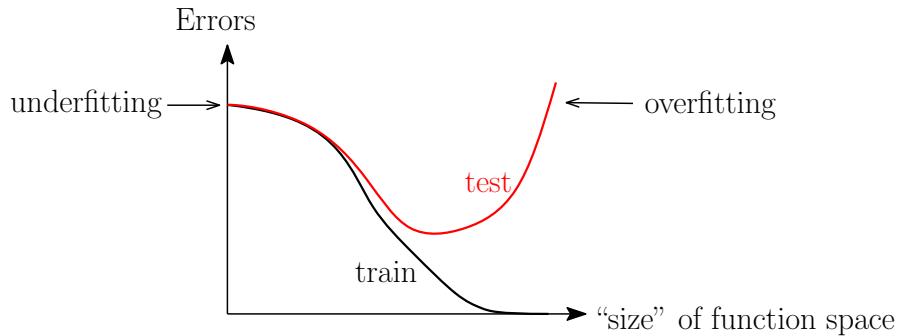
Exercise 11.1 Extend the analysis above to the stochastic gradient algorithm.

11.2 Double descent

In this section, we consider a recent and interesting phenomenon described in several recent works ([Belkin et al., 2019](#); [Mei and Montanari, 2022](#); [Geiger et al., 2020](#); [Hastie et al., 2019](#)).

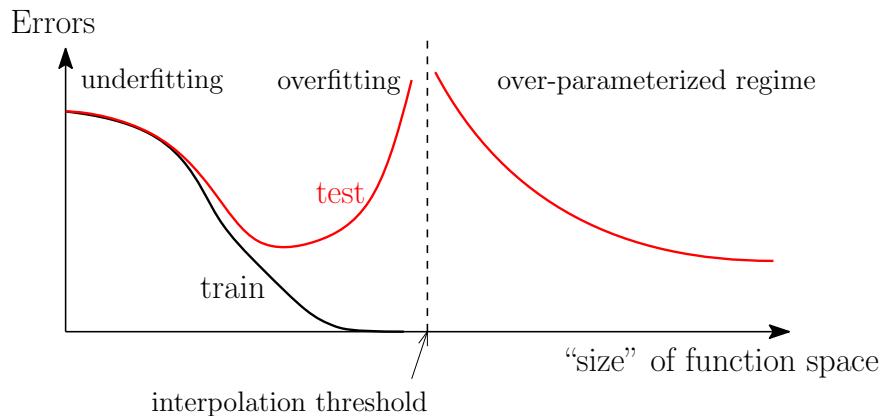
11.2.1 The double descent phenomenon

As seen in Chapter 2 and Chapter 4, typical learning curves look like the one below



Typically the “capacity” of the space of functions \mathcal{H} used to estimate the prediction function is controlled either by the number of parameters or by some norms of its parameters. In particular, at the extreme right of the curve, when there is zero training error, the testing error may be arbitrarily bad. The bound that we have used in Chapter 4, such as Rademacher averages for \mathcal{H} controlled by the ℓ_2 -norm of some parameters (with a bound D), grows as D/\sqrt{n} , which can typically be quite large. These bounds were true for *all* empirical risk minimizers. In this section, we will focus on a particular one, namely **the one obtained by unconstrained gradient descent**.

When the model is over-parameterized (in other words, the capacity gets very large), that is, when the number of parameters is large, or the norm constraint allows for exact fitting, a new phenomenon occurs, where after the test error explodes as the capacity grows, it goes down again:



This section aims to understand why, starting from empirical evidence.



There may be no double descent phenomenon if other empirical risk minimizers are used, instead of the one obtained by (stochastic) gradient descent.

11.2.2 Empirical evidence

Toy example with random features. We consider a random feature models like in Chapter 7 and Chapter 9, with the features $(v^\top x)_+$, for neurons $v \in \mathbb{R}^d$ sampled uniformly on the unit sphere. We consider $n = 200$, $d = 5$ with input data distributed uniformly on the unit sphere, and we consider $y = (\frac{1}{4} + (v_*^\top x)^2)^{-1} + \mathcal{N}(0, \sigma^2)$, with $\sigma = 2$, for some random v_* .

We sample m random features $v_1, \dots, v_m \in \mathbb{R}^d$ uniformly at random on the sphere, and we learn parameters $\theta \in \mathbb{R}^m$ by minimizing

$$\frac{1}{n} \sum_{i=1}^n \left(y_i - \sum_{j=1}^m \theta_j (v_j^\top x_i)_+ \right)^2 + \lambda \|\theta\|_2^2. \quad (11.9)$$

We report in Figure 11.2 train and test errors after learning with gradient descent until convergence: (left) varying m with $\lambda = 0$, (right) varying λ with $m = +\infty$ (we can perform estimation for $m = +\infty$ efficiently because we can compute the corresponding positive-definite kernel $k(x, x') = \mathbb{E}_v[(v^\top x)_+(v^\top x')_+]$, see Section 9.4).

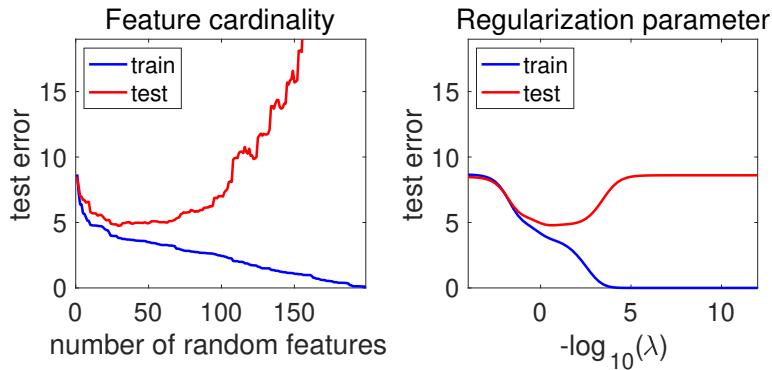


Figure 11.2: Classical learning curve: (left) train and test errors as functions of the number of random features, always less than the number of observations, (right) train and test errors for ridge regression with the same features (i.e., using ℓ_2 -regularization).

In the left curve in Figure 11.2, the number of random features m is less than n as the test error diverges. But, when this number m is allowed to grow past n , we see the double descent phenomenon in Figure 11.3. Similar experiments are shown by Belkin et al. (2019); Geiger et al. (2020); Mei and Montanari (2022), in particular for neural networks.

No phenomenon when using regularization. When an extra regularizer is used, that is $\lambda \neq 0$ in Eq. (11.9), then the double descent phenomenon is reduced. In particular, if the regularization parameter λ is adapted for each m , then the phenomenon totally disappears (see Mei and Montanari, 2022, for more details).

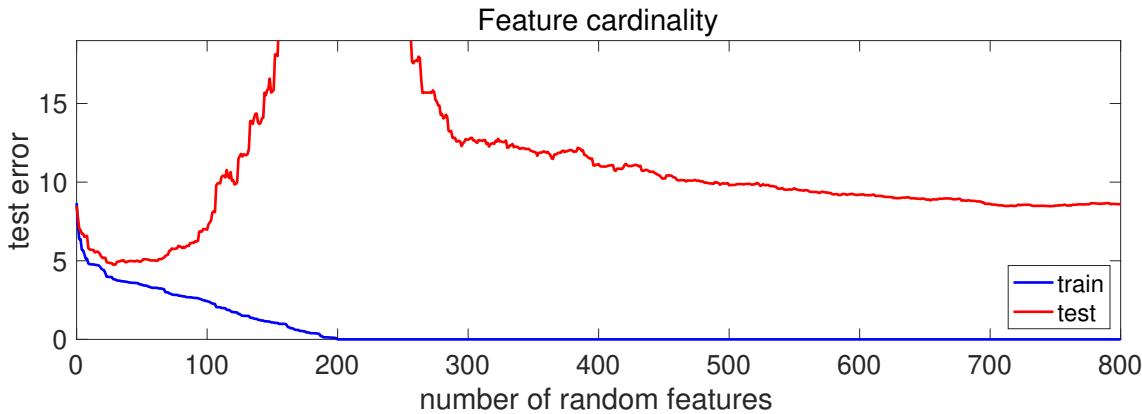


Figure 11.3: Double descent curve: train and test errors as functions of the number of random features. For $m \leq n = 200$, this is exactly the curves from Figure 11.2 (left).

11.2.3 Analysis for linear regression with Gaussian projections (♦)

In order to provide some theoretical justification for the double descent phenomenon, we consider a linear regression model in the random design setting, with Gaussian inputs and Gaussian noise.

That is, we consider a Gaussian random variable with mean 0 and covariance matrix Σ the identity matrix, with n observations x_1, \dots, x_n , and responses $y_i = x_i^\top \theta_* + \varepsilon_i$, with ε_i normal with mean zero and variance $\sigma^2 I$.

In order to have a unique prediction problem with a varying number of features, we consider additional random projections, that is, like in Section 10.2.2,² we consider a matrix $S \in \mathbb{R}^{d \times m}$ with independent components all sampled from a standard Gaussian distribution (mean 0 and variance 1). The main differences are that (a) we will perform an analysis in the random design setting, and (b) we will also need to tackle the overparameterized regime $m > n$.

We will compute the expectation of the risk of the minimum norm empirical risk minimizer (as detailed in Section 11.1.1), which is the one gradient descent converges to. See Bach (2023) for further more precise asymptotic results using random matrix theory.

We denote by $X \in \mathbb{R}^{n \times d}$ the design matrix, and $\hat{\Sigma} = \frac{1}{n} X^\top X$ the non-centered covariance matrix, and by $K = X X^\top \in \mathbb{R}^{n \times n}$ the kernel matrix. We will need to compute expectations with respect to the data X, ε and the random projection matrix S . The estimator $\hat{\theta}$ is equal to $S\hat{\eta}$ with $\hat{\eta} \in \mathbb{R}^m$ a minimizer of $\|y - XS\eta\|_2^2$.

The excess risk is $\mathcal{R}(\hat{\theta}) = (\hat{\theta} - \theta_*)^\top \Sigma (\hat{\theta} - \theta_*)$, and we now consider the two regimes $m > n$ (underparameterized) and $m > n$ (overparameterized). In both cases, as already seen in

²For an analysis without random projections, see Hastie et al. (2019).

Chapter 3, the expectation of the excess risk will be composed of two terms: a (squared) “bias term” $\mathcal{R}^{(\text{bias})}(\hat{\theta})$ corresponding to $\sigma = 0$, and a “variance term” $\mathcal{R}^{(\text{var})}(\hat{\theta})$ corresponding to $\theta_* = 0$.

Underparameterized regime. In the under-parameterized regime, the minimum norm empirical risk minimizer is simply the ordinary least-squares estimator. We denote by $\eta_* = (S^\top \Sigma S)^{-1} S^\top \Sigma \theta_* \in \mathbb{R}^m$ the minimizer of $(\theta_* - S\eta)^\top \Sigma (\theta_* - S\eta)$. We have $S\eta_* = \Pi_S \theta_*$ with $\Pi_S = S(S^\top \Sigma S)^{-1} S^\top \Sigma \in \mathbb{R}^{d \times d}$, which is a projection matrix such that $\Pi_S S = S$ and $\Pi_S^2 = \Pi_S$.

If $m \leq n$, the estimator is obtained from the normal equations $S^\top X^\top X S \hat{\theta} = S^\top X^\top y$, and can be expanded using θ_* as follows:

$$\begin{aligned}\hat{\theta} &= S\hat{\eta} = S(S^\top X^\top X S)^{-1} S^\top X^\top y \\ &= S(S^\top X^\top X S)^{-1} S^\top X^\top X \theta_* + S(S^\top X^\top X S)^{-1} S^\top X^\top \varepsilon \quad \text{using } y = X\theta_* + \varepsilon, \\ &= N\theta_* + S(S^\top X^\top X S)^{-1} S^\top X^\top \varepsilon,\end{aligned}$$

with $N = S(S^\top X^\top X S)^{-1} S^\top X^\top X$. Conditioned on S and X , the expected risk is equal to:

$$\begin{aligned}\mathbb{E}_\varepsilon[\mathcal{R}(\hat{\theta})] &= \sigma^2 \text{tr}(XS(S^\top X^\top X S)^{-1} S^\top \Sigma S(S^\top X^\top X S)^{-1} S^\top X^\top) + \|\Sigma^{1/2}(N\theta_* - \theta_*)\|_2^2 \\ &= \sigma^2 \text{tr}(S^\top \Sigma S(S^\top X^\top X S)^{-1}) + \text{tr}((N\theta_* - \theta_*)^\top \Sigma(N\theta_* - \theta_*)).\end{aligned}$$

For the variance term (first term above), for S fixed, since X has a Gaussian distribution, the matrix $S^\top X^\top X S$ is distributed as a Wishart distribution with parameter $S^\top \Sigma S$ and n degrees of freedom (see, e.g., Haff, 1979, for computations of moments of the Wishart distribution). Thus, if $n > m + 1$, we have:

$$\mathbb{E}_X[(S^\top X^\top X S)^{-1}] = \frac{1}{n-m-1}(S^\top \Sigma S)^{-1},$$

which in turn implies $\mathbb{E}_{S,X,\varepsilon}[\mathcal{R}^{(\text{var})}(\hat{\theta})] = \mathbb{E}_{X,\varepsilon}[\mathcal{R}^{(\text{var})}(\hat{\theta})] = \frac{\sigma^2 m}{n-m-1}$, independently of the choice of the sketching matrix S .

For the bias term, the computation is more involved. We expand

$$\begin{aligned}\mathbb{E}_{X,\varepsilon}[\mathcal{R}^{(\text{bias})}(\hat{\theta})] &= \mathbb{E}_X \left[\text{tr}((N\theta_* - \theta_*)^\top \Sigma(N\theta_* - \theta_*)) \right] \\ &= \theta_*^\top \Sigma \theta_* + 2\theta_*^\top \Sigma S(S^\top X^\top X S)^{-1} S^\top X^\top X \theta_* \\ &\quad + \theta_*^\top X^\top X S(S^\top X^\top X S)^{-1} S^\top \Sigma S(S^\top X^\top X S)^{-1} S^\top X^\top X \theta_*.\end{aligned}$$

In order to compute the expectation, we will first condition on XS , and use the Gaussian conditioning formulas from Section 1.1.3, which leads to, for any matrices A and B of

appropriate sizes (proof left as an exercise):

$$\begin{aligned}\mathbb{E}[X|XS] &= XS(S^\top \Sigma S)^{-1}S^\top \Sigma = X\Pi_S \\ \mathbb{E}[\text{tr}(AX^\top BX)|XS] &= \text{tr}(A\Pi_S^\top X^\top BX\Pi_S) + \text{tr}(B)\text{tr}(A\Sigma(I - \Pi_S))\end{aligned}$$

This leads to

$$\begin{aligned}\mathbb{E}_{X,\varepsilon}[\mathcal{R}^{(\text{bias})}(\hat{\theta})] &= \theta_*^\top \Sigma \theta_* + \mathbb{E}_X[2\theta_*^\top \Sigma S(S^\top X^\top XS)^{-1}S^\top X^\top X\Pi_S \theta_*] \\ &\quad + \mathbb{E}_X[\theta_*^\top \Pi_S^\top X^\top XS(S^\top X^\top XS)^{-1}S^\top \Sigma S(S^\top X^\top XS)^{-1}S^\top X^\top X\Pi_S \theta_*] \\ &\quad + \mathbb{E}_X[\text{tr}(XS(S^\top X^\top XS)^{-1}S^\top \Sigma S(S^\top X^\top XS)^{-1}S^\top X^\top) \cdot \text{tr}(\theta_* \theta_*^\top \Sigma(I - \Pi_S))] \\ &= \theta_*^\top \Sigma \theta_* + \mathbb{E}_X[2\theta_*^\top \Sigma S(S^\top \Sigma S)^{-1}S^\top \Sigma \theta_*] \\ &\quad + \mathbb{E}_X[\theta_*^\top \Sigma S(S^\top \Sigma S)^{-1}S^\top \Sigma S(S^\top \Sigma S)^{-1}S^\top \Sigma \theta_*] \\ &\quad + \mathbb{E}_X[\text{tr}(S^\top \Sigma S(S^\top X^\top XS)^{-1}) \cdot \text{tr}(\theta_* \theta_*^\top \Sigma(I - S(S^\top \Sigma S)^{-1}S^\top \Sigma))] \\ &= \theta_*^\top (I - \Pi_S)^\top \Sigma (I - \Pi_S) \theta_* \cdot (1 + \mathbb{E}_X[\text{tr}(S^\top \Sigma S(S^\top X^\top XS)^{-1})]) \\ &= \theta_*^\top (I - \Pi_S)^\top \Sigma (I - \Pi_S) \theta_* \cdot (1 + \text{tr}\left(\frac{1}{n-m-1}(S^\top \Sigma S)^{-1}S^\top \Sigma S\right)).\end{aligned}$$

Overall we get:

$$\begin{aligned}\mathbb{E}_{X,\varepsilon}[\mathcal{R}^{(\text{bias})}(\hat{\theta})] &= \theta_*^\top (I - \Pi_S)^\top \Sigma (I - \Pi_S) \theta_* \cdot \frac{n-1}{n-m-1} \\ &= \theta_*^\top (\Sigma - \Sigma S(S^\top \Sigma S)^{-1}S^\top \Sigma) \theta_* \cdot \frac{n-1}{n-m-1}.\end{aligned}$$

We can further bound the bias term; we have, for S Gaussian, following the same reasoning as in Section 10.2.2:

$$\begin{aligned}\mathbb{E}_S[\theta_*^\top (I - \Pi_S)^\top \Sigma (I - \Pi_S) \theta_*] &= \mathbb{E}_S[\min_{\eta \in \mathbb{R}^m} (\theta_* - S\eta)^\top \Sigma (\theta_* - S\eta)] \\ &\leq \mathbb{E}_S[\min_{\xi \in \mathbb{R}^d} (\theta_* - SS^\top \xi)^\top \Sigma (\theta_* - SS^\top \xi)] \\ &\leq \min_{\xi \in \mathbb{R}^d} \mathbb{E}_S[(\theta_* - SS^\top \xi)^\top \Sigma (\theta_* - SS^\top \xi)] \\ &= \min_{\xi \in \mathbb{R}^d} \left(\theta_*^\top \Sigma \theta_* - 2\xi^\top \mathbb{E}[SS^\top] \Sigma \theta_* + \xi^\top \mathbb{E}[SS^\top \Sigma SS^\top] \xi \right) \\ &= \theta_*^\top \left(\Sigma - \Sigma \mathbb{E}[SS^\top] (\mathbb{E}[SS^\top \Sigma SS^\top])^{-1} \mathbb{E}[SS^\top] \Sigma \right) \theta_* \\ &= \theta_*^\top \left(\Sigma - m\Sigma((m+1)\Sigma + \text{tr}(\Sigma)I)^{-1}\Sigma \right) \theta_* \\ &= \theta_*^\top (\Sigma + \text{tr}(\Sigma)I)((m+1)\Sigma + \text{tr}(\Sigma)I)^{-1}\Sigma \theta_* \\ &\leq \frac{2\text{tr}(\Sigma)}{m+1} \cdot \theta_*^\top \left(\Sigma + \frac{\text{tr}(\Sigma)}{m+1}I \right)^{-1} \Sigma \theta_* \leq \frac{2\text{tr}(\Sigma)}{m+1} \cdot \|\theta_*\|_2^2.\end{aligned}$$

Overall, for the underparameterized regime, we obtain an upper-bound equal to $\frac{1}{1-m/n}$ times $\frac{\sigma^2 m}{n} + \frac{2 \text{tr}(\Sigma)}{m+1} \cdot \|\theta_*\|_2^2$, which leads to a classical bias-variance trade-off, with a U-shaped curve. See [Bach \(2023\)](#) for sharper results.

Overparameterized regime. In the overparameterized regime, when $m \geq n$, then the kernel matrix is almost surely invertible, and the minimum ℓ_2 -norm interpolator $\hat{\theta}$ is equal to (using the formulas from Section 11.1.1)

$$\hat{\theta} = S\hat{\eta} = SS^\top X^\top (XSS^\top X^\top)^{-1}(X\theta_* + \varepsilon).$$

We can decompose the expectation with respect to ε of $\mathcal{R}(\hat{\theta})$ as follows:

$$\begin{aligned} \mathbb{E}_\varepsilon[\mathcal{R}(\hat{\theta})] &= \sigma^2 \text{tr}((XSS^\top X^\top)^{-1} XSS^\top \Sigma SS^\top X^\top (XSS^\top X^\top)^{-1}) \\ &\quad + \|\Sigma^{1/2}(SS^\top X^\top (XSS^\top X^\top)^{-1} X - I)\theta_*\|_2^2. \end{aligned}$$

We can now use the same reasoning as in the under-parameterized regime, but now taking expectation with respect to S . We have for any symmetric matrices A and B of compatible sizes (proof left as an exercise):

$$\begin{aligned} \mathbb{E}[\text{tr}(ASBS^\top)|S^\top X^\top] &= \text{tr}(X^\top(XX^\top)^{-1} XAX^\top(XX^\top)^{-1} XSB S^\top) \\ &\quad + \text{tr}(B) \text{tr}[A(I - X^\top(XX^\top)^{-1} X)] \\ \mathbb{E}[S|S^\top X^\top] &= X^\top(XX^\top)^{-1} X. \end{aligned}$$

Therefore, for the variance term, for which we take $B = S^\top X^\top (XSS^\top X^\top)^{-2} XS$ and $A = \Sigma$, the second part of the variance term becomes:

$$\begin{aligned} &\text{tr}[S^\top X^\top (XSS^\top X^\top)^{-2} XS] \cdot \text{tr}[\Sigma(I - X^\top(XX^\top)^{-1} X)] \\ &= \text{tr}[(XSS^\top X^\top)^{-1}] \cdot \text{tr}[\Sigma(I - X^\top(XX^\top)^{-1} X)]. \end{aligned}$$

The first part of the variance term is:

$$\begin{aligned} &\text{tr}(X^\top(XX^\top)^{-1} X \Sigma X^\top(XX^\top)^{-1} XSS^\top X^\top (XSS^\top X^\top)^{-2} XSS^\top) \\ &= \text{tr}((XX^\top)^{-1} X \Sigma X^\top(XX^\top)^{-1}). \end{aligned}$$

Thus, using expectation of the inverse Wishart distribution, the variance term is

$$\mathbb{E}_{\varepsilon, S}[\mathcal{R}^{(\text{var})}(\hat{\theta})] = \text{tr}((XX^\top)^{-1} X \Sigma X^\top(XX^\top)^{-1}) + \frac{\text{tr}((XX^\top)^{-1})}{m-n-1} \cdot \text{tr}[\Sigma(I - X^\top(XX^\top)^{-1} X)].$$

For the bias term we have:

$$\begin{aligned} &\|\Sigma^{1/2}(SS^\top X^\top (XSS^\top X^\top)^{-1} X - I)\theta_*\|_2^2 \\ &= \theta_*^\top \Sigma \theta_* + \theta_*^\top X^\top (XSS^\top X^\top)^{-1} XSS^\top \Sigma SS^\top X^\top (XSS^\top X^\top)^{-1} X \theta_* \\ &\quad - 2\theta_*^\top \Sigma SS^\top X^\top (XSS^\top X^\top)^{-1} X \theta_* \\ &= \theta_*^\top \Sigma \theta_* + \text{tr}(ASBS^\top) - 2\theta_*^\top \Sigma SS^\top X^\top (XSS^\top X^\top)^{-1} X \theta_*, \end{aligned}$$

with $A = \Sigma$, and $B = S^\top X^\top (XSS^\top X^\top)^{-1} X \theta_* \theta_*^\top X^\top (XSS^\top X^\top)^{-1} XS$, with conditional expectation given XS :

$$\begin{aligned}
& \theta_*^\top \Sigma \theta_* \\
& + \text{tr}(X^\top (XX^\top)^{-1} X \Sigma X^\top (XX^\top)^{-1} XSS^\top X^\top (XSS^\top X^\top)^{-1} X \theta_* \theta_*^\top X^\top (XSS^\top X^\top)^{-1} XSS^\top) \\
& + \text{tr}(S^\top X^\top (XSS^\top X^\top)^{-1} X \theta_* \theta_*^\top X^\top (XSS^\top X^\top)^{-1} XS) \cdot \text{tr}[\Sigma(I - X^\top (XX^\top)^{-1} X)] \\
& - 2\theta_*^\top \Sigma X^\top (XX^\top)^{-1} XSS^\top X^\top (XSS^\top X^\top)^{-1} X \theta_* \\
& = \theta_*^\top \Sigma \theta_* \\
& + \theta_*^\top X^\top (XX^\top)^{-1} X \Sigma X^\top (XX^\top)^{-1} X \theta_* \\
& + \text{tr}((XSS^\top X^\top)^{-1} X \theta_* \theta_*^\top X^\top) \cdot \text{tr}[\Sigma(I - X^\top (XX^\top)^{-1} X)] \\
& - 2\theta_*^\top \Sigma X^\top (XX^\top)^{-1} X \theta_* \\
& = \theta_*^\top (I - X^\top (XX^\top)^{-1} X) \Sigma (I - X^\top (XX^\top)^{-1} X) \theta_* \\
& + \text{tr}((XSS^\top X^\top)^{-1} X \theta_* \theta_*^\top X^\top) \cdot \text{tr}[\Sigma(I - X^\top (XX^\top)^{-1} X)]
\end{aligned}$$

leading to

$$\begin{aligned}
\mathbb{E}_{\varepsilon, S}[\mathcal{R}^{(\text{bias})}(\hat{\theta})] &= \theta_*^\top (I - X^\top (XX^\top)^{-1} X) \Sigma (I - X^\top (XX^\top)^{-1} X) \theta_* \\
&\quad + \frac{1}{m-n-1} \theta_*^\top X^\top (XX^\top)^{-1} X \theta_* \cdot \text{tr}[\Sigma(I - X^\top (XX^\top)^{-1} X)].
\end{aligned}$$

When m tends to infinity, we get the performance:

$$\begin{aligned}
\mathbb{E}_{\varepsilon, S}[\mathcal{R}_\infty(\hat{\theta})] &= \theta_*^\top (I - X^\top (XX^\top)^{-1} X) \Sigma (I - X^\top (XX^\top)^{-1} X) \theta_* \\
&\quad + \sigma^2 \text{tr}((XX^\top)^{-1} X \Sigma X^\top (XX^\top)^{-1}).
\end{aligned}$$

Overall, we get:

$$\mathbb{E}_{\varepsilon, S}[\mathcal{R}_\infty(\hat{\theta})] + \frac{1}{m-n-1} \text{tr}[\Sigma(I - X^\top (XX^\top)^{-1} X)] \cdot (\theta_*^\top X^\top (XX^\top)^{-1} X \theta_* + \sigma^2 \text{tr}((XX^\top)^{-1})).$$

Thus we do get a descent curve on the right of $m = n$. While the limiting bias term typically has a better value than for the under-parameterized regime, for the variance term, the limit when m tends to $+\infty$ does not always go to zero when n tends to infinity. See [Bartlett et al. \(2020\)](#) for conditions under which the end of the double descent curve can lead to good performance when $\sigma^2 > 0$. See illustration in Figure 11.4.

11.3 Global convergence of gradient descent

In Section 9.2.1, arguments were presented, highlighting that gradient descent neural networks with a single hidden layer and infinite widths could be shown to converge to a

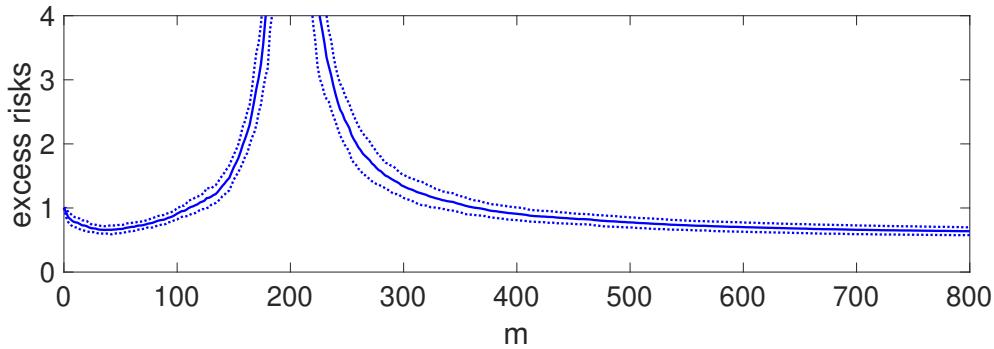


Figure 11.4: Example of a double descent curve, for linear regression with random projections with $n = 200$ observations, in dimension $d = 400$ and a non-isotropic covariance matrix. The data are normalized so that predicting zero leads to an excess risk of 1 and the noise so that the optimal expected risk is $1/4$. The empirical estimate is obtained by sampling 20 datasets and 20 different random projections from the same distribution and averaging the corresponding excess risks

global minimum. This was based on works by Chizat and Bach (2018); Bach and Chizat (2022).³ When applied to logistic regression, then combining these results with Section 11.1, we also obtain that in the infinite width limit, we get a predictor that interpolates the data, with a minimum norm, for norms which are exactly the ones obtained in Section 9.3 (Chizat and Bach, 2020).⁴

In this section, in order to present a simpler analysis, we focus on linear neural networks and first reformulate them as optimizing over positive definite matrices.

11.3.1 From linear networks to positive definite matrices

We consider “linear” neural networks, that is, neural networks with no activation function. For example, for $x \in \mathbb{R}^d$, we consider $f(x) = UV^\top x \in \mathbb{R}^k$, where $U \in \mathbb{R}^{k \times m}$ and $V \in \mathbb{R}^{d \times m}$. This is a linear function $f(x) = \Theta x$, with Θ of the form $\Theta = UV^\top \in \mathbb{R}^{k \times d}$. Assuming that we minimize some smooth convex risk $R : \mathbb{R}^{k \times d} \rightarrow \mathbb{R}$, we aim to minimize $R(UV^\top)$.

It can be rewritten as the function R applied to a linear projection of $\begin{pmatrix} U \\ V \end{pmatrix} \begin{pmatrix} U \\ V \end{pmatrix}^\top = \begin{pmatrix} UU^\top & UV^\top \\ VU^\top & VV^\top \end{pmatrix}$, which is of the form WW^\top with $W = \begin{pmatrix} U \\ V \end{pmatrix} \in \mathbb{R}^{(k+d) \times m}$. Thus, we can

³See also <https://francisbach.com/gradient-descent-neural-networks-global-convergence/>.

⁴See <https://francisbach.com/gradient-descent-for-wide-two-layer-neural-networks-implicit-bias/> for more details.

analyze instead the minimization of functions of the form $R(WW^\top)$ for $W \in \mathbb{R}^{d \times m}$, where R is a smooth convex function defined on positive semidefinite matrices of size d .

The goal of this section is now to minimize a convex function R over positive-semidefinite (PSD) matrices, using plain gradient descent techniques on a non-linear parameterization of such matrices. This is done to illustrate optimization for neural networks, noting that faster algorithms based on projected gradient descent presented in Chapter 5 could be used as well.

11.3.2 Global convergence for positive definite matrices

We consider a twice continuously differentiable convex function $R : \mathbb{R}^{d \times d} \rightarrow \mathbb{R}$ (which only needs to be defined on symmetric matrices). We consider m vectors $w_1, \dots, w_m \in \mathbb{R}^d$ put into a matrix $W = (w_1, \dots, w_m) \in \mathbb{R}^{d \times m}$, and the cost function $F(W) = R(WW^\top)$, where we have $WW^\top = \sum_{j=1}^m w_j w_j^\top$.

We consider the gradient flow $\dot{W} = -\frac{1}{2}F'(W)$, where the factor $\frac{1}{2}$ was added so simplify formulas later. Since F is twice differentiable, this ordinary differential equation (ODE) is defined for all $t \geq 0$. In order to compute the gradient of F , we perform an asymptotic expansion as follows:

$$\begin{aligned} F(W + \Delta) &= R(WW^\top + \Delta W^\top + W\Delta^\top + o(\|\Delta\|_2)) \\ &= F(W) + \text{tr}[R'(WW^\top)(\Delta W^\top + W\Delta^\top)] + o(\|\Delta\|_2) \\ &= F(W) + 2\text{tr}[\Delta^\top R'(WW^\top)W] + o(\|\Delta\|_2), \end{aligned}$$

so that $F'(W) = 2R'(WW^\top)W$, and the flow becomes $\dot{W} = -R'(WW^\top)W$. By projecting onto each of the m columns of W , this leads to the following flow for each “particle” $w_j \in \mathbb{R}^d$:

$$\dot{w}_j = -R'(WW^\top)w_j,$$

which is a linear ODE, but with a time-dependent matrix $R'(WW^\top)$ which depends on the aggregation of all particles since $WW^\top = \sum_{j=1}^m w_j w_j^\top$.

We denote $M = WW^\top$ and $A = R'(M)$, which are functions of time defined for all time $t \geq 0$. We then have:

$$\dot{M} = \dot{W}W^\top + W\dot{W}^\top = -R'(M)M - MR'(M) = -AM - MA.$$

Preservation of rank. If at time zero $M = WW^\top$ has full rank, then the rank is preserved throughout the flow. This is a simple consequence of the ODE for $r(M) = \log \det(M)$, equal to

$$\dot{r} = \text{tr}[M^{-1}\dot{M}] = \text{tr}[M^{-1}(-AM - MA)] = -2\text{tr}(A).$$

Thus, since A is continuous for all positive times, the log determinant is finite for all times as soon as it exists at initialization, and we thus obtain a full rank matrix. If $m \geq d$, which corresponds to an over-parameterized situation, and the columns of W are initialized randomly (e.g., from a standard Gaussian random variable), then WW^\top indeed has full rank.

Exercise 11.2 (♦) Show that if at initialization, $M = WW^\top$ has rank $r \leq \min\{d, m\}$, then M has rank r at all times.

Global optimality conditions. The problem of minimizing $R(M)$ over PSD matrices has the following optimality condition: (a) $\text{tr}[MR'(M)] = 0$ and (b) $R'(M) \succcurlyeq 0$. Note that once (b) is satisfied, (a) is equivalent to $MR'(M) = 0$.⁵

- *Necessary conditions (no need for convexity).* If M is optimal, then for all Δ such that $M + \Delta \succcurlyeq 0$, $R(M + \Delta) - R(M) \geq 0$. When Δ is small, this leads to $\text{tr}[\Delta R'(M)] \geq 0$. Taking Δ small along $-M$ or M , we get: $\text{tr}[MR'(M)] = 0$ as necessary condition. Taking $\Delta = uu^\top$ for all $u \in \mathbb{R}^d$, we get $R'(M) \succcurlyeq 0$ as a necessary condition.
- *Sufficient conditions.* If the conditions are met, then for any matrix $N \succcurlyeq 0$, we get from the subgradient inequality for the convex function R :

$$R(N) \geq R(M) + \text{tr}[R'(M)(N - M)].$$

Using condition (a), we get : $\text{tr}[R'(M)M] = 0$, while condition (b) ensures that $\text{tr}[R'(M)N] \geq 0$. Thus M is a global optimum.

If M is invertible, then the optimality conditions simplify to $R'(M) = 0$.

Global convergence. (♦) If the flow in M is initialized with a full-rank matrix and converges to some M_∞ ,⁶ we now show that it satisfies the two optimality conditions above (and thus it has to be a global optimum). Note that while we know that M is invertible for all time $t \geq 0$, it is often not the case for M_∞ (see examples below).

The first condition (a) is a direct consequence of $-R'(M_\infty)M_\infty - M_\infty R'(M_\infty) = 0$ (by taking the trace), which is satisfied at convergence (this is the stationary condition, stating that all particles stop). The difficult part is to show the second condition (b), which can be interpreted as ensuring that no other potential particles could enter and increasing the rank of M while reducing the cost function.

⁵For two PSD matrices A and B of same sizes, $AB = 0 \Leftrightarrow \text{tr}(AB) = 0$.

⁶It does under basic assumptions on R , such as piecewise analyticity, see [Bolte et al. \(2006\)](#).

We now assume that $A_\infty = R'(M_\infty)$ is not PSD, that is, $\lambda_{\min}(A_\infty) < 0$. We choose $\eta > 0$ such that $\lambda_{\min}(A_\infty) < -\eta$, and $-\eta$ is not an eigenvalue of A_∞ (which is possible because there are at most d distinct eigenvalues). This implies that for u such that $\|u\|_2 = 1$ and $u^\top A_\infty u = -\eta$,

$$\eta = -u^\top A_\infty u < \|u\|_2 \|A_\infty u\|_2 = \|A_\infty u\|_2$$

by Cauchy-Schwarz inequality and the impossibility of having $A_\infty u = -\eta u$ (which is the equality condition for Cauchy-Schwarz inequality). We denote by $\beta > \eta$ the minimal value of such $\|A_\infty u\|_2$ (for all u that satisfies $\|u\|_2 = 1$ and $u^\top A_\infty u = -\eta$).

The idea is to show that sufficiently close to convergence, once a particle has a direction in

$$K = \{u \in \mathbb{R}^d, \|u\|_2 = 1, u^\top A_\infty u < -\eta\},$$

its direction never gets out of K , and that it leads to a contradiction (the set K is not empty because $\lambda_{\min}(A_\infty) < -\eta$).

We now introduce the time dependence explicitly.

Choice of particle close to convergence (\blacklozenge). We have $M(t) \rightarrow M_\infty$. Thus there exists t_0 such that $\|A(t) - A_\infty\|_{\text{op}} \leq \varepsilon$, for all $t \geq t_0$, with ε well chosen (small enough).

Let $y_0 \in \mathbb{R}_+ K$, $y_0 \neq 0$ (it exists since K is not empty). Since $W(t_0) \in \mathbb{R}^{d \times m}$ has full rank equal to d , then there exists $\alpha_0 \in \mathbb{R}^m$ such that $y_0 = W(t_0)\alpha_0$.

We then consider a particle $z(t) = W(t)\alpha_0 \in \mathbb{R}^d$. By construction, $\dot{z}(t) = \dot{W}(t)\alpha_0 = -A(t)W(t)\alpha_0 = -A(t)z(t)$, and $z(t_0) = y_0 \in \mathbb{R}_+ K$. We now show by contradiction that we must have $z(t) \in \mathbb{R}_+ K$ for all $t \geq t_0$. If t_1 is the smallest $t \geq t_0$ such that $z(t) \notin \mathbb{R}_+ K$ (which is assumed to exist by contradiction), then by continuity, $z(t_1) \in \mathbb{R}_+ \partial K$, that is, $z(t_1)^\top A_\infty z(t_1) = -\eta z(t_1)^\top z(t_1)$. We then have, with $z_1 = z(t_1)$, and using $\dot{z}(t_1) = -A(t_1)z(t_1)$:

$$\begin{aligned} \frac{d}{dt} \frac{z(t)^\top A_\infty z(t)}{z(t)^\top z(t)} \Big|_{t=t_1} &= 2 \frac{z(t_1)^\top A_\infty \dot{z}(t_1)}{z(t_1)^\top z(t_1)} - 2 \frac{z(t_1)^\top A_\infty z(t_1)}{z(t_1)^\top z(t_1)} \frac{\dot{z}(t_1)^\top z(t_1)}{z(t_1)^\top z(t_1)} \\ &= -2 \frac{z_1^\top A_\infty A(t_1) z_1}{z_1^\top z_1} + 2 \frac{z_1^\top A_\infty z_1}{z_1^\top z_1} \frac{z_1^\top A(t_1) z_1}{z_1^\top z_1} \\ &= -2 \frac{z_1^\top A_\infty^2 z_1}{z_1^\top z_1} + 2 \frac{z_1^\top A_\infty (A_\infty - A(t_1)) z_1}{z_1^\top z_1} + 2 \frac{z_1^\top A_\infty z_1}{z_1^\top z_1} \frac{z_1^\top A(t_1) z_1}{z_1^\top z_1}. \end{aligned}$$

Using that $\|A(t_1) - A_\infty\|_{\text{op}} \leq \varepsilon$ and $z(t_1)^\top A_\infty z(t_1) = -\eta z(t_1)^\top z(t_1)$, this leads to

$$\begin{aligned} \frac{d}{dt} \frac{z(t)^\top A_\infty z(t)}{z(t)^\top z(t)} \Big|_{t=t_1} &\leq -2 \frac{z_1^\top A_\infty^2 z_1}{z_1^\top z_1} + 2 \frac{\|A_\infty z_1\|_2 \varepsilon}{\|z_1\|_2} + 2\eta^2 + 2\eta\varepsilon \\ &\leq -2\beta^2 + 2\eta^2 + 2\|A_\infty\|_{\text{op}} \varepsilon + 2\eta\varepsilon, \end{aligned}$$

which is strictly negative for ε small enough, which is a contradiction because it would imply that for t just above t_1 , $\frac{z(t)^\top A_\infty z(t)}{z(t)^\top z(t)} < \frac{z(t_1)^\top A_\infty z(t_1)}{z(t_1)^\top z(t_1)} = -\eta$, and thus, $z(t) \in \mathbb{R}_+ K$.

Final contradiction. (♦) We now have that the particule $z(t)$ is in $\mathbb{R}_+ K$ for all $t \geq t_0$. We then have for all $t \geq t_0$,

$$\frac{d}{dt} z(t)^\top z(t) = -2z(t)^\top A(t)z(t) \geq 2(-z(t)^\top A_\infty z(t) - \|z(t)\|_2^2 \varepsilon) \geq 2(\eta - \varepsilon) \|z\|_2^2,$$

leading to, after integration, $\|z(t)\|_2^2 \geq \|z(t_0)\|_2^2 \exp(2(\eta - \varepsilon)(t - t_0))$, and thus a divergence. This contradicts the convergence of $z(t) = W(t)\alpha_0$.

11.3.3 Special case of Oja flow

As an illustration of the convergence results above, we consider the function

$$R(M) = \frac{1}{2} \|M - C\|_F^2,$$

for a symmetric matrix $C \in \mathbb{R}^{d \times d}$, for which the flow can integrated in closed form. We have $R'(M) = M - C$, and thus the following gradient flows:

$$\dot{W} = -R'(WW^\top)W = CW - WW^\top W \quad \text{and} \quad \dot{M} = CM + MC - 2M^2.$$

If we initialize $W(0) = V \in \mathbb{R}^{d \times m}$, we obtain a solution in closed-form (as can be checked by taking derivatives and showing that $\dot{M} = CM + MC - 2M^2$), as

$$M = WW^\top = \exp(Ct)V(I + V^\top C^{-1}(\exp(2Ct) - 1)V)^{-1}V^\top \exp(Ct).$$

This is the Oja flow, up to a change of variable [Yan et al. \(1994\)](#). It is interesting to note that if we use $m \leq d$ particles, the rank of WW^\top is always less than $m \leq d$, and in fact the same as the rank of the initialization. The global minimizer of R on PSD matrices is the positive part of C , whose rank can be strictly smaller than m , and thus, it cannot converge to the global optimum of R . The minimum number of particles is the number of positive eigenvalues of C .

Vanishing initialization. If $V = \sqrt{\alpha}I \in \mathbb{R}^{d \times d}$, we get:

$$M = \alpha \exp(2Ct)(I + \alpha C^{-1}(\exp(2Ct) - 1))^{-1}.$$

Then, M is a spectral variant of C , thus with the same eigenvector, and eigenvalue $m = \frac{\alpha e^{2ct}}{1 + \alpha c^{-1}(e^{2ct} - 1)} \approx \frac{c}{1 + e^{-2ct}c/\alpha}$ for small α , where c is the corresponding eigenvalue of C .

Thus, when α tends to zero (and thus closer to the stationary point), the eigenvalues m stay at zero until they increase to the final positive values c , and this increase happens around $t = \frac{1}{2c} \log \frac{1}{\alpha}$. We thus observe an incremental learning of each eigenvector, with each eigenvector corresponding to a positive eigenvalue c , which is a very different optimization dynamics from the one obtained from projected gradient descent, which corresponds to $m = c(1 - e^{-t})$ where all eigenvectors come together.

Chapter 12

Lower bounds on performance

Chapter summary

- Statistical lower bounds: for least-squares regression, the optimal performance of supervised learning with target functions that are linear in some feature vector or in Sobolev spaces on \mathbb{R}^d happens to be achieved by several algorithms presented earlier in the book. The lower bounds can be obtained through information theory or Bayesian analysis.
- Optimization lower bounds: for the classical problem classes from Chapter 5, hard functions can be designed so that gradient-descent-based algorithms that linearly combine gradients are shown to be optimal.
- Lower bounds for stochastic gradient descent: The rates proportional to $O(1/\sqrt{n})$ for convex functions and $O(1/n\mu)$ for μ -strongly convex problems are optimal.

In this textbook, we have shown various convergence rates for statistical procedures when the number of observations n goes to infinity, and optimization methods, as the number of iterations k goes to infinity. Most of them were non-asymptotic upper bounds on the error measures, with a precise dependence on the problem parameters (e.g., smoothness of the target function or the objective function).

In this chapter, we are looking at lower bounds on performance, that is, we aim to show that for a particular problem class and a specific class of algorithms, the error measures cannot go to zero too quickly. Lower bounds are useful, in particular when they match upper bounds up to constants (we can then claim that we have an “optimal” method). They

sometimes provide hard problems (like for optimization), sometimes not (when they are based on information theory, such as for prediction performance).



Lower bounds will be obtained in a “minimax” setting where we look at the worst-case performance over the entire problem class. As for upper bounds, looking at worst-case performance is, in essence, pessimistic, and algorithms often behave better than their bounds. The key is to identify classes of problems that are not too large (or the bounds will be very bad) but still contains interesting problems.

12.1 Statistical lower bounds

In this section, our goal is to obtain lower bounds for regression problems in \mathbb{R}^d with the square loss when assuming the target function $f^* : \mathbb{R}^d \rightarrow \mathbb{R}$ (here the conditional expectation of y given x) is in a particular set, such as:

- linear function of some d -dimensional features, that is, $f_*(x) = \langle \theta_*, \varphi(x) \rangle$, for $\theta_* \in \mathbb{R}^d$, potentially in a ℓ_2 -ball, and/or with less than k non-zero elements,
- functions with all partial derivatives up to order s bounded in L_2 -norm (e.g., Sobolev spaces).

Since we are looking for lower bounds, we are free to make extra assumptions (that can only make the problem simpler) and lower the lower bounds. For example, we will focus on Gaussian noise with constant variance σ^2 that is independent of x .

We can either consider fixed design assumptions or random designs with the simplest input distributions (that can only make the problem simpler).

Classification. Lower bounds for classification problems are more delicate and out of scope (see, e.g., [Yang, 1999](#)). However, we can get lower bounds for the convex surrogates that are typically used (but note that this does not translate to lower bounds for the 0-1 loss), see for example Section 12.3 for Lipschitz-continuous loss functions.

12.1.1 Minimax lower bounds

We consider a set of probability distributions indexed by some set Θ (that can characterize input distributions and the smoothness of the target function). We consider some data \mathcal{D} , generated from this distribution, and we denote \mathbb{E}_θ expectations with respect to data coming from the distribution indexed by θ .

We consider an estimator $\mathcal{A}(\mathcal{D})$ of $\theta \in \Theta$, with some squared distance d^2 between two elements of Θ , so that $d(\theta, \theta')^2$ measures the performance of θ' when the true estimator is θ . The performance of \mathcal{A} when the data come from θ_* is

$$\mathbb{E}_{\theta_*} [d(\theta_*, \mathcal{A}(\mathcal{D}))^2].$$

The goal is to find an algorithm so that $\sup_{\theta_* \in \Theta} \mathbb{E}_{\theta_*} [d(\theta_*, \mathcal{A}(\mathcal{D}))^2]$ is as small as possible, and the lower bound of performance is thus:

$$\inf_{\mathcal{A}} \sup_{\theta_* \in \Theta} \mathbb{E}_{\theta_*} [d(\theta_*, \mathcal{A}(\mathcal{D}))^2]. \quad (12.1)$$

This is often referred to as “minimax” lower bounds.

Since by Markov’s inequality, $\mathbb{E}_{\theta_*} [d(\theta_*, \mathcal{A}(\mathcal{D}))^2] \geq A \mathbb{P}_{\theta_*}(d(\theta_*, \mathcal{A}(\mathcal{D}))^2 > A)$, it is sufficient to lower bound

$$\inf_{\mathcal{A}} \sup_{\theta_* \in \Theta} \mathbb{P}_{\theta_*}(d(\theta_*, \mathcal{A}(\mathcal{D}))^2 > A),$$

for some $A > 0$. This will be useful for techniques based on information theory.

We will see two principles for obtaining statistical minimax lower bounds:

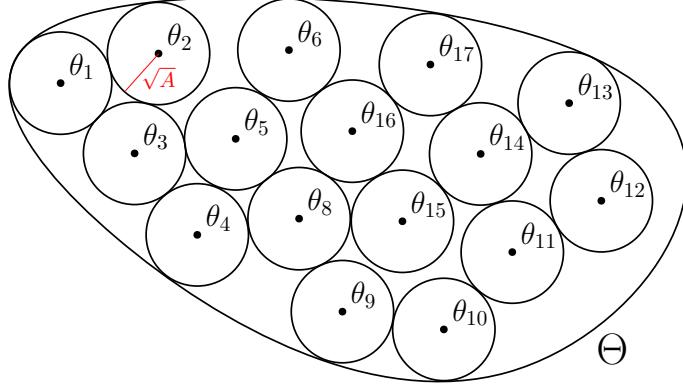
- **Reduction to a hypothesis test:** by selecting a finite subset $\{\theta_1, \dots, \theta_M\}$ of distributions Θ which is maximally spread, a good estimator leads to a good hypothesis test that can identify which θ_j was used to generate the data. We can then use information theory to lower-bound the probability of error of such a test. This very versatile technique can deal with most situations, from fixed to random design.
- **Bayesian analysis:** We can lower bound the supremum for all Θ by any expectation over a distribution supported on Θ . Once we have an expectation, we can use the same decision-theoretic argument as the ones we used to compute the Bayes risk is Chapter 4, e.g., for Hilbertian or Euclidean performance measures, the optimal estimator is the conditional expectation $\mathbb{E}[\theta_* | \mathcal{D}]$. The key is choosing distributions so they can be computed in closed form. This approach is less flexible but the simplest in situations where it can be applied (fixed design regression on balls, with potentially sparse assumptions).

12.1.2 Reduction to a hypothesis test

The principle is simple: pack the set Θ with “balls” of some radius $4A$, that is find $\theta_1, \dots, \theta_M \in \Theta$ such that

$$\forall i \neq j, d(\theta_i, \theta_j)^2 \geq 4A, \quad (12.2)$$

and transform the estimation problem into a hypothesis test, that is, an algorithm going from the data \mathcal{D} to one out of M potential outcomes (see illustration below).



Then, because we take the supremum over a smaller set:

$$\sup_{\theta_* \in \Theta} \mathbb{P}_{\theta_*}(d(\theta_*, \mathcal{A}(\mathcal{D}))^2 > A) \geq \max_{j \in \{1, \dots, M\}} \mathbb{P}_{\theta_j}(d(\theta_j, \mathcal{A}(\mathcal{D}))^2 > A).$$

Any algorithm $A(\mathcal{D}) \in \Theta$ gives a “test”, that is, a function $g \circ \mathcal{A} : \mathcal{D} \rightarrow \{1, \dots, m\}$ defined as

$$g(\mathcal{A}(\mathcal{D})) = \arg \min_{j \in \{1, \dots, m\}} d(\theta_j, \mathcal{A}(\mathcal{D})) \in \{1, \dots, m\},$$

where ties are broken arbitrarily (e.g., by selecting the minimal index). Because of the packing condition in Eq. (12.2), the performance of \mathcal{A} can be lower-bounded by the classification performance of $g \circ \mathcal{A}$.

Indeed, if, for some $j \in \{1, \dots, M\}$, $g(\mathcal{A}(\mathcal{D})) \neq j$, there exists $k \neq j$, such that $d(\theta_k, \mathcal{A}(\mathcal{D})) < d(\theta_j, \mathcal{A}(\mathcal{D}))$. Moreover, using the triangle inequality for d , we get:

$$d(\theta_j, \theta_k)^2 \leq 2[d(\theta_j, \mathcal{A}(\mathcal{D}))^2 + d(\mathcal{A}(\mathcal{D}), \theta_k)^2],$$

then,

$$\begin{aligned} d(\theta_j, \mathcal{A}(\mathcal{D}))^2 &\geq \frac{1}{2}d(\theta_j, \theta_k)^2 - d(\mathcal{A}(\mathcal{D}), \theta_k)^2 \\ &\geq \frac{1}{2}d(\theta_j, \theta_k)^2 - d(\mathcal{A}(\mathcal{D}), \theta_j)^2 \text{ using the optimal } k, \end{aligned}$$

which implies $d(\theta_j, \mathcal{A}(\mathcal{D}))^2 \geq \frac{1}{4}d(\theta_j, \theta_k)^2 \geq A$. Thus, we have

$$\mathbb{P}_{\theta_j}(d(\theta_j, \mathcal{A}(\mathcal{D}))^2 > A) \geq \mathbb{P}_{\theta_j}(g(\mathcal{A}(\mathcal{D})) \neq j),$$

leading to

$$\begin{aligned} \inf_{\mathcal{A}} \sup_{\theta_* \in \Theta} \mathbb{E}_{\theta_*}[d(\theta_*, \mathcal{A}(\mathcal{D}))^2] &\geq A \cdot \inf_h \max_{j \in \{1, \dots, M\}} \mathbb{P}_{\theta_j}(g(\mathcal{D}) \neq j) \\ &\geq A \cdot \inf_h \frac{1}{M} \sum_{j=1}^M \mathbb{P}_{\theta_j}(g(\mathcal{D}) \neq j), \end{aligned} \tag{12.3}$$

where h is any function from \mathcal{D} to $\{1, \dots, M\}$. We have lower-bounded the minimax statistical performance by the minimax performance of a hypothesis test $h : \mathcal{D} \rightarrow \{1, \dots, M\}$. Information theory can then be used to lower-bound this minimax error. We first provide a quick review of information theory (see [Cover and Thomas, 1999](#), for more details).

12.1.3 Information theory

Entropy. Given a random variable y taking finitely many values in \mathcal{Y} , its entropy is equal to

$$H(y) = - \sum_{y' \in \mathcal{Y}} \mathbb{P}(y = y') \log \mathbb{P}(y = y').$$

Since $\mathbb{P}(y = y') \in [0, 1]$, the entropy is always non-negative. Moreover, using Jensen's inequality for the logarithm, we have $H(y) = \sum_{y' \in \mathcal{Y}} \mathbb{P}(y = y') \log \frac{1}{\mathbb{P}(y = y')} \leq \log \left(\sum_{y' \in \mathcal{Y}} \mathbb{P}(y = y') \frac{1}{\mathbb{P}(y = y')} \right) = \log |\mathcal{Y}|$.

The entropy $H(y)$ represents the uncertainty associated with the random variable y , going from $H(y) = 0$ if y is deterministic (that is $\mathbb{P}(y = y') = 1$ for some $y' \in \mathcal{Y}$), to $\log |\mathcal{Y}|$ when y has a uniform distribution.

Joint and conditional entropies. Given two random variables x, y with finitely many values in \mathcal{X} and \mathcal{Y} , we can define the joint entropy

$$H(x, y) = - \sum_{x' \in \mathcal{X}} \sum_{y' \in \mathcal{Y}} \mathbb{P}(x = x', y = y') \log \mathbb{P}(x = x', y = y').$$

It can be decomposed as

$$\begin{aligned} H(x, y) &= - \sum_{x' \in \mathcal{X}} \sum_{y' \in \mathcal{Y}} \mathbb{P}(y = y', x = x') \log [\mathbb{P}(y = y' | x = x') \mathbb{P}(x = x')] \\ &= - \sum_{x' \in \mathcal{X}} \sum_{y' \in \mathcal{Y}} \mathbb{P}(y = y', x = x') \log \mathbb{P}(y = y' | x = x') \\ &\quad - \sum_{x' \in \mathcal{X}} \sum_{y' \in \mathcal{Y}} \mathbb{P}(y = y', x = x') \log \mathbb{P}(x = x') \\ &= \sum_{x' \in \mathcal{X}} \mathbb{P}(x = x') \log H(y | x = x') + H(x), \end{aligned}$$

where $H(y | x = x')$ is the entropy of the conditional distribution of y given $x = x'$. By defining the conditional entropy $H(y | x)$ as $H(y | x) = \sum_{x' \in \mathcal{X}} \mathbb{P}(x = x') H(y | x = x')$, we exactly have:

$$H(x, y) = H(y | x) + H(x).$$

This leads to a first version of Fano's inequality, which lower bounds the probability that $y \neq \hat{y}$ from the conditional entropy $H(y|\hat{y})$; the main idea is that if y remains very uncertain given \hat{y} , then the probability that they are equal cannot be too large.

Proposition 12.1 (Fano's inequality) *If the random variables y and \hat{y} have values in the same finite set \mathcal{Y} , then*

$$\mathbb{P}(\hat{y} \neq y) \geq \frac{H(y|\hat{y}) - \log 2}{\log |\mathcal{Y}|}.$$

Proof Let $e = 1_{y \neq \hat{y}} \in \{0, 1\}$ be the indicator function of errors, then, by decomposing the joint entropy through conditional and marginal entropies in the two different ways, we get:

$$H(e|\hat{y}) + H(y|e, \hat{y}) = H(e, y|\hat{y}) = H(y|\hat{y}) + H(e|y, \hat{y}).$$

We then have $H(e|y, \hat{y}) = 0$ (since e is deterministic given y and \hat{y}), $H(e|\hat{y}) \leq H(e) \leq \log 2$ (because $e \in \{0, 1\}$), and $H(y|e, \hat{y}) = \mathbb{P}(e = 1)H(y|\hat{y}, e = 1) + \mathbb{P}(e = 0)H(y|\hat{y}, e = 0) = \mathbb{P}(e = 1)H(y|\hat{y}, e = 1) + 0 \leq \mathbb{P}(\hat{y} \neq y) \log |\mathcal{Y}|$. Expressing $\mathbb{P}(\hat{y} \neq y)$ in function of other quantities leads to the desired result. ■

Data processing inequality. A fundamental result in information theory allows to lower-bound conditional entropies where conditional independencies are present. That is, if we have three random variables x, y, z , such that z and x are conditionally independent given y , then $H(x|z) \geq H(x|y)$: in words, the uncertainty of x given z has to be larger than the uncertainty of $x|y$, which is “normal” because the statistical dependence between x and z is occurs through y . In other words, the sequence $x \rightarrow y \rightarrow z$ forms a Markov chain.

The data processing inequality is a simple application of the concavity of the entropy as a function of the probability mass function; indeed, using that by conditional independence $\mathbb{P}(x = x'|z = z') = \sum_{y' \in \mathcal{Y}} \mathbb{P}(x = x', y = y'|z = z') = \sum_{y' \in \mathcal{Y}} \mathbb{P}(x = x'|y = y')\mathbb{P}(y = y'|z = z')$, we have:

$$\begin{aligned} H(x|z) &= \sum_{z' \in \mathcal{Z}} \mathbb{P}(z = z') H(x|z = z') \\ &\geq \sum_{z' \in \Theta} \mathbb{P}(z = z') \sum_{y' \in \mathcal{Y}} \mathbb{P}(y = y'|z = z') H(x|y = y') \\ &= \sum_{y' \in \mathcal{Y}} \mathbb{P}(y = y') H(x|y = y') = H(x|y). \end{aligned}$$

This leads immediately to the following full version of Fano's inequality:

Proposition 12.2 (Fano's inequality) *If the random variable y and \hat{y} have values in the same finite set \mathcal{Y} , and if we have a Markov chain $y \rightarrow z \rightarrow \hat{y}$, then*

$$\mathbb{P}(\hat{y} \neq y) \geq \frac{H(y|\hat{y}) - \log 2}{\log |\mathcal{Y}|} \geq \frac{H(y|z) - \log 2}{\log |\mathcal{Y}|}.$$

We need a last concept from information theory, namely mutual information and Kullback-Leibler divergence, both for discrete-valued random variables and continuous-valued random variables.

Mutual information. Given two random variables x and y , then we can define their mutual information as

$$I(x, y) = H(x) - H(x|y) = H(x) + H(y) - H(x, y) = H(y) - H(y|x).$$

This can be seen as the reduction of uncertainty in x when observing y . It is symmetric, always less than $\log |\mathcal{X}|$ and $\log |\mathcal{Y}|$. Moreover, it can be written as:

$$\begin{aligned} I(x, y) &= H(x) + H(y) - H(x, y) \\ &= \sum_{x' \in \mathcal{X}} \sum_{y' \in \mathcal{Y}} \mathbb{P}(x = x', y = y') \log \frac{\mathbb{P}(x = x', y = y')}{\mathbb{P}(x = x') \mathbb{P}(y = y')}, \end{aligned}$$

which can be seen as the Kullback-Leibler (KL) divergence between the distribution of (x, y) and the product of marginals of x and y . Indeed, given two distributions on \mathcal{Z} , p and q (which are non-negative functions on \mathcal{Z} that sum to one), then the KL divergence is defined as

$$D_{\text{KL}}(p||q) = \sum_{z \in \mathcal{Z}} p(z) \log \frac{p(z)}{q(z)}.$$

The KL divergence is always non-negative by convexity of the function $t \mapsto t \log t$, and equal to zero, if and only if $p = q$. Moreover, the KL divergence is jointly convex in (p, q) . Thus, one can see the mutual information between the KL divergences between the joint distribution of (x, y) and the corresponding product of marginals (which is thus non-negative).

From discrete to continuous distributions. Many of the information theory concepts can be extended to continuous random variables on \mathbb{R}^d , by replacing the probability mass function with the probability density with respect to some base measures. Then many properties (which were obtained through convex arguments) extend. In particular, the data processing inequality and Fano's inequality when z is continuous-valued.

Moreover, the KL divergence between two distributions can be defined as

$$D_{\text{KL}}(p||q) = \mathbb{E}_p \log \frac{dp}{dq}(x).$$

A short calculation shows that for two normal distributions of means μ_1, μ_2 and equal covariance matrices Σ , the KL divergence is equal to $\frac{1}{2}(\mu_1 - \mu_2)^\top \Sigma^{-1}(\mu_1 - \mu_2)$.

12.1.4 Lower-bound on hypothesis testing based on information theory

We consider a joint random variable (y, \mathcal{D}) distributed as y uniform in $\{1, \dots, M\}$, and, given $y = j$, \mathcal{D} distributed as the distribution associated with θ_j . We consider $\hat{y} = h(\mathcal{D})$. This defines a Markov chain: $y \rightarrow \mathcal{D} \rightarrow h(\mathcal{D})$, that is, even for a randomized test, $h(\mathcal{D})$ is independent of y given \mathcal{D} . The last term in Eq. (12.3) is exactly the probability that $\hat{y} \neq y$. This is exactly what Fano's inequality from information theory gives us, leading to the following corollary.

Corollary 12.1 (Fano's inequality for multiple hypothesis testing) *Given M probability distributions p_j on \mathcal{D} , then*

$$\inf_h \frac{1}{M} \sum_{j=1}^M \mathbb{P}_j(h(\mathcal{D}) \neq j) \geq 1 - \frac{1}{M^2 \log M} \sum_{j,j'=1}^M D_{\text{KL}}(p_j || p_{j'}) - \frac{\log 2}{\log M}. \quad (12.4)$$

Proof We consider a joint random variable (y, \mathcal{D}) distributed as y uniform in $\{1, \dots, M\}$, and, given $y = j$, \mathcal{D} distributed as the distribution p_j . We have:

$$\begin{aligned} H(y|z) &= H(y) - I(y, z) = \log M - \frac{1}{M} \sum_{j=1}^M D_{\text{KL}}(p_j || \frac{1}{M} \sum_{j'=1}^M p_{j'}) \\ &\geq H(y) - I(y, z) = \log M - \frac{1}{M^2} \sum_{j,j'=1}^M D_{\text{KL}}(p_j || p_{j'}), \end{aligned}$$

by the convexity of the Kullback-Leibler divergence. We can then apply Prop. 12.2 and conclude. ■

Using Gaussian noise to compute KL divergences. For regression with Gaussian errors such as $y_i = f_\theta(x_i) + \varepsilon_i$, with $\varepsilon \sim \mathcal{N}(0, \sigma^2 I)$, then, for fixed designs (all x_i 's deterministic), we get exactly

$$D_{\text{KL}}(p_{\theta_j} || p_{\theta_{j'}}) = \frac{1}{2\sigma^2} \sum_{i=1}^n [f_{\theta_j}(x_i) - f_{\theta_{j'}}(x_i)]^2 = \frac{n}{2\sigma^2} d(\theta_j, \theta_{j'})^2,$$

where $d(\theta, \theta')^2 = \frac{1}{n} \sum_{i=1}^n [f_\theta(x_i) - f_{\theta'}(x_i)]^2$.

For random designs, we consider distributions on $(x_i, y_i)_{i=1, \dots, n}$. If we consider a common distribution for x , then

$$D_{\text{KL}}(p_{\theta_j} || p_{\theta_{j'}}) = \frac{1}{2\sigma^2} \int_X [f_{\theta_j}(x) - f_{\theta_{j'}}(x)]^2 dp(x) = \frac{1}{2\sigma^2} \|f_{\theta_j} - f_{\theta_{j'}}\|_{L_2(p)}^2,$$

which we define to be $\frac{1}{2\sigma^2} d(\theta_j, \theta_{j'})^2$.

Overall, to obtain a lower bound with Gaussian noise, we need to find $\theta_1, \dots, \theta_M$ in Θ such that:

- $\frac{1}{M^2} \sum_{j,j'=1}^M \frac{n}{2\sigma^2} d(\theta_j, \theta_{j'})^2 \leq \log(M)/4$. and $\log 2/\log M \leq 1/4$ (that is $M \geq 16$), so that Eq. (12.4) leads to a lower bound of $A/2$.
- $\min_{j \neq k} d(\theta_j, \theta_k)^2 \geq 4A$, so that we can apply Eq. (12.3).

Then the minimax lower bound is $A/2$. Thus, the lower bound is essentially the largest possible A for a given M such that we can find M points in Θ , which are all $2\sqrt{A}$ apart. There are two main tools to find such packings: (1) a direct volume argument and (2) using Varshamov-Gilbert's lemma. We present them before going over examples.

Volume argument. The following lemma provides the simplest argument.

Lemma 12.1 (Packing ℓ_2 -balls) *Let M be the maximal number of elements of the Euclidean ball of radius 1, which are at least 2ε -apart in ℓ_2 -norm. Then $(2\varepsilon)^{-d} \leq M \leq (1 + \varepsilon^{-1})^d$.*

Proof Let $\theta_1, \dots, \theta_M$ be the corresponding M points.

(a) All balls of center θ_j and radius ε are disjoint and included in the ball of radius $1 + \varepsilon$. Thus, the sum of the volumes of the small balls is smaller than the volume of the large balls, that is, $M\varepsilon^d \leq (1 + \varepsilon)^d$.

(b) Since M is maximal, for any θ such that $\|\theta\|_2 \leq 1$, there exists a $j \in \{1, \dots, M\}$ such that $\|\theta_j - \theta\|_2 \leq 2\varepsilon$ (otherwise, we can add a new point to $\{\theta_1, \dots, \theta_M\}$ and M is not maximal). Thus the ball of radius 1 is covered by the M balls of radius θ_j and radius 2ε . Thus, by using volumes, we get $1 \leq M(2\varepsilon)^d$. ■

Packing with Varshamov-Gilbert lemma. The maximal number of points in the hypercube $\{0, 1\}^d$ that are at least $d/4$ -apart in Hamming loss (i.e., ℓ_1 -distance) is greater than $\exp(d/8)$.

Lemma 12.2 (Varshamov-Gilbert's lemma) *For any $\alpha \in (0, 1)$, there exists a subset \mathcal{B} of the hypercube $\{0, 1\}^d$ such that*

- (a) for all $x, x' \in \mathcal{B}$ such that $x \neq x'$, $\|x - x'\|_1 \geq (1 - \alpha)\frac{d}{2}$,
- (b) $|\mathcal{B}| \geq \exp(d\alpha^2/2)$.

Proof We consider the largest family satisfying (a). By maximality, the union of ℓ_1 -balls of radius $(1 - \alpha)\frac{d}{2}$ includes all of $\{0, 1\}^d$. Therefore, by comparing cardinalities,

$$2^d \leq \sum_{x \in \mathcal{B}} |\{y \in \{0, 1\}^d, \|y - x\|_1 \leq (1 - \alpha)\frac{d}{2}\}|.$$

Consider a random variable z , which is binomial with parameters d and $1/2$ (that is, the sum of d independent uniform Bernoulli random variables). Then,

$$2^{-d} |\{y \in \{0, 1\}^d, \|y - x\|_2^2 = \|y - x\|_1 \leq (1 - \alpha)\frac{d}{2}\}| = \mathbb{P}(z \leq (1 - \alpha)\frac{d}{2}) = \mathbb{P}(z \geq (1 + \alpha)\frac{d}{2}).$$

Using Hoeffding's inequality (Prop. 1.1), we get $\mathbb{P}(z \geq (1 + \alpha)\frac{d}{2}) = \mathbb{P}(\frac{z}{d} - \frac{\mathbb{E}[z]}{d} \geq \alpha\frac{d}{2}) \leq \exp(-2d(\alpha/2)^2) = \exp(-d\alpha^2/2)$. This leads to the result. ■

12.1.5 Examples

Fixed design linear regression. We consider linear regression with $\Phi \in \mathbb{R}^{n \times d}$ a design matrix with $\frac{1}{n}\Phi^\top\Phi = I$ (which imposes $n \geq d$). We consider the ball $\Theta = \{\theta \in \mathbb{R}^d, \|\theta\|_2 \leq D\}$. By rotational invariance of the Gaussian distribution of the noise variable ε , we can assume that the first d rows of Φ are equal to $\sqrt{n}I$ and the rest of the rows are equal to zero. Thus we can assume the model $y = \theta_* + \frac{1}{\sqrt{n}}\varepsilon$, where $\varepsilon \in \mathbb{R}^d$ with normal distribution with mean zero and covariance $\sigma^2 I$, and $y \in \mathbb{R}^d$. We are thus in the situation where $d(\theta, \theta')^2 = \|\theta - \theta'\|_2^2$.

In order to find M points in $\Theta = \{\theta \in \mathbb{R}^d, \|\theta\|_2 \leq D\}$, we consider the $M \geq \exp(d/8)$ elements x_1, \dots, x_M of $\{0, 1\}^d$ from Lemma 12.2 with $\alpha = 1/2$, and define $\theta_i = \beta(2x_i - 1_d) \in \{-\beta, \beta\}$. Thus $\|\theta_i\|_2^2 = \beta^2 d$, and, for $i \neq j$,

$$\|\theta_i - \theta_j\|_2^2 \leq 4\beta^2 d \leq 32\beta^2 \log(M) \text{ and } \|\theta_i - \theta_j\|_2^2 \geq \beta^2 d.$$

We thus need, $\beta^2 d \leq D^2$, and $32\beta^2 \log(M) \frac{n}{2\sigma^2} \leq \frac{\log M}{4}$, that is, $64\beta^2 \frac{n}{\sigma^2} \leq 1$. Thus, the optimal rate is greater than

$$\frac{1}{8}\beta^2 d \geq \frac{1}{8} \min \left\{ D^2, \frac{\sigma^2 d}{64n} \right\}.$$

Therefore, when $D^2 \geq \frac{\sigma^2 d}{64n}$, we get a lower bound of $\frac{\sigma^2 d}{512n}$, which is the upper-bound obtained in Chapter 3 (note that in Section 3.7 we provided a sharper lower-bound using similar tools as in Section 12.1.6).

The sparse regression setting could also be considered with the same tool, but the proof is simpler with the Bayesian arguments from Section 12.1.6. We now turn to the random design setting.

Exercise 12.1 Use Lemma 12.1 instead of Lemma 12.2 to obtain the same result.

Random design linear regression. We consider the same model as above, but with (x_i, y_i) sampled i.i.d. from a given distribution such that $\mathbb{E}[\varphi(x)\varphi(x)^\top] = I$, so that $d(\theta, \theta')^2 = \|\theta - \theta'\|_2^2$. Thus the result above for fixed design regression also applies to the random design setting.

Non-parametric estimation with Hilbert spaces (♦). We consider random design regression with a fixed distribution for the inputs, with Gaussian independent noise and target functions which are in a certain ellipsoid of $L_2(p)$. That is, we assume that there exists a compact self-adjoint operator T on $L_2(p)$ such that $\langle \theta, T^{-1}\theta \rangle_{L_2(p)} \leq D^2$. We denote by $(\lambda_m)_{m \geq 1}$ the non-increasing sequence of eigenvalues of T , with the associated eigenvectors ψ_m in $L_2(p)$.

We consider a certain integer K , and $M \geq \exp(K/8)$ elements x_1, \dots, x_M of $\{0, 1\}^K$. We define $\theta_i = \beta \sum_{m=1}^K (2(x_i)_m - 1)\psi_m$. Then $\langle \theta, T^{-1}\theta \rangle_{L_2(p)} = \beta^2 \sum_{m=1}^K \lambda_m^{-1} \leq K\beta^2 \lambda_K^{-1}$, and, for $i \neq j$,

$$\|\theta_i - \theta_j\|_{L_2(p)}^2 \leq 4\beta^2 K \leq 32\beta^2 \log(M) \text{ and } \|\theta_i - \theta_j\|_{L_2(p)}^2 \geq \beta^2 K.$$

We thus need, $\beta^2 K \leq D^2 \lambda_K$, and $32\beta^2 \log(M) \frac{n}{2\sigma^2} \leq \frac{\log M}{4}$, that is, $64\beta^2 \frac{n}{\sigma^2} \leq 1$. Thus, the minimax lower bound is greater than

$$\frac{1}{8}\beta^2 K \geq \frac{1}{8} \min \left\{ D^2 \lambda_K, \frac{\sigma^2 K}{64n} \right\}.$$

We can now specialize to Sobolev spaces where it can be shown that for compact supports with piecewise smooth boundaries. The sum of all L_2 -norms of partial derivatives corresponds to an operator for which $\lambda_K \geq C \cdot K^{-\alpha}$, with $\alpha = 2s/d$ when all s -th order derivatives are taken, for a constant C (Adams and Fournier, 2003). The lower bound becomes

$$\max_{K \geq 1} \frac{1}{8} \min \left\{ D^2 C K^{-\alpha}, \frac{\sigma^2 K}{64n} \right\},$$

which can be balanced to obtain $K \propto \left(\frac{nD^2}{\sigma^2}\right)^{1/(1+\alpha)}$, leading to lower bound proportional to

$$D^{2/(1+\alpha)} \left(\frac{\sigma^2}{n}\right)^{\alpha/(1+\alpha)}.$$

For $\alpha = 2s/d$, we get $\alpha/(1+\alpha) = \frac{2s}{2s+d}$, and the lower matches the upper-bound obtained with kernel ridge regression in Chapter 7. It turns out that the lower bound on the minimax

rate for Lipschitz-continuous functions is the same as for $s = 1$ ([Tsybakov, 2008](#), Section 2.6).

12.1.6 Minimax lower bounds through Bayesian analysis

As outlined for least-squares in Section [3.7](#), we can use a Bayesian analysis as follows. We consider a certain probability distribution $p(\theta_*)$ whose support is included in Θ . Then we have:

$$\inf_{\mathcal{A}} \sup_{\theta_* \in \Theta} \mathbb{E}_{\theta_*} [d(\theta_*, \mathcal{A}(\mathcal{D}))^2] \geq \inf_{\mathcal{A}} \mathbb{E}_{p(\theta_*)} \mathbb{E}_{\theta_*} [d(\theta_*, \mathcal{A}(\mathcal{D}))^2].$$

This reasoning is particularly simple when the optimal algorithm \mathcal{A} is simple to estimate, which is the case in particular where d is a Euclidean norm so that $\mathcal{A}^*(\mathcal{D}) = \mathbb{E}[\theta_* | \mathcal{D}]$. If the prior $p(\theta_*)$ and the likelihood $p(\mathcal{D} | \theta_*)$ are simple enough, then the conditional expectation can be computed in closed form. In Section [3.7](#), these were all Gaussians, which was possible for the prior distribution on Θ because Θ was unbounded. When dealing with bounded balls, we need to use different distributions, as used originally by [Donoho and Johnstone \(1994\)](#).

Least-squares on a Euclidean ball. We consider linear regression with a fixed design like in the previous section (with a bound $\|\theta_*\|_2 \leq D$), which corresponds to the model $y = \theta_* + \frac{1}{\sqrt{n}}\varepsilon$, where $\varepsilon \in \mathbb{R}^d$ with normal distribution with mean zero and covariance $\sigma^2 I$, and $y, \theta_* \in \mathbb{R}^d$.

We then consider a prior distribution on θ_* as $\theta_* = \beta x$, where $x \in \{-1, 1\}^d$ are independent Rademacher random variables. We need $\beta^2 d \leq D^2$ to be in the correct set. We then need to compute $\mathbb{E}[\theta_* | y]$. The posterior probability of θ_* is supported on $\beta\{-1, 1\}^n$. Moreover, given the independence by component, we can treat each of them separately. Then, by keeping only terms that depend on the posterior value, we get:

$$\mathbb{P}((\theta_*)_i = \pm\beta | y_i) \propto \exp\left(-\frac{n}{2\sigma^2}(y_i - \pm\beta)^2\right) \propto \exp\left(\pm\frac{n}{\sigma^2}y_i\beta\right).$$

Thus,

$$\mathbb{E}[(\theta_*)_i | y_i] = \beta \frac{\exp(\frac{n}{\sigma^2}y_i\beta) - \exp(-\frac{n}{\sigma^2}y_i\beta)}{\exp(\frac{n}{\sigma^2}y_i\beta) + \exp(-\frac{n}{\sigma^2}y_i\beta)} = \beta \frac{1 - \exp(-2\frac{n}{\sigma^2}y_i\beta)}{1 + \exp(-2\frac{n}{\sigma^2}y_i\beta)} = \beta [\text{sigmoid}\left(2\frac{n}{\sigma^2}y_i\beta\right) - 1],$$

where $\text{sigmoid}(\alpha) = 1/(1 + \exp(-\alpha))$.

The posterior variance for the i -th component is equal to

$$\begin{aligned}\mathbb{E}[(\theta_*)_i - \mathbb{E}[(\theta_*)_i|y_i])^2] &= \frac{1}{2}\mathbb{E}_{\varepsilon_i}(\beta - \beta[2\text{sigmoid}(2\frac{n}{\sigma^2}\beta(\beta + \varepsilon_i/\sqrt{n})) - 1])^2 \\ &\quad + \frac{1}{2}\mathbb{E}_{\varepsilon_i}(-\beta - \beta[2\text{sigmoid}(2\frac{n}{\sigma^2}\beta(-\beta + \varepsilon_i/\sqrt{n})) - 1])^2 \\ &= 4\beta^2\mathbb{E}_{\varepsilon_i \sim \mathcal{N}(0, \sigma^2)}\left[\left(\text{sigmoid}\left(-2\frac{n}{\sigma^2}\beta^2 + 2\frac{\sqrt{n}}{\sigma^2}\beta\varepsilon_i\right)\right)^2\right] \\ &= 4\beta^2\mathbb{E}_{\tilde{\varepsilon}_i \sim \mathcal{N}(0, 1)}\left[\left(\text{sigmoid}\left(-2\frac{n}{\sigma^2}\beta^2 + 2\frac{\beta\sqrt{n}}{\sigma}\tilde{\varepsilon}_i\right)\right)^2\right].\end{aligned}$$

We consider the function $\psi : \alpha \mapsto \mathbb{E}_{\varepsilon \sim \mathcal{N}(0, 1)}\left[\left(\text{sigmoid}(-2\alpha^2 + 2\alpha\varepsilon)\right)^2\right]$. We have $\psi(0) = 1/4$, and $\psi(\alpha) \rightarrow 0$ when $\alpha \rightarrow +\infty$, and $\psi(\alpha) \geq \frac{1}{4}\mathbb{P}_{\varepsilon \sim \mathcal{N}(0, 1)}(\varepsilon > \alpha) \geq \frac{1}{8}\exp(-\alpha^2)$, by using simple Gaussian tail bounds (and since the sigmoid function is greater than 1/2 for positive numbers).

Thus, the total posterior variance $\mathbb{E}[\|\theta_* - \mathbb{E}[\theta_*|y]\|_2^2]$ is greater than

$$\frac{\beta^2 d}{2} \exp(-n\beta^2/\sigma^2) = \frac{\sigma^2 d}{n} \times \frac{\beta^2 n}{2\sigma^2} \exp(-n\beta^2/\sigma^2),$$

which is maximized for $\beta^2 \propto \sigma^2/n$, and thus if $\sigma^2 d/n$ is smaller than D^2 , we obtain the usual $\sigma^2 d/n$, while if it is greater than D^2 , we take $\beta_2^2 = D^2/d$, to obtain the lower bound

$$D^2 \exp(-4nD^2/(\sigma^2 d)) \geq D^2 \exp(-4),$$

which leads to the same bound as the previous section but with a more direct argument.

Sparse case (\blacklozenge). To deal with the sparse case, we could consider a prior on θ_* that is only selecting k non-zero elements out of d and perform an analysis based on the posterior probability of θ_* . Following [Donoho and Johnstone \(1994\)](#), it is easier to divide the set of d variables into k blocks of size d/k (for simplicity, we assume that d/k is an integer). We then consider a prior probability defined independently on each of the k blocks by selecting one of the d/k variables uniformly at random and setting its value to β , while all others are set to zero.

To compute the posterior probability of θ_* , we can treat each block independently and sum the posterior variances; we thus consider the first block, composed of d/k variables, and compute the probability that the selected variable is the j -th one, which is proportional to

$$\exp(-n/(2\sigma^2)(y_j - \beta)^2) \prod_{i \neq j} \exp(-n/(2\sigma^2)(y_i)^2) \propto \exp(n\beta y_j/\sigma^2).$$

The conditional expectation of θ_* then satisfies

$$\mathbb{E}[(\theta_*)_i|y] = \beta \frac{\exp(n\beta y_i/\sigma^2)}{\sum_{j=1}^{d/k} \exp(n\beta y_j/\sigma^2)}.$$

To compute the posterior variance, we need to sample from the prior θ_* . By symmetry, we may consider that $\theta_1 = \beta$. If $y_1 \leq \max_{j \neq 1} y_j$, then

$$\mathbb{E}[(\theta_*)_1|y] = \beta \frac{\exp(n\beta y_1/\sigma^2)}{\sum_{j=1}^{d/k} \exp(n\beta y_j/\sigma^2)} \leq \beta t \frac{\exp(n\beta y_1/\sigma^2)}{\exp(n\beta y_1/\sigma^2) + \exp(n\beta \max_{j \neq 1} y_j/\sigma^2)} \leq \beta/2,$$

and then the risk is at least $(\beta - \mathbb{E}[(\theta_*)_1|y])^2 \geq \beta^2/4$.

In order to lower-bound the probability that $y_1 \leq \max_{j \neq 1} y_j$, we can consider the events $\{y_1 \leq \beta\}$ and $\{\beta \leq \max_{j \neq 1} y_j\}$. The probability that $y_1 = \beta + \varepsilon_1$ is less than β is greater than $1/2$. Moreover, by independence of all y_j , $j \neq 1$,

$$\mathbb{P}(\{\beta \leq \max_{j \neq 1} y_j\}) \geq 1 - (1 - \mathbb{P}_{t \sim \mathcal{N}(0,1)}(t \geq \beta\sqrt{n}/\sigma))^{d/k-1}.$$

Thus, the lower bound is greater than

$$k \frac{\beta^2}{8} \left[1 - (1 - \mathbb{P}_{t \sim \mathcal{N}(0,1)}(t \geq \beta\sqrt{n}/\sigma))^{d/k-1} \right] \geq k \frac{\beta^2}{8} \left[1 - \left(1 - \frac{1}{2} \exp(-\beta^2 n/\sigma^2) \right)^{d/k-1} \right],$$

using the Gaussian tail bound $\mathbb{P}_{t \sim \mathcal{N}(0,1)}(t \geq z) \geq \frac{1}{2} \exp(-z^2)$. We can then consider $\beta^2 = \frac{\sigma^2}{n} \sqrt{2 \log(d/k)}$, leading to a lower bound

$$\frac{\sigma^2 k}{4n} \log(d/k) \left[\left(1 - \left(1 - \frac{1}{2} (k/d) \right)^{d/k-1} \right) \right]$$

which is greater than $\frac{\sigma^2 k}{8n} \log(d/k)$ if $k \leq 2d$. We obtain the same lower-bound as the upper-bound for ℓ_0 -penalty-based methods in Chapter 8.

12.2 Optimization lower bounds

In this section, we consider ways of obtaining lower bounds of performance for optimization algorithms. While the statistical lower bounds from the previous section were not obtained by explicitly building hard problems, the algorithmic lower bounds of this section will explicitly build such hard problems.

12.2.1 Convex optimization

To obtain computational lower bounds for convex optimization, which is notoriously hard in general in computer science, we will rely on a simple model of computation; that is, we will restrict ourselves to methods that access gradients of the objective function and combine them linearly to select a new query point.

We follow the results from [Nesterov \(2018, Section 2.1.2\)](#) and [Bubeck \(2015, Section 3.5\)](#), and assume that we want to minimize a convex function F defined on \mathbb{R}^d . The algorithm starts from $\theta_0 = 0$ and can only query points in the span of the observed gradients or some sub-gradients of F at the previously observed points.

The key is finding functions with the proper regularity properties, for which we know that a few iterations provably lead to suboptimal performance. These functions will only reveal one new variable at each iteration and, after k iterations, can only achieve the minimum on the first k variables.

Non-smooth functions. We consider the following function, which will be dedicated to a given number of iterations k :

$$F(\theta) = \eta \max_{i \in \{1, \dots, k+1\}} \theta_i + \frac{\mu}{2} \|\theta\|_2^2,$$

for $k < d$, and η, μ positive parameters that will be set later.

The subdifferential of $F(\theta)$ is equal to

$$\mu\theta + \eta \cdot \text{hull}(\{e_i, \theta_i = \max_{i' \in \{1, \dots, k+1\}} \theta_{i'}\}),$$

which is bounded in ℓ_2 -norm on the ball of radius R , by $\mu R + \eta$ (here e_i denotes the i -th basis vector). We consider the oracle where the output gradient is $\mu\theta + \eta e_i$, where i is the smallest index within maximizers of $\theta_{i'}$.

Starting from $\theta_0 = 0$, θ_1 is supported on the first variable, and by recursion, after $k \leq d$ steps of subgradient descent, θ_k is supported on the first k variables. Since $k < d$, then $(\theta_k)_{k+1} = 0$, so $F(\theta_k) \geq 0$. Minimizing over the span of the first $k+1$ variables leads to, by symmetry, $\theta_* = \kappa \sum_{i=1}^{k+1} e_i$, for a certain κ which minimizes $\eta\kappa + \frac{(k+1)\mu}{2}\kappa^2$, so that $\kappa = -\frac{\eta}{\mu(k+1)}$, and thus $\theta_* = -\frac{\eta}{\mu(k+1)} \sum_{i=1}^{k+1} e_i$, with value $F(\theta_*) = -\frac{\eta^2}{2\mu(k+1)}$. Thus

$$F(\theta_k) - F(\theta_*) \geq 0 - F(\theta_*) = \frac{\eta^2}{2\mu(k+1)},$$

with $\|\theta_*\|_2^2 = \frac{\eta^2}{\mu^2(k+1)}$.

In order to build a B -Lipschitz-continuous function on a ball of center 0 and radius D , we can take $\eta = B/2$, and $D = B/(2\mu)$, and we get a lower bound of $\frac{B^2}{8\mu k}$.

With $\mu = \frac{B}{D} \frac{1}{1+\sqrt{k+1}}$ and $\eta = B \frac{\sqrt{k+1}}{1+\sqrt{k+1}}$, we also get a B -Lipschitz continuous function, and we get the lower bound $\frac{DB}{2(1+\sqrt{k+1})}$, which is valid as long as $k < d$.

⚠ The lower bounds are only valid for $k < d$ because there exist algorithms that are linearly convergent in this setting with a constant that depends on d , such as the ellipsoid method or the center of mass method (see [Bubeck, 2015](#), for details).

Smooth functions (♦). We consider a sequence of quadratic functions on \mathbb{R}^d . We need that the gradient for iterates supported on the first i components is supported on the first $i+1$ components. We consider the example from Nesterov (2018, Section 2.1.2), and highlight the main arguments without proof:

$$F_k(\theta) = \frac{L}{4} \left\{ \frac{1}{2} \left[\theta_1^2 + \theta_k^2 + \sum_{i=1}^{k-1} (\theta_i - \theta_{i+1})^2 \right] - \theta_1 \right\}.$$

The function F_k is convex and smooth, with a smoothness constant less than L . Moreover, its global minimizer is attained at $\theta_*^{(k)}$ such that $(\theta_*^{(k)})_i = 1 - \frac{i}{k+1}$ for $i \in \{1, \dots, k\}$ and 0 otherwise, with an optimal value of $F_k(\theta_*^{(k)}) = \frac{L}{8} \frac{-k}{k+1}$, and with

$$\|\theta_*^{(k)}\|_2^2 = \sum_{i=1}^k \left(1 - \frac{i}{k+1}\right)^2 \leq \frac{k+1}{3}.$$

By construction, if θ is supported in the first i components for $i < k$, then $F'_k(\theta)$ is supported on the first $i+1$ components. Thus, the i -th iterate is supported on the first i components, and therefore the lowest attainable value is $F_i(\theta_*^{(i)})$.

Given this set of functions, for a given k such that $k \leq \frac{d-1}{2}$, we consider F_{2k+1} , for which $\theta_*^{(2k+1)}$ is the global minimizer with value $\frac{L}{8} \frac{-2k-1}{2k+2}$, while after k iterations, we can only achieve $F_k(\theta_*^{(k)}) = \frac{L}{8} \frac{-k}{k+1}$. Thus, we have:

$$\frac{F_{2k+1}(\theta_k) - F_{2k+1}^*}{\|\theta_0 - \theta_*\|_2^2} \geq \frac{L}{8} \frac{\frac{1}{k+1} - \frac{1}{2k+2}}{\frac{2k+2}{3}} \geq \frac{3L}{32} \frac{1}{(k+1)^2}.$$

We thus obtain the lower bounds corresponding to the upper bounds obtained from Nesterov acceleration.

⚠ The number of iterations has to be less than half the dimension for the lower bound to hold.

Smooth strongly-convex functions (♦). Following Nesterov (2018), we consider a function defined on the space ℓ_2 of square-summable sequences as

$$F(\theta) = \frac{L-\mu}{4} \left\{ \frac{1}{2} \left[\theta_1^2 + \sum_{i=1}^{\infty} (\theta_i - \theta_{i+1})^2 \right] - \theta_1 \right\} + \frac{\mu}{2} \|\theta\|_2^2.$$

This function is L -smooth and μ -strongly convex. Its global minimizer is θ_* such that

$$(\theta_*)_k = \left(\frac{1 - \sqrt{\mu/L}}{1 + \sqrt{\mu/L}} \right)^k = q^k,$$

with $\|\theta_*\|_2^2 = \sum_{k=1}^{\infty} q^{2k} = \frac{q^2}{1-q^2}$. Moreover, it can be shown that $\|\theta_k - \theta_*\|_2^2 \geq \sum_{i=k+1}^{\infty} q^{2i} = q^{2k} \|\theta_*\|_2^2$. This leads to $F(\theta_k) - F_* \geq \frac{\mu}{2} \|\theta_k - \theta_*\|_2^2 \geq q^{2k} \|\theta_0 - \theta_*\|_2^2$.

12.2.2 Non-convex optimization (♦)

While upper and lower bounds can have a good behavior with respect to dimension in the convex case, this is not the case when removing the convexity assumption. In this section, we show that when optimizing a Lipschitz-continuous function on a compact subset of \mathbb{R}^d , we cannot hope to have guarantees which are not exponential in dimension.

 This does not mean that all problem instances will require exponential time, but that in the worst-case sense, for any algorithm, there will always be a bad function.

We consider minimizing a function F on a bounded subset Θ of \mathbb{R}^d , based only on function evaluations, a problem often referred to as zero-th order optimization or derivative-free optimization (see algorithms for convex functions in Section 13.2). No convexity is assumed in this section, so we should not expect fast rates and, again, no efficient algorithms that can provably find a global minimizer. Clearly, such algorithms are not made to be used to find millions of parameters for logistic regression or neural networks. Still, they are often used for hyperparameter tuning (regularization parameters, size of neural network layers, etc.). See, e.g., [Snoek et al. \(2012\)](#) for applications.

We will assume some regularity for the functions we want to minimize, typically bounded derivatives. We will thus assume that $f \in \mathcal{F}$, for a space \mathcal{F} of functions from Θ to \mathbb{R} . We will take a worst-case approach, where we characterize convergence over all members of \mathcal{F} . That is, we want our guarantees to hold for *all* functions in \mathcal{F} . Note that this worst-case analysis may not predict well what is happening for a particular function; in particular, it is (by design) pessimistic.

An algorithm \mathcal{A} will be characterized by (a) the choice of points $\theta_1, \dots, \theta_n \in \Theta$ to query the function, and (b) the algorithm to output a candidate $\hat{\theta} \in \Theta$ such that $F(\hat{\theta}) - \inf_{\theta \in \Theta} F(\theta)$ is small. The estimate $\hat{\theta}$ can only depend on $(\theta_i, F(\theta_i))$, for $i \in \{1, \dots, n\}$. In this section, the choice of points $\theta_1, \dots, \theta_n$ is made once (without seeing any function values).¹

Given a selection of points and the algorithm \mathcal{A} , the rate of convergence is the supremum over all functions $F \in \mathcal{F}$ of the error $F(\hat{\theta}) - \inf_{\theta \in \Theta} F(\theta)$. This is a function $\varepsilon_n(\mathcal{A})$ of the number n of sampled points (and of the class of functions \mathcal{F}). The optimal algorithm (minimizing $\varepsilon_n(\mathcal{A})$) will lead to a rate we denote $\varepsilon_n^{\text{opt}}$, and which we aim to characterize.

Direct lower/upper bounds for Lipschitz-continuous functions. The argument is particularly simple for a bounded metric space Θ with distance δ , and \mathcal{F} the class of L -Lipschitz-continuous functions, that is, such that for all $\theta, \theta' \in \Theta$, $|F(\theta) - F(\theta')| \leq L\delta(\theta, \theta')$. This is a very large set of functions, so we expect weak convergence rates.

¹It turns out that going *adaptive*, where the point θ_{i+1} is selected after seeing $(\theta_j, F(\theta_j))$ for all $j \leq i$, does not bring much (at least in the worst-case sense) ([Novak, 2006](#)).

Like in Section 4.4.4, we will need to cover the set Θ with balls of a given radius. The minimal radius r of a cover of Θ by n balls of radius r is denoted $r_n(\Theta, \delta)$. This corresponds to n ball centers $\theta_1, \dots, \theta_n$. See example below for the unit cube $\Theta = [0, 1]^2$ and the metric obtained from the ℓ_∞ -norm, with $n = 16$, and $r_n([0, 1]^2, \ell_\infty) = 1/8$.

| | | | |
|---------------|---------------|---------------|---------------|
| r | | | |
| θ_1 | \bullet | \bullet | \bullet |
| | θ_2 | \bullet | \bullet |
| | | θ_3 | \bullet |
| | | | θ_4 |
| | | | |
| θ_5 | \bullet | \bullet | \bullet |
| | θ_6 | \bullet | \bullet |
| | | θ_7 | \bullet |
| | | | θ_8 |
| | | | |
| θ_9 | \bullet | \bullet | \bullet |
| | θ_{10} | \bullet | \bullet |
| | | θ_{11} | \bullet |
| | | | θ_{12} |
| | | | |
| θ_{13} | \bullet | \bullet | \bullet |
| | θ_{14} | \bullet | \bullet |
| | | θ_{15} | \bullet |
| | | | θ_{16} |

More generally, for the unit cube $\Theta = [0, 1]^d$, we have $r_n([0, 1]^d, \ell_\infty) \approx \frac{1}{2}n^{-1/d}$ (which is not an approximation when n is the d -th power of an integer). For other normed metrics (since all norms are equivalent), the scaling as $r_n \sim \text{diam}(\Theta)n^{-1/d}$ is the same on any bounded set in \mathbb{R}^d (with an extra constant that depends on d).

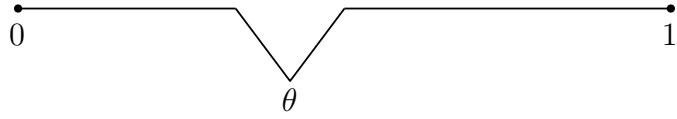
Naive algorithm. Given the ball centers $\theta_1, \dots, \theta_n$, outputting the minimum of function values $F(\theta_i)$ for $i = 1, \dots, n$, leads to an error which is less than $Lr_n(\Theta, \delta)$, as the optimal $\theta_* \in \Theta$ is at most at distance $r_n(\Theta, \delta)$ from one of the cluster centers, let's say θ_k , and thus $F(\theta_k) - F(\theta_*) \leq L\delta(\theta_k, \theta_*) \leq Lr_n(\Theta, \delta)$. This provides an upper bound on $\varepsilon_n^{\text{opt}}$. The algorithm we just described seems naive, but it turns out to be optimal for this class of problems.

Lower bound. Consider any optimization algorithm, with its first n point queries and its estimate $\hat{\theta}$. By considering the functions which are zero in these $n + 1$ points, the algorithm can only output an arbitrary fixed real number for the optimal value (let's say zero). We now simply need to construct a function $F \in \mathcal{F}$ such that F is zero at these points but maximally smaller than zero at a different point.

Given the $n + 1$ points above, there is at least a point $\eta \in \Theta$ which is at a distance at most $r_{n+1}(\Theta, \delta)$ from all of them (otherwise, we obtain a cover of Θ with $n + 1$ points). We can then construct the function

$$F(\theta) = -L(r_{n+1}(\Theta, \delta) - d(\theta, \eta))_+ = -L \max \{r_{n+1}(\Theta, \delta) - d(\theta, \eta), 0\},$$

which is L -Lipschitz-continuous, equal to zero on all points of the algorithm and the output point $\hat{\theta}$, and with minimum value $-Lr_{n+1}(\Theta, \delta)$ attained at η . Thus, we must have $\varepsilon_n^{\text{opt}} \geq 0 - (-Lr_{n+1}(\Theta, \delta)) = Lr_{n+1}(\Theta, \delta)$. This difficult function is plotted below in one dimension.



Thus, the performance of any algorithm from n function values has to be larger than $Lr_{n+1}(\Theta, \delta)$. Thus, so far, we have shown that

$$Lr_{n+1}(\Theta, \delta) \leq \varepsilon_n^{\text{opt}} \leq Lr_n(\Theta, \delta).$$

For $\Theta \subset \mathbb{R}^d$, $r_n(\Theta, \delta)$ is typically of order $\text{diam}(\Theta)n^{-1/d}$, and thus the difference between n and $n+1$ above is negligible. Note that the rate in $n^{-1/d}$ is *very* slow and symptomatic of the classical curse of dimensionality. The appearance of a covering number is not totally random here and comes from the equivalence in terms of worst-case guarantees between optimization and uniform approximation (Novak, 2006).

Random search. We can have a similar bound up to logarithmic terms for random search, that is, after selecting independently n points $\theta_1, \dots, \theta_n$, uniformly at random in Θ , and selecting the points with smallest function value $F(\theta_i)$. The performance can be shown to be proportional to $L\text{diam}(\Theta)(\log n)^{1/d}n^{-1/d}$ in high probability, leading to an additional logarithmic term (the proof can be obtained with a simple covering argument, see exercise below). Therefore, random search is optimal up to logarithmic terms for this very large class of functions to optimize.

To go beyond Lipschitz-continuous functions, we can leverage smoothness like in supervised learning and hopefully avoid the dependence in $n^{-1/d}$. This can be done by a somewhat surprising equivalence between worst-case guarantees from optimization and worst-case guarantees for uniform approximation.²

Exercise 12.2 (♦) Consider sampling independently and uniformly in Θ n points $\theta_1, \dots, \theta_n$.

(a) For a given L -Lipschitz-continuous function F , show that the worst-case performance of outputting the lower function value is less than $L \max_{\theta \in \Theta} \min_{i \in \{1, \dots, n\}} \delta(\theta, \theta_i)$.

(b) Considering an optimal cover with m points and radius $r = r_m(\Theta, d)$, show that

$$\mathbb{P}\left(\max_{\theta \in \Theta} \min_{i \in \{1, \dots, n\}} \delta(\theta, \theta_i) \geq 2r\right) \leq m(1 - 1/m)^n.$$

(c) By the appropriate choice of m , show that when $r \sim m^{-1/d}\text{diam}(\mathcal{X})$, we get an overall performance proportional to $L\left(\frac{\log n}{n}\right)^{1/d}$ with probability greater than $1 - \frac{\log n}{n}$.

²See <https://francisbach.com/optimization-is-as-hard-as-approximation/> for more details, as well as Novak (2006).

12.3 Lower bounds for stochastic gradient descent (♦)

In this section, our goal is to show that the convergence rates for stochastic gradient descent (SGD) shown in Section 5.4 are “optimal”, in a sense to be made precise. We consider a class \mathcal{F} of functions, here the convex B -Lipschitz-continuous functions on the ball of center zero and radius D (for the Euclidean norm). We consider the class \mathcal{A} of algorithms that can sequentially access independent random unbiased estimates of the gradients of a function F in \mathcal{F} , with squared norm bounded by B^2 , and we denote $A_t(F) \in \mathbb{R}^d$ the output of algorithm A . Our goal is to find upper and lower bounds on

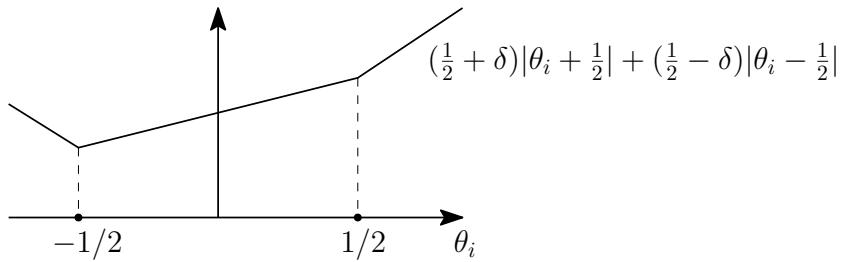
$$\varepsilon_t(\mathcal{A}, \mathcal{F}) = \inf_{A \in \mathcal{A}} \sup_{f \in \mathcal{F}} \mathbb{E}[F(A_t(F)) - \inf_{\|\theta\|_2 \leq D} F(\theta)].$$

SGD is an algorithm in \mathcal{A} achieving a bound proportional to BD/\sqrt{t} , thus, up to a constant, $\varepsilon_t(\mathcal{A}, \mathcal{F}) \leq BD/\sqrt{t}$. We now prove a matching lower-bound by exhibiting a set of functions that will make any algorithm have this desired performance. Note that, as opposed to Section 12.2.1 on deterministic convex optimization, we make no assumption on the running-time complexity of algorithms in \mathcal{A} .

We follow the exposition from Agarwal et al. (2012) and consider a function

$$F_\alpha(\theta) = \frac{B}{2d} \sum_{i=1}^d \left\{ \left(\frac{1}{2} + \alpha_i \delta \right) \cdot \left| \theta_i + \frac{1}{2} \right| + \left(\frac{1}{2} - \alpha_i \delta \right) \cdot \left| \theta_i - \frac{1}{2} \right| \right\}, \quad (12.5)$$

with $\alpha \in \{-1, 1\}^d$ a well chosen vector and $\delta \in (0, 1/4]$, and $B > 0$. One element of the sum is plotted below.



The function F_α is convex and Lipschitz-continuous with gradients bounded in L_2 -norm by $B/(2\sqrt{d})$. Moreover, the global minimizer of F_α is $\theta = -\frac{\alpha}{2}$, with an optimal value equal to $F_\alpha^* = \frac{B}{4}(1 - 2\delta)$. That is, minimizing F_α on $[-1/2, 1/2]^d$ exactly corresponds to finding an element of the hypercube α . Moreover, it turns out that minimizing it approximately also leads to identifying α among a set of α 's, which are sufficiently different.

Lemma 12.3 *If $\alpha, \beta \in \{-1, 1\}^d$, and $F_\alpha(\theta) - F_\alpha^* \leq \varepsilon$, then $F_\beta(\theta) - F_\beta^* \geq \frac{B\delta}{2d}\|\alpha - \beta\|_1 - \varepsilon$.*

Proof (♦) We have: $F_\beta(\theta) - F_\beta^* = F_\beta(\theta) + F_\alpha(\theta) - F_\beta^* - F_\alpha^* + [F_\alpha^* - F_\alpha(\theta)]$. We then notice that for all $\theta \in \mathbb{R}^d$,

$$F_\beta(\theta) + F_\alpha(\theta) - F_\beta^* - F_\alpha^* \geq \frac{B}{2d} \sum_{i, \alpha_i \neq \beta_i} \left\{ \left| \theta_i + \frac{1}{2} \right| + \left| \theta_i - \frac{1}{2} \right| + 2\delta - 1 \right\} \geq \frac{B\delta}{2d} \|\alpha - \beta\|_1.$$

■

Thus, if we consider M points $\alpha^{(1)}, \dots, \alpha^{(M)} \in \{-1, 1\}^d$ such that $\|\alpha^{(i)} - \alpha^{(j)}\|_1 \geq \frac{d}{2}$ (with potentially $M \geq \exp(d/8)$ such points from Lemma 12.2), then, if $\varepsilon < \frac{B\delta}{8}$, because of Lemma 12.3, minimizing up to ε exactly identifies which of the functions $F_{\alpha^{(i)}}$ was being minimized.

Moreover, if $\hat{\theta}$ is random then, denoting $\mathcal{A} = \{\alpha^{(1)}, \dots, \alpha^{(M)}\}$, following the same reasoning as in Section 12.1.2:

$$\sup_{\alpha \in \mathcal{A}} \mathbb{E}_\alpha [F_\alpha(\hat{\theta}) - F_\alpha^*] \geq \varepsilon \cdot \sup_{\alpha \in \mathcal{A}} \mathbb{P}_\alpha (F_\alpha(\hat{\theta}) - F_\alpha^* > \varepsilon) \geq \varepsilon \cdot \frac{1}{|\mathcal{A}|} \sum_{\alpha \in \mathcal{A}} \mathbb{P}_\alpha (F_\alpha(\hat{\theta}) - F_\alpha^* > \varepsilon).$$

From an estimate $\hat{\theta}$, we can build a test $g(\hat{\theta}) \in \mathcal{A}$ by selecting the (unique if $\varepsilon < \frac{B\delta}{8}$) $\alpha \in \mathcal{A}$ such that $F_\alpha(\hat{\theta}) - F_\alpha^* \leq \varepsilon$ if it exists, and uniformly at random in \mathcal{A} otherwise. Therefore, the minimax performance is greater than ε times the probability of mistake of the best possible test.

We consider the following stochastic oracle:

- (1) pick some coordinate $i \in \{1, \dots, d\}$ uniformly at random,
- (2) draw a Bernoulli random variable $b_i \in \{0, 1\}$ with parameter $\frac{1}{2} + \alpha_i \delta$,
- (3) consider $\hat{F}(\theta) = b_i |\theta_i + \frac{1}{2}| + (1 - b_i) |\theta_i - \frac{1}{2}|$, with gradient with components

$$\hat{F}'_\alpha(\theta)_i = \frac{B}{2} [b_i \text{sign}(\theta_i + 1/2) + (1 - b_i) \text{sign}(\theta_i - 1/2)].$$

The stochastic gradients have an ℓ_2 -norm bounded by B and are unbiased. Moreover, observation of the gradient for a $\theta \in [-1/2, 1/2]^d$ reveals the outcome of the Bernoulli random variable b_i .

Therefore, after t steps, we can apply Fano's inequality to the following set-up: the random variable $\alpha \in \mathcal{A}$ is uniform, and given α , we sample independently t times, one variable i in $\{1, \dots, d\}$ and observe (a potentially noisy version of) a Bernoulli random variable b , with parameter α_i .

We then need to upper bound the mutual information between α and (i, b) and multiply the result t times because each of the t gradients is sampled independently.

The mutual information can be decomposed as

$$I(\alpha, (i, b)) = I(\alpha, i) + I(\alpha, b|i) = 0 + \mathbb{E}_i \mathbb{E}_\alpha [D_{\text{KL}}(p(b|i, \alpha) || p(b|i))],$$

where $p(b|i, \alpha)$ and $p(b|i)$ denotes the probability distribution of b . Thus, by convexity of the KL divergence,

$$\begin{aligned} I(\alpha, (i, b)) &= \mathbb{E}_i \mathbb{E}_\alpha \left[D_{\text{KL}} \left(p(b|i, \alpha) \middle\| \frac{1}{|\mathcal{A}|} \sum_{\alpha' \in \mathcal{A}} p(b|i, \alpha') \right) \right] \\ &\leq \frac{1}{|\mathcal{A}|} \sum_{\alpha' \in \mathcal{A}} \mathbb{E}_i \mathbb{E}_\alpha [D_{\text{KL}}(p(b|i, \alpha) || p(b|i, \alpha'))]. \end{aligned}$$

Since $p(b|i, \alpha)$ is Bernoulli random variable with parameter $\frac{1}{2} + \delta$ or $\frac{1}{2} - \delta$, the KL divergences above are bounded by the KL between two Bernoulli random variables with the two different parameters, that is,

$$\begin{aligned} I(\alpha, (i, b)) &\leq \left(\frac{1}{2} + \delta \right) \log \frac{\frac{1}{2} + \delta}{\frac{1}{2} - \delta} + \left(\frac{1}{2} - \delta \right) \log \frac{\frac{1}{2} - \delta}{\frac{1}{2} + \delta} = 2\delta \log \frac{1 + 2\delta}{1 - 2\delta} \\ &= 2\delta \log \left(1 + \frac{4\delta}{1 - 2\delta} \right) \leq \frac{8\delta^2}{1 - 2\delta} \leq 16\delta^2 \text{ if } \delta \in [0, 1/4]. \end{aligned}$$

Therefore, applying Corollary 12.1, the minimax lower bound is greater than

$$\varepsilon \left(1 - \frac{16t\delta^2 - \log 2}{\log M} \right) \geq \varepsilon \left(1 - \frac{16t\delta^2 - \log 2}{d/8} \right).$$

Thus, we need $256t\delta^2 \geq d$, and then $B\delta/4$ is the lower bound on the rate so that the lower bound is

$$\frac{1}{16} \sqrt{\frac{d}{t}},$$

which is the desired lower-bound (up to a constant) $\varepsilon_t(\mathcal{A}, \mathcal{F}) \geq DB/\sqrt{t}$ where D is the diameter of the set of θ . The lower-bound is thus the same as the upper-bound achieved by stochastic gradient descent in Chapter 5. The result above can be extended to strongly-convex problems (Agarwal et al., 2012).

Chapter 13

From online learning to bandits

Chapter summary

- Online convex optimization with gradients: stochastic gradient descent still works with the regret criterion and potentially adversarial functions, with essentially the same rates.
- Zero-th order optimization: Randomization can be used to obtain a gradient from function values with an additional dimension dependence.
- Multi-armed bandits: to tackle exploration / exploitation trade-offs, several algorithms can be used, from simple algorithms based on alternating exploration and exploitation to more refined ones utilizing the principle of “optimism in the face of uncertainty.”

In traditional stochastic optimization such as presented in Chapter 5 (e.g., Section 5.4), we observe a sequence of gradients of loss functions obtained from a pair of observations $(x_t, y_t) \in \mathcal{X} \times \mathcal{Y}$:

$$F'_t(\theta_{t-1}) = \frac{\partial \ell(y_t, f_\theta(x_t))}{\partial \theta} \Big|_{\theta=\theta_{t-1}},$$

and our performance measure was

$$\mathbb{E}[F(\theta_t)] - F_*,$$

where the expectation is taken with respect to the training data, and $F(\theta) = \mathbb{E}[\ell(y_s, f_\theta(x_s))]$ is the expected test error, assuming that all (x_s, y_s) (and thus the functions $F_s(\theta) = \ell(y_s, f_\theta(x_s))$), $s = 1, \dots, t$, are independent and identically distributed, and $F_* = \inf_{\theta \in \mathcal{C}} F(\theta)$, where \mathcal{C} is the optimization domain.

There are several important extensions corresponding to specific applications:

- **Regret instead of final performance:** The performance criterion can take into account performance along iterations such as $\frac{1}{t} \sum_{s=1}^t F(\theta_{s-1})$, and not only at the last

iteration, that is $F(\theta_t)$. This is important in situations where the loss functions can be interpreted as actual financial losses incurred while learning the parameter θ (such as in applications in advertising or finance).

Performance measures such as the *regret* can then be considered, here equal to

$$\frac{1}{t} \sum_{s=1}^t F(\theta_{s-1}) - \inf_{\theta \in \mathcal{C}} F(\theta),$$

often after taking the expectation (since θ_s is random because it depends on the past data).

 In this book, we choose to study what is often called the *normalized* regret since we divide $\sum_{s=1}^t [F(\theta_s) - \inf_{\theta \in \mathcal{C}} F(\theta)]$ by t . This is done to make comparisons with the usual stochastic framework easier.

- **Adversarial instead of stochastic:** The consideration of the regret criterion opens up the possibility of functions F_s to be different or sampled from different distributions, with a potentially adversarial choice that depends on the past. The regret is then $\frac{1}{t} \sum_{s=1}^t F_s(\theta_{s-1}) - \inf_{\theta \in \mathcal{C}} \frac{1}{t} \sum_{s=1}^k F_s(\theta)$, which is the comparison to the optimal constant prediction. This allows it to be robust to adversarial functions and adapted to non-stationary environments where very few assumptions can be made. Note here that the regret can be negative. This is presented in Section 13.1.
- **Partial feedback (zero-th order):** Independently of the regret framework, the feedback given to the algorithm may be less precise than the full gradient (e.g., only the function value). This is crucial in applications where function values are expensive to obtain with no access to gradients.

This is the domain of zero-th order optimization, which can be treated through gradient-based algorithms (Section 13.2) or through the framework of multi-armed bandits (Section 13.3).

In this chapter, we briefly cover three topics from this large literature. For more details, see [Shalev-Shwartz \(2011\)](#); [Bubeck and Cesa-Bianchi \(2012\)](#); [Hazan \(2022\)](#); [Slivkins \(2019\)](#); [Lattimore and Szepesvári \(2020\)](#).

13.1 First-order online convex optimization

In this section, we consider a sequence of arbitrary deterministic convex functions $F_s : \mathbb{R}^d \rightarrow \mathbb{R}$, $s \geq 1$, and a compact convex set \mathcal{C} . The goal of online convex optimization is, starting

from a certain $\theta_0 \in \mathcal{C}$, to obtain a sequence $(\theta_s)_{s \geq 1}$ so that the regret at time t , defined as

$$\frac{1}{t} \sum_{s=1}^t F_s(\theta_{s-1}) - \inf_{\theta \in \mathcal{C}} \frac{1}{t} \sum_{s=1}^t F_s(\theta),$$

is as small as possible.

We assume that at time s , we can access a gradient of F_s at any point $\theta_{s-1} \in \mathcal{C}$ that depends on past information. We also consider the possibility that we only observe a random, unbiased version g_s , that is, if \mathcal{F}_s denotes the information up to (and including) time s ,

$$\mathbb{E}[g_s | \mathcal{F}_{s-1}] = F'_s(\theta_{s-1}).$$

Given the added randomness, we consider the expected regret as a criterion.

For simplicity, we assume that almost surely, $\|g_s\|_2^2 \leq B^2$ (which in the context of machine learning corresponds to Lipschitz-continuous loss functions, which include the logistic loss, the hinge loss, and the square loss since we have assumed that we optimize on a bounded set¹).

Applications. This is adapted to a non-stationary environment, where the data distribution varies over time, either stochastically or even adversarially (based on earlier predictions).

In this section, we only present the non-smooth case. The smooth case will be proposed as exercises but leads to similar results compared to the regular stochastic case.

13.1.1 Convex case

We consider the projected stochastic gradient descent recursion:

$$\theta_s = \Pi_{\mathcal{C}}(\theta_{s-1} - \gamma_s g_s),$$

for a certain positive step-size γ_s (which we assume deterministic for simplicity), where $\Pi_{\mathcal{C}}$ is the orthogonal projection onto the set \mathcal{C} . We then have, for any $\theta \in \mathcal{C}$ (as opposed to a fixed $\theta = \eta_*$ the global optimum, like in regular optimization in Chapter 5),

$$\begin{aligned} \|\theta_s - \theta\|_2^2 &\leq \|\theta_{s-1} - \theta\|_2^2 - 2\gamma_s g_s^\top (\theta_{s-1} - \theta) + \gamma_s^2 B^2 \text{ by contractivity of projections,} \\ \mathbb{E}[\|\theta_s - \theta\|_2^2 | \mathcal{F}_{s-1}] &\leq \|\theta_{s-1} - \theta\|_2^2 - 2\gamma_s F'_s(\theta_{s-1})^\top (\theta_{s-1} - \theta) + \gamma_s^2 B^2, \\ &\quad \text{using the unbiasedness of the gradient,} \\ &\leq \|\theta_{s-1} - \theta\|_2^2 - 2\gamma_s [F_s(\theta_{s-1}) - F_s(\theta)] + \gamma_s^2 B^2, \text{ using convexity.} \end{aligned}$$

¹The square loss is not Lipschitz-continuous on an unbounded domain, but is once constrained to a bounded domain.

Taking full expectations and isolating $F_s(\theta_{s-1}) - F_s(\theta)$, we get:

$$\mathbb{E}[F_s(\theta_{s-1}) - F_s(\theta)] \leq \frac{1}{2\gamma_s} (\mathbb{E}[\|\theta_{s-1} - \theta\|_2^2] - \mathbb{E}[\|\theta_s - \theta\|_2^2]) + \frac{\gamma_s}{2} B^2.$$

We can then sum between $s = 1$ to $s = t$, to obtain

$$\frac{1}{t} \sum_{s=1}^t \mathbb{E}[F_s(\theta_{s-1})] - \frac{1}{t} \sum_{s=1}^t F_s(\theta) \leq \frac{1}{t} \sum_{s=1}^t \frac{1}{2\gamma_s} (\mathbb{E}[\|\theta_{s-1} - \theta\|_2^2] - \mathbb{E}[\|\theta_s - \theta\|_2^2]) + \frac{1}{t} \sum_{s=1}^t \frac{\gamma_s}{2} B^2.$$

At this point, the proof is exactly the same as the one of Theorem 5.4, with only the appearances of functions F_s that depend on s .

In Chapter 5 (that is, the proof of Theorem 5.4), we considered non-uniform averaging, which is not adapted to the online setting (because the regret is based on a uniform average). We could also use a constant step-size that depends on the horizon t (which then needs to be known in advance). By using Abel's summation formula (discrete integration by part), we can use a time-dependent step-size sequence, as, using the notation $\delta_s = \mathbb{E}[\|\theta_s - \theta\|_2^2]$, and for decreasing step-sizes:

$$\begin{aligned} \frac{1}{t} \sum_{s=1}^t \mathbb{E}[F_s(\theta_{s-1})] - \frac{1}{t} \sum_{s=1}^t F_s(\theta) &\leq \frac{1}{t} \sum_{s=1}^t \frac{1}{2\gamma_s} (\delta_{s-1} - \delta_s) + \frac{1}{t} \sum_{s=1}^t \frac{\gamma_s}{2} B^2 \text{ from the last equation,} \\ &= \frac{1}{t} \sum_{s=1}^{t-1} \delta_s \left(\frac{1}{2\gamma_{s+1}} - \frac{1}{2\gamma_s} \right) + \frac{\delta_0}{2t\gamma_1} - \frac{\delta_t}{2t\gamma_1} + \frac{1}{t} \sum_{s=1}^t \frac{\gamma_s}{2} B^2 \\ &\quad \text{using Abel's summation formula,} \\ &\leq \frac{1}{t} \sum_{s=1}^{t-1} \text{diam}(\mathcal{C})^2 \left(\frac{1}{2\gamma_{s+1}} - \frac{1}{2\gamma_s} \right) + \frac{\text{diam}(\mathcal{C})^2}{2t\gamma_1} + \frac{1}{t} \sum_{s=1}^t \frac{\gamma_s}{2} B^2 \\ &\quad \text{using that } \delta_s \leq \text{diam}(\mathcal{C})^2 \text{ for all } s, \\ &= \frac{\text{diam}(\mathcal{C})^2}{2t\gamma_t} + \frac{1}{t} \sum_{s=1}^t \frac{\gamma_s}{2} B^2. \end{aligned}$$

By choosing $\gamma_s = \frac{\text{diam}(\mathcal{C})}{B\sqrt{s}}$, we get, using the same inequalities as for the proof of Theorem 5.4:

$$\frac{1}{t} \sum_{s=1}^t \mathbb{E}[F_s(\theta_{s-1})] - \frac{1}{t} \sum_{s=1}^t F_s(\theta) \leq \frac{3B\text{diam}(\mathcal{C})}{2\sqrt{t}}. \quad (13.1)$$

This is exactly the expected regret and essentially the same bound as stochastic optimization in Section 5.4. Note that from such a bound, if all F_s 's are equal, we can do an “online-to-batch” conversion using Jensen’s inequality and exactly get the bound for regular projected stochastic gradient descent (which is no surprise, as the proof is essentially the same).

We show in Section 13.1.3 that the rate in Eq. (13.1) is, up to constants, the best possible over all Lipschitz-continuous functions over a compact set.

Exercise 13.1 (♦) In the unconstrained online optimization with smooth functions, that is, assuming that each F_t is L -smooth, and $\mathcal{C} = \mathbb{R}^d$, provide a regret bound for online gradient descent.

13.1.2 Strongly-convex case (♦)

Assuming strong-convexity (e.g., by adding $\frac{\mu}{2}\|\theta\|_2^2$ to the objective function), we will get a rate proportional to $\frac{B^2 \log(k)}{\mu k}$. Indeed, assuming that the functions F_s are all μ -strongly-convex on \mathcal{C} . We can indeed modify the proof above with the step-size $\gamma_s = 1/(\mu s)$, to get (with modifications in red):

$$\begin{aligned}\|\theta_s - \theta\|_2^2 &\leq \|\theta_{s-1} - \theta\|_2^2 - 2\gamma_s g_s^\top (\theta_{s-1} - \theta) + \gamma_s^2 B^2 \\ \mathbb{E}[\|\theta_s - \theta\|_2^2 | \mathcal{F}_{s-1}] &\leq \|\theta_{s-1} - \theta\|_2^2 - 2\gamma_s F'_s(\theta_{s-1})^\top (\theta_{s-1} - \theta) + \gamma_s^2 B^2 \\ &\leq \|\theta_{s-1} - \theta\|_2^2 - 2\gamma_s [F_s(\theta_{s-1}) - F_s(\theta) + \frac{\mu}{2}\|\theta_{s-1} - \theta\|_2^2] + \gamma_s^2 B^2.\end{aligned}$$

Taking full expectations, we get:

$$\mathbb{E}[F_s(\theta_{s-1}) - F_s(\theta)] \leq (\frac{1}{2\gamma_s} - \frac{\mu}{2}) E[\|\theta_{s-1} - \theta\|_2^2] - \frac{1}{2\gamma_s} \mathbb{E}[\|\theta_s - \theta\|_2^2] + \frac{\gamma_s}{2} B^2.$$

We can then use the specific form of step-size to get

$$\mathbb{E}[F_s(\theta_{s-1}) - F_s(\theta)] \leq \frac{\mu}{2}(s-1) E[\|\theta_{s-1} - \theta\|_2^2] - \frac{\mu}{2}s \mathbb{E}[\|\theta_s - \theta\|_2^2] + \frac{1}{2\mu s} B^2.$$

Then, summing between $s = 1$ to $s = t$, we obtain, with a telescoping sum:

$$\frac{1}{t} \sum_{s=1}^t \mathbb{E}[F_s(\theta_{s-1})] - \frac{1}{t} \sum_{s=1}^t F_s(\theta) \leq \frac{1}{t} \sum_{s=1}^t \frac{1}{2\mu s} B^2 \leq \frac{1}{2\mu t} (1 + \log t),$$

using the classical $\log(t)$ upper bound on the harmonic series. Note the appearance of $\log(t)$, which would not be the case if we had used the step-size $\gamma_s = \frac{2}{s+1}$ like in Exercise 5.24 (but which would require a different averaging scheme with weights proportional to s). For online learning, it turns out that the logarithmic term is unavoidable (Hazan and Kale, 2014).

13.1.3 Lower bounds (♦♦)

In order to prove a lower bound, following Abernethy et al. (2008), we consider the set $\mathcal{C} = \{\theta \in \mathbb{R}^d, \|\theta\|_\infty \leq 1\}$, and the linear (hence convex) function $F_t^{(\varepsilon)} : \mathbb{R}^d \rightarrow \mathbb{R}$ defined as $F_t^{(\varepsilon)}(\theta) = \varepsilon_t^\top \theta$, for $\varepsilon_s \in \{-1, 1\}^d$ for all $s \in \{1, \dots, t\}$. The gradient vectors g_t are then

simply equal to ε_t . We here have the exact deterministic gradient, with constants $B = \sqrt{d}$ and $\text{diam}(\mathcal{C}) = 2\sqrt{d}$.

To obtain a lower bound of performance, it suffices to show that for any sequence (θ_s) ,

$$\sup_{\varepsilon \in \mathcal{E}} \frac{1}{t} \sum_{s=1}^t F_s^{(\varepsilon)}(\theta_{s-1}) - \inf_{\theta \in \mathcal{C}} \frac{1}{t} \sum_{s=1}^t F_s^{(\varepsilon)}(\theta)$$

is lower-bounded for \mathcal{E} a well-chosen set. As already used in proving lower bounds in Section 3.7 and in Chapter 12, this is lower-bounded by the expectation for any distribution on \mathcal{E} , which we take to be all independent Rademacher random variables (note that the algorithm is deterministic, with no noise in the gradients, but the problem itself is random).

The regret of any algorithm is $\frac{1}{t} \sum_{s=1}^t \varepsilon_s^\top \theta_{s-1}$, which has zero expectation because θ_{s-1} does not use the information of ε_s . Moreover, using that the ℓ_1 -norm is dual to the ℓ_∞ -norm:

$$\inf_{\theta \in \mathcal{C}} \frac{1}{t} \sum_{s=1}^t \varepsilon_s^\top \theta = -\left\| \frac{1}{t} \sum_{s=1}^t \varepsilon_s \right\|_1 = -d \left| \frac{1}{t} \sum_{s=1}^t (\varepsilon_s)_1 \right|.$$

Therefore, from the following lemma, the regret is greater than $d \left| \frac{1}{t} \sum_{s=1}^t (\varepsilon_s)_1 \right| \geq d/(8\sqrt{t}) = \frac{B \text{diam}(\mathcal{C})}{16\sqrt{t}}$, a lower bound that matches the upper-bound from SGD from Eq. (13.1), up to a constant factor.

Lemma 13.1 (Khintchine's inequality) *Let $\eta \in \{-1, 1\}^t$ be a vector of independent Rademacher random variables (with equal probabilities for -1 and $+1$) and $x \in \mathbb{R}^d$. Let $p \in [0, \infty)$. Then*

$$(\mathbb{E}[|x^\top \eta|^p])^{1/p} \leq B_p \|x\|_2, \quad (13.2)$$

with $B_p = (p^{2p/2} \Gamma(p/2))^{1/2}$, where Γ is the Gamma function.² The bound B_p is less than $3\sqrt{p}$ for $p \geq 1$ and $\frac{3}{2}\sqrt{p}$ for $p \geq 2$. Moreover, if $p \geq 2$, $(\mathbb{E}[|x^\top \eta|^p])^{1/p} \geq \|x\|_2$, and if $p \leq 2$, we have:

$$(\mathbb{E}[|x^\top \eta|^p])^{1/p} \geq B_{4-p}^{2-p/2} \|x\|_2. \quad (13.3)$$

We also have when $p \geq 1$, with $1/p + 1/q = 1$, $(\mathbb{E}[|x^\top \eta|^p])^{1/p} \geq B_q^{-1} \|x\|_2$.

Proof (♦) We have, for $s = x^\top \eta$, and $p > 0$:

$$\mathbb{E}[|s|^p] = p \int_0^{+\infty} \lambda^{p-1} \mathbb{P}(|s| \geq \lambda) d\lambda,$$

²See https://en.wikipedia.org/wiki/Gamma_function.

(which can be checked using Fubini's theorem). We then compute directly:

$$\mathbb{E}[e^{ts}] = \prod_{i=1}^d \left(\frac{1}{2} e^{ts} + \frac{1}{2} e^{-ts} \right) = \prod_{i=1}^d \cosh(tx_i) \leq \exp(t^2 \|x\|_2^2 / 2),$$

using that $\cosh \alpha \leq \exp(\alpha^2/2)$ for any $\alpha \in \mathbb{R}$. Thus, for $\lambda \geq 0$,

$$\begin{aligned} \mathbb{P}(|s| \geq \lambda) &\leq 2\mathbb{P}(s \geq \lambda) = 2\mathbb{P}(e^{ts} \geq e^{t\lambda}) \leq 2 \inf_{t \geq 0} e^{-\lambda t} \mathbb{E}[e^{ts}] \text{ using Markov's inequality,} \\ &\leq 2 \inf_{t \geq 0} e^{-\lambda t} \exp(t^2 \|x\|_2^2 / 2) = 2 \exp(-\lambda^2 / (2\|x\|_2^2)), \text{ with } t = \lambda/\|x\|_2. \end{aligned}$$

Thus, through the change of variable $\mu = \lambda/\|x\|_2$:

$$\mathbb{E}[|s|^p] \leq 2p \int_0^{+\infty} \lambda^{p-1} \exp(-\lambda^2 / (2\|x\|_2^2)) d\lambda = \|x\|_2^p \times 2p \int_0^{+\infty} \mu^{p-1} \exp(-\mu^2 / 2) d\mu.$$

Thus, for Eq. (13.2), we can take $B_p^p = 2p \int_0^{+\infty} \lambda^{p-1} e^{-\lambda^2/2} d\lambda = p 2^{p/2} \int_0^{+\infty} u^{p/2-1} e^{-u} du = p 2^{p/2} \Gamma(p/2)$, with the change of variable $u = \lambda^2/2$. Through Stirling formula $\Gamma(p/2)^{1/p} \sim \sqrt{p/(2e)}$, and thus $B_p \sim \sqrt{p/e}$, and one can then check the bound $B_p \leq 3\sqrt{p}$ for $p \geq 1$, and $B_p \leq \frac{3}{2}\sqrt{p}$ for $p \geq 2$.

Assuming $\|x\|_2 = 1$ without loss of generality, we have, using Hölder's inequality:

$$1 = \mathbb{E}[|x^\top \eta|^2] \leq (\mathbb{E}[|x^\top \eta|^p])^{1/p} (\mathbb{E}[|x^\top \eta|^q])^{1/q},$$

which leads to the last lower bound.

Moreover, for $p \geq 2$, we have directly $\|x\|_2 \leq (\mathbb{E}[|x^\top \eta|^p])^{1/p}$, and to prove Eq. (13.3), for $p \in [0, 2]$, we have by Cauchy-Schwarz inequality:

$$\begin{aligned} 1 &= \mathbb{E}[|x^\top \eta|^2] = \mathbb{E}[|x^\top \eta|^{p/2} |x^\top \eta|^{2-p/2}] \leq (\mathbb{E}[|x^\top \eta|^p])^{1/2} (\mathbb{E}[|x^\top \eta|^{4-p}])^{1/2} \\ &\leq (\mathbb{E}[|x^\top \eta|^p])^{1/2} B_{4-p}^{2-p/2}. \end{aligned}$$

■

Thus, with the notations of the lemma above:

$$(\mathbb{E}[|x^\top \eta|^p])^{1/p} \geq B_{4-p}^{1-4/p} \|x\|_2.$$

This leads to $\mathbb{E}|x^\top \eta| \geq \|x\|_2 B_3^{-3} \geq \|x\|_2 (3 \cdot 2^{3/2} \Gamma(3/2))^{-1} \geq \|x\|_2 / 8$ for the lower bound for online learning.

Exercise 13.2 (♦) What would upper and lower bounds be if the regret criterion is replaced by $\mathbb{E} \left[\sum_{s=1}^t \alpha_s F_s(\theta_{s-1}) \right] - \inf_{\theta \in \mathcal{C}} \frac{1}{t} \sum_{s=1}^t \alpha_s F_s(\theta)$ for an arbitrary sequence (α_s) of positive numbers?

13.2 Zero-th order convex optimization

In this section, we consider the task of unconstrained minimization of a convex function F , given only access to function values, which is typically referred to as *zero-th order optimization* (since the function value is the zero-th order derivative of F , while the gradient is the vector of first-order derivatives).

If the function values are accessible with no noise and the function is smooth, then one can get a gradient by finite differences by defining the following estimate:

$$\hat{F}'(\theta) = \sum_{i=1}^d \frac{1}{\delta} [F(\theta + \delta e_i) - F(\theta)] e_i \in \mathbb{R}^d, \quad (13.4)$$

where $(e_i)_{i \in \{1, \dots, d\}}$ is the canonical orthonormal basis of \mathbb{R}^d , with arbitrary precision when δ tends to zero. Indeed, using the smoothness inequality from Eq. (5.10):

$$\|\hat{F}'(\theta) - F'(\theta)\|_2^2 = \frac{1}{\delta^2} \sum_{i=1}^d [F(\theta + \delta e_i) - F(\theta) - F'(\theta)^\top \delta e_i]^2 \leq \frac{d}{\delta^2} (L\delta^2/2)^2 = \frac{dL^2\delta^2}{4}.$$

Therefore, assuming for simplicity that algorithms have infinite numerical precision at the expense of $d + 1$ noiseless function evaluations (one at θ , and d at each $\theta + \delta e_i$), we can compute the exact gradient, and use gradient descent. Note also that for many functions, the gradient can be computed easily with automatic differentiation techniques (see, e.g., Baydin et al., 2018, and references therein). The problem is more interesting with noisy evaluations.

In this section, we first consider for simplicity the case where f is convex and smooth (that is, essentially with bounded second-order derivatives) but only accessible with a stochastic first-order oracle (unbiased, with variance σ^2), for which, in Eq. (13.4), the noise in the function values explodes when δ goes to zero.

That is, we will consider the iteration

$$\theta_t = \theta_{t-1} - \gamma \left[\frac{1}{\delta} (F(\theta_{t-1} + \delta z_t) + \zeta_t - F(\theta_{t-1}) - \zeta'_t) z_t \right],$$

where ζ_t and ζ'_t are zero-mean random variables with variance σ^2 , corresponding to the additive noise on the two function evaluations. By writing $\varepsilon_t = \zeta_t - \zeta'_t$, we get:

$$\theta_t = \theta_{t-1} - \gamma \left[\frac{1}{\delta} (F(\theta_{t-1} + \delta z_t) - F(\theta_{t-1}) + \varepsilon_t) z_t \right], \quad (13.5)$$

where ε_t corresponds to the noise with the two function evaluations at θ_{t-1} and $\theta_{t-1} + \delta z_t$, thus of variance $2\sigma^2$, and z_t is sampled from a distribution so that $\mathbb{E}[z_t] = 0$ and $\mathbb{E}[z_t z_t^\top] = I$.

There are two natural candidates: (1) z a signed canonical basis vectors selected uniformly at random (that is, $\pm\sqrt{d}e_i$, with i selected uniformly at random in $\{1, \dots, d\}$, and a factor \sqrt{d} to obtain an identity covariance matrix), which corresponds to a single coordinate change like in Eq. (13.4), or (2) z standard Gaussian vector (with mean zero and identity covariance matrix). We consider the second option, as this will lead to an interesting property relating the stochastic gradient estimate to the gradient of a modified function.

Note that if F is defined as an expectation $F(\theta) = \mathbb{E}_\xi[f(\theta, \xi)]$, the stochasticity at time t comes from a sample ξ_t . We then compute the function values $f(\theta, \xi_t)$ at *two* different points with the same ξ_t , and we can get an improved bound (see the end of Section 13.2.1).

The key in analyzing the iteration in Eq. (13.5) is to study the quantity $g = \frac{1}{\delta}(F(\theta + \delta z) - F(\theta))z$, for a certain θ and z and a standard Gaussian vector.

For δ small, a simple Taylor expansion around θ leads to

$$g = \frac{1}{\delta}(F(\theta + \delta z) - F(\theta))z = \frac{1}{\delta}(\delta z^\top F'(\theta) + O(\delta^2))z = zz^\top F'(\theta) + O(\delta).$$

Thus, by taking an expectation with respect to z , we get $\mathbb{E}[g] = F'(\theta) + O(\delta)$, that is, we have an almost unbiased gradient (for δ small), and we can thus expect to use stochastic gradient techniques. It turns out that the analysis will be made even simpler through the use of integration by parts and the property of the Gaussian distribution.

In terms of variance linked to noisy evaluations, the term $\frac{1}{\delta}\varepsilon_t z_t$ has zero mean, but its squared norm has expectation $\mathbb{E}[\|\frac{1}{\delta}\varepsilon_t z_t\|_2^2] = \frac{1}{\delta^2}2\sigma^2 d$. Thus, it explodes when δ goes to zero, thus leading to some trade-offs that we now look at.

13.2.1 Smooth stochastic gradient descent

For simplicity, we consider an L -smooth function F defined on \mathbb{R}^d (see next section for the non-smooth version).

An important tool will be to consider the function $F_\delta : \mathbb{R}^d \rightarrow \mathbb{R}$ defined as

$$F_\delta(\theta) = \mathbb{E}_{z \sim \mathcal{N}(0, I)}[F(\theta + \delta z)], \quad (13.6)$$

which is the expectation of F taken at point distributed as a Gaussian with mean θ and covariance matrix $\delta^2 I$.

Approximation properties. We can analyze the difference between F and F_δ when F is L -smooth:

$$\forall \theta \in \mathbb{R}^d, F_\delta(\theta) - F(\theta) = \mathbb{E}_{z \sim \mathcal{N}(0, I)}[F(\theta + \delta z) - F(\theta) - \delta F'(\theta)^\top z].$$

Thus, using Jensen's inequality, we get $F_\delta(\theta) \geq F(\theta)$ and using the smoothness bound from Eq. (5.10), we get:

$$\forall \theta \in \mathbb{R}^d, 0 \leq F_\delta(\theta) - F(\theta) \leq \frac{L\delta^2}{2} \mathbb{E}_{z \sim \mathcal{N}(0, I)} [\|z\|_2^2] = \frac{L}{2} \delta^2 d. \quad (13.7)$$

Moreover, we can compute the expectation of the squared norm of the gradient estimate as

$$\begin{aligned} & \mathbb{E} \left[\left\| \frac{1}{\delta} (F(\theta + \delta z) - F(\theta)) z \right\|_2^2 \right] \\ & \leq 2 \mathbb{E} \left[\left\| \frac{1}{\delta} (F(\theta + \delta z) - F(\theta) - \delta F'(\theta)^\top z) z \right\|_2^2 \right] + 2 \mathbb{E} [\|zz^\top F'(\theta)\|_2^2] \\ & \leq 2 \mathbb{E} \left[\frac{L^2 \delta^2}{4} \|z\|_2^6 \right] + 2 F'(\theta)^\top \mathbb{E} [\|z\|_2^2 z z^\top] F'(\theta) \text{ using smoothness,} \\ & = \frac{L^2 \delta^2}{2} d(d+2)(d+4) + 2 \|F'(\theta)\|_2^2 \cdot 3d \leq \frac{L^2 \delta^2}{2} 15d^3 + 6d \|F'(\theta)\|_2^2, \end{aligned} \quad (13.8)$$

where we have used that $\|z\|_2^2$ is a chi-squared random variable, and that we get in closed form $\mathbb{E}[\|z\|_2^6] = d(d+2)(d+4)$ and $\mathbb{E}[\|z\|_2^2 z z^\top] = 3dI$ (see the exercise below).

Exercise 13.3 Show that for a standard Gaussian vector $z \in \mathbb{R}^d$ (with zero mean and covariance matrix identity), then $\mathbb{E}[\|z\|_2^6] = d(d+2)(d+4)$ and $\mathbb{E}[\|z\|_2^2 z z^\top] = 3dI$.

Stochastic gradient descent. We can now analyze gradient descent and take conditional expectations given the information \mathcal{F}_{s-1} up to time $s-1$, and use the standard manipulations from Chapter 5, starting from:

$$\theta_s - \theta_* = \theta_{s-1} - \theta_* - \gamma \frac{1}{\delta} (F(\theta_{s-1} + \delta z_s) - F(\theta_{s-1})) z_s - \frac{\gamma}{\delta} \varepsilon_s z_s,$$

to get, by expanding the squared norm:

$$\begin{aligned} & \mathbb{E} [\|\theta_s - \theta_*\|_2^2 | \mathcal{F}_{s-1}] \\ & \leq \|\theta_{s-1} - \theta_*\|_2^2 - 2\gamma F'_\delta(\theta_{s-1})^\top (\theta_{s-1} - \theta_*) \\ & \quad + 2\gamma^2 \mathbb{E} \left[\left\| \frac{1}{\delta} (F(\theta_{s-1} + \delta z_s) - F(\theta_{s-1})) z_s \right\|_2^2 | \mathcal{F}_{s-1} \right] + 2 \frac{\gamma^2}{\delta^2} \mathbb{E} [\varepsilon_s^2 \|z_s\|_2^2] \\ & \leq \|\theta_{s-1} - \theta_*\|_2^2 - 2\gamma F'_\delta(\theta_{s-1})^\top (\theta_{s-1} - \theta_*) \\ & \quad + 2\gamma^2 \cdot \left[\frac{L^2 \delta^2}{2} 15d^3 + 6d \|F'(\theta_{s-1})\|_2^2 \right] + 2 \frac{\gamma^2}{\delta^2} \cdot 2d\sigma^2 \text{ using Eq. (13.8),} \\ & \leq \|\theta_{s-1} - \theta_*\|_2^2 - 2\gamma [F_\delta(\theta_{s-1}) - F_\delta(\theta_*)] \\ & \quad + 15\gamma^2 L^2 \delta^2 d^3 + 24L\gamma^2 d [F(\theta_{s-1}) - F(\theta_*)] + 4d \frac{\gamma^2}{\delta^2} \sigma^2 \text{ using co-coercivity,} \\ & \leq \|\theta_{s-1} - \theta_*\|_2^2 - 2\gamma [F(\theta_{s-1}) - F(\theta_*)] + 2\gamma \cdot \frac{L}{2} \delta^2 d \\ & \quad + 15\gamma^2 L^2 \delta^2 d^3 + 24L\gamma^2 d [F(\theta_{s-1}) - F(\theta_*)] + 4d \frac{\gamma^2}{\delta^2} \sigma^2, \text{ using Eq. (13.7).} \end{aligned}$$

Thus, if $\gamma \leq \frac{1}{24dL}$, we have $24L\gamma^2d \leq \gamma$, and we get:

$$\begin{aligned}\mathbb{E}[\|\theta_s - \theta_*\|_2^2 | \mathcal{F}_{s-1}] &\leq \|\theta_{s-1} - \theta_*\|_2^2 - \gamma[F(\theta_{s-1}) - F(\theta_*)] + \gamma L\delta^2 d + \frac{15}{24}\gamma L\delta^2 d^2 + 4d\frac{\gamma^2}{\delta^2}\sigma^2 \\ &\leq \|\theta_{s-1} - \theta_*\|_2^2 - \gamma[F(\theta_{s-1}) - F(\theta_*)] + 2\gamma L\delta^2 d^2 + 4d\frac{\gamma^2}{\delta^2}\sigma^2,\end{aligned}$$

leading to, taking full expectations:

$$\mathbb{E}[F(\theta_{s-1})] - F(\theta_*) \leq \frac{1}{\gamma} \left(\mathbb{E}[\|\theta_{s-1} - \theta_*\|_2^2] - \mathbb{E}[\|\theta_s - \theta_*\|_2^2] \right) + 2L\delta^2 d^2 + 4d\frac{\gamma}{\delta^2}\sigma^2.$$

Summing from $s = 1$ to $s = t$, we get

$$\frac{1}{t} \sum_{s=1}^t \mathbb{E}[F(\theta_{s-1})] - F(\theta_*) \leq \frac{1}{\gamma t} \|\theta_0 - \theta_*\|_2^2 + 2L\delta^2 d^2 + 4d\frac{\gamma}{\delta^2}\sigma^2. \quad (13.9)$$

We can now analyze various situations depending on the presence or absence of noise (see empirical illustration in Figure 13.1):

- If $\sigma = 0$, then we can take δ as close to zero as possible and get the rate, with $\gamma = \frac{1}{24dL}$, for the average iterate $\bar{\theta}_t = \frac{1}{t} \sum_{s=1}^t \theta_{s-1}$, and using Jensen's inequality:

$$\mathbb{E}[F(\bar{\theta}_t)] - F(\theta_*) \leq \frac{24Ld}{t} \|\theta_0 - \theta_*\|_2^2. \quad (13.10)$$

As suggested at the beginning of Section 13.2, we only lose a factor of d compared to regular gradient descent in Section 5.2.4.

- If $\sigma > 0$, we can optimize over δ to get (assuming σ is known), with $\delta^4 = 2\gamma\sigma^2 L^{-1}d^{-1}$,

$$\mathbb{E}[F(\bar{\theta}_t)] - F(\theta_*) \leq \frac{1}{\gamma t} \|\theta_0 - \theta_*\|_2^2 + 2\sqrt{2} \cdot \gamma^{1/2} L^{1/2} \sigma d^{3/2}.$$

With the maximal allowed step-size $\gamma = \frac{1}{24dL}$, this leads to

$$\mathbb{E}[F(\bar{\theta}_t)] - F(\theta_*) \leq \frac{24Ld}{t} \|\theta_0 - \theta_*\|_2^2 + \sigma d.$$

There is convergence only up to the noise level with a limiting bound σd . We can also use a step-size γ that depends on the horizon t , by taking $\gamma = \frac{1}{24Ld} t^{-2/3}$, leading to:

$$\mathbb{E}[F(\bar{\theta}_t)] - F(\theta_*) \leq \frac{d}{t^{1/3}} [24L\|\theta_0 - \theta_*\|_2^2 + \sigma].$$

We not only lose a factor of d in the bound but the dependence in t is worsened from $1/t$ to $1/t^{1/3}$. Note that (a) the natural rate for convex stochastic first-order methods is $O(1/\sqrt{t})$, and (b) the dependence in σ could be improved if the noise level were known.

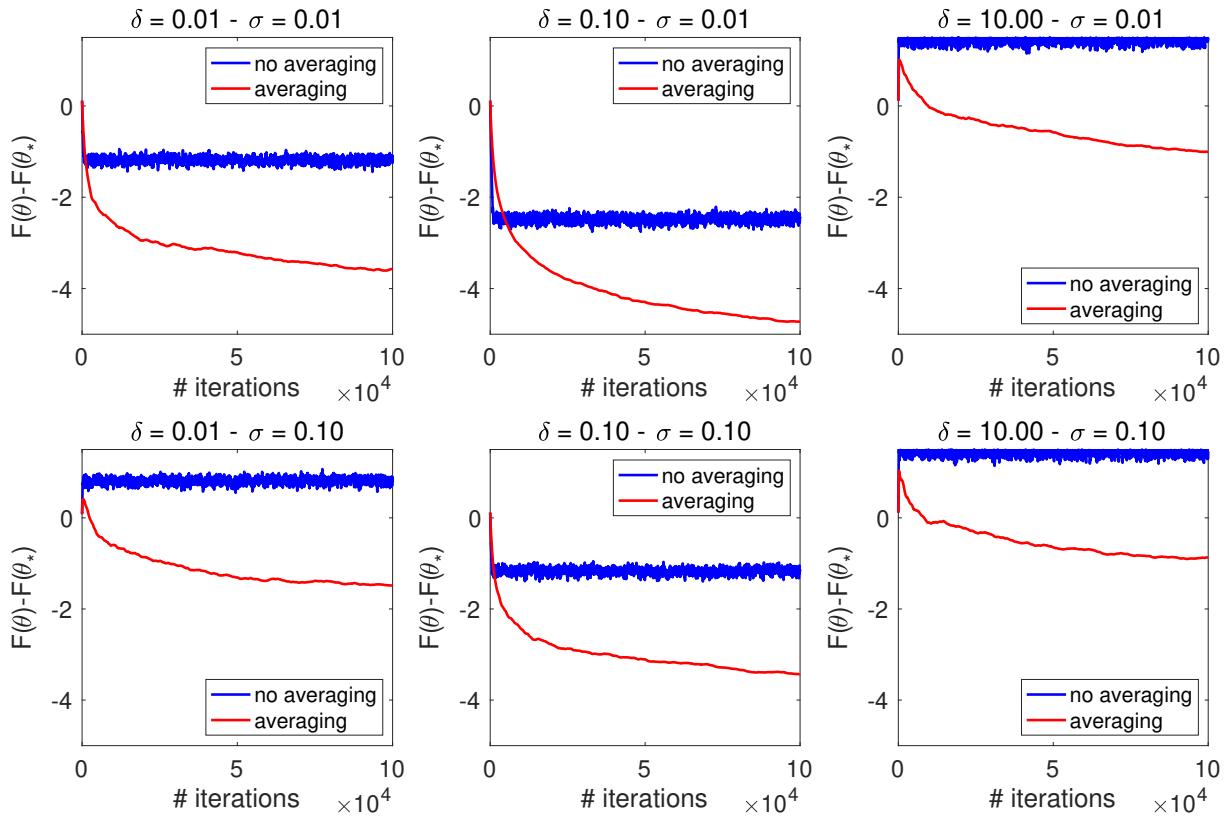


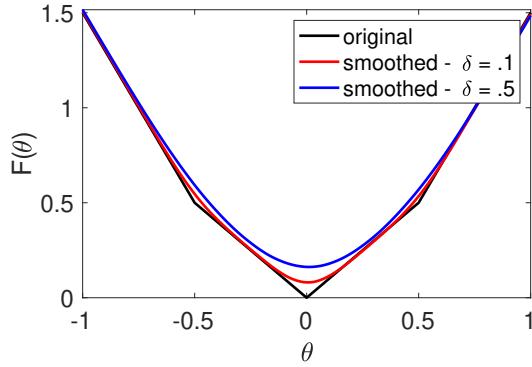
Figure 13.1: Zero-th order optimization with Gaussian smoothing on a quadratic function F in dimension $d = 10$, with step-size $\gamma = 1/(4Ld)$: two different levels of noise added to the function values, $\sigma = 0.01$ (top), and $\sigma = 0.1$ (bottom), with three different smoothing constants, $\delta = 0.01$ (left), $\delta = 0.1$ (middle), and $\delta = 10.00$ (right). Performance improves with smaller noise variance σ^2 , while δ should be chosen not too large (then two much bias) and not too small (too much variance).

Extensions. We can also consider the case where we can do two function evaluations, where one can check that we can essentially remove the variance term in $d\frac{\gamma^2}{\delta^2}\sigma^2$ due to two noisy evaluations, removing in Eq. (13.9) the last term, and thus with improved behavior. For related lower bounds, see Duchi et al. (2015).

Exercise 13.4 When two function evaluations are available, compute optimal values of δ and γ and provide an improved convergence rate.

13.2.2 Stochastic smoothing (\blacklozenge)

In this section, we consider the case where F may not be smooth, which leads to considering the nice effect of randomized smoothing. This randomized smoothing can simply be explained by seeing F_δ as the convolution of the function F by the density of the Gaussian distribution with mean zero and covariance matrix $\delta^2 I$. Since this density is infinitely differentiable, a continuous function will be turned into an infinitely differentiable function. One particular instance of this phenomenon is shown precisely below.



Proposition 13.1 (Randomized smoothing) *Assume F is B -Lipschitz-continuous. Then the function $F_\delta : \mathbb{R}^d \rightarrow \mathbb{R}$ defined in Eq. (13.6) is also B -Lipschitz-continuous. Moreover, it is $(\frac{\sqrt{d}}{\delta}B)$ -smooth, with gradient equal to*

$$F'_\delta(\theta) = \frac{1}{\delta} \mathbb{E}_{z \sim \mathcal{N}(0, I)} [F(\theta + \delta z) z] = \frac{1}{\delta} \mathbb{E}_{z \sim \mathcal{N}(0, I)} [(F(\theta + \delta z) - F(\theta)) z].$$

Moreover, $\forall \theta \in \mathbb{R}^d$, $|F_\delta(\theta) - F(\theta)| \leq B\delta\sqrt{d}$.

Proof If F is B -Lipschitz-continuous, then for any $\theta, \theta' \in \mathbb{R}^d$, we have

$$\begin{aligned} |F_\delta(\theta) - F_\delta(\theta')| &= |\mathbb{E}[F(\theta + \delta z) - F(\theta' + \delta z)]| \leq \mathbb{E}[|F(\theta + \delta z) - F(\theta' + \delta z)|] \\ &\leq \mathbb{E}[B\|\theta - \theta'\|_2] = B\|\theta - \theta'\|_2, \end{aligned}$$

which shows Lipschitz-continuity of F_δ . In terms of approximation, we have:

$$\forall \theta \in \mathbb{R}^d, |F_\delta(\theta) - F(\theta)| \leq \mathbb{E}_{z \sim \mathcal{N}(0, I)} [|F(\theta + \delta z) - F(\theta)|] \leq B\delta\mathbb{E}_{z \sim \mathcal{N}(0, I)} [\|z\|_2] \leq B\delta\sqrt{d}.$$

We can now use the expression of the multivariate standard Gaussian density to get:

$$F_\delta(\theta) = \frac{1}{(2\pi)^{d/2}} \int_{\mathbb{R}^d} F(\theta + \delta\eta) \exp\left(-\frac{1}{2}\|\eta\|_2^2\right) d\eta.$$

Then, assuming for simplicity that we can differentiate through the expectation, we get, by integration by parts:

$$\begin{aligned}
F'_\delta(\theta) &= \frac{1}{(2\pi)^{d/2}} \int_{\mathbb{R}^d} F'(\theta + \delta\eta) \exp\left(-\frac{1}{2}\|\eta\|_2^2\right) d\eta \\
&= \frac{1}{(2\pi)^{d/2}} \frac{1}{\delta} \int_{\mathbb{R}^d} \delta F'(\theta + \delta\eta) \exp\left(-\frac{1}{2}\|\eta\|_2^2\right) d\eta \\
&= \frac{1}{(2\pi)^{d/2}} \frac{1}{\delta} \int_{\mathbb{R}^d} \frac{\partial F(\theta + \delta\eta)}{\partial \eta} \exp\left(-\frac{1}{2}\|\eta\|_2^2\right) d\eta \\
&= -\frac{1}{(2\pi)^{d/2}} \frac{1}{\delta} \int_{\mathbb{R}^d} F(\theta + \delta\eta) \frac{\partial \exp\left(-\frac{1}{2}\|\eta\|_2^2\right)}{\partial \eta} d\eta \text{ by integration by parts,} \\
&= -\frac{1}{(2\pi)^{d/2}} \frac{1}{\delta} \int_{\mathbb{R}^d} F(\theta + \delta\eta) \exp\left(-\frac{1}{2}\|\eta\|_2^2\right) (-\eta) d\eta = \mathbb{E}\left[\frac{1}{\delta} F(\theta + \delta z) z\right].
\end{aligned}$$

That is, the gradient is equal to

$$F'_\delta(\theta) = \mathbb{E}\left[\frac{1}{\delta} F(\theta + \delta z) z\right] = \mathbb{E}\left[\frac{1}{\delta} (F(\theta + \delta z) - F(\theta)) z\right].$$

The function F_δ is $(\frac{\sqrt{d}}{\delta}B)$ -smooth, since for $\theta, \theta' \in \mathbb{R}^d$,

$$\|F'_\delta(\theta) - F'_\delta(\theta')\|_2 \leq \frac{1}{\delta} \mathbb{E}_{z \sim \mathcal{N}(0, I)} [|F(\theta + \delta z) - F(\theta' + \delta z)| \|z\|] \leq \frac{B}{\delta} \|\theta - \theta'\|_2 \mathbb{E}_{z \sim \mathcal{N}(0, I)} [\|z\|_2].$$

■

In other words, the expectation of the gradient estimate happens to be exactly the gradient of a smoothed version F_δ of F . This will be used in the proof below. Moreover, the expression of F'_δ as an expectation leads naturally to the stochastic gradient $\hat{F}'_\delta(\theta) = \frac{1}{\delta} F(\theta + \delta z) z - \frac{1}{\delta} F(\theta) z$, for which we have: $\mathbb{E}[\hat{F}'_\delta(\theta)] = F'_\delta(\theta)$ and

$$\mathbb{E}[\|\hat{F}'_\delta(\theta)\|_2^2] \leq \mathbb{E}[B^2 \|z\|_2^4] \leq 4B^2 d^2.$$

Stochastic gradient descent. We have, for θ_* a minimizer of F on \mathbb{R}^d , by expanding the square,

$$\begin{aligned}
\|\theta_s - \theta_*\|_2^2 &= \|\theta_{s-1} - \theta_*\|_2^2 - 2\frac{\gamma}{\delta} ([F(\theta_{s-1} + \delta z_s) - F(\theta_{s-1}) + \varepsilon_s] z_s)^\top (\theta_{s-1} - \theta_*) \\
&\quad + \frac{\gamma^2}{\delta^2} \| [F(\theta_{s-1} + \delta z_s) - F(\theta_{s-1}) + \varepsilon_s] z_s \|_2^2.
\end{aligned}$$

We have, using the previous inequalities:

$$\mathbb{E}[\|\theta_s - \theta\|_2^2 | \mathcal{F}_{s-1}] = \|\theta_{s-1} - \theta\|_2^2 - 2\gamma F'_\delta(\theta_{s-1})^\top (\theta_{s-1} - \theta) + 2\gamma^2 \cdot 4B^2 d^2 + 2\frac{\gamma^2}{\delta^2} \cdot \sigma^2 d,$$

leading to

$$\begin{aligned} F_\delta(\theta_{s-1}) - F_\delta(\theta) &\leq \frac{1}{2\gamma} \left(\mathbb{E}[\|\theta_{s-1} - \theta\|_2^2] - \mathbb{E}[\|\theta_s - \theta\|_2^2] \right) + 4\gamma B^2 d^2 + \frac{\gamma}{\delta^2} \sigma^2 d \\ F(\theta_{s-1}) - F(\theta) &\leq \frac{1}{2\gamma} \left(\mathbb{E}[\|\theta_{s-1} - \theta\|_2^2] - \mathbb{E}[\|\theta_s - \theta\|_2^2] \right) + 4\gamma B^2 d^2 + \frac{\gamma}{\delta^2} \sigma^2 d + 2B\delta\sqrt{d}. \end{aligned}$$

We thus get

$$\frac{1}{t} \sum_{s=1}^t F(\theta_{s-1}) - F(\theta) \leq \frac{1}{2\gamma t} \|\theta_0 - \theta\|_2^2 + 4\gamma B^2 d^2 + \frac{\gamma}{\delta^2} \sigma^2 d + 2B\delta\sqrt{d}.$$

This leads to a similar discussion as for the smooth case in Section 13.2.1, for the choice of step-sizes:

- When $\sigma = 0$ (no noise in function evaluations), we can take δ as small as possible so that rounding errors do not perturb the finite differences, and we then only lose a factor of d compared to the standard subgradient method studied in Section 5.3.
- When $\sigma > 0$, then we can optimize over δ , with $\delta^3 = \gamma\sigma^2 B^{-1}\sqrt{d}$. We then get

$$\frac{1}{t} \sum_{s=1}^t F(\theta_{s-1}) - F(\theta) \leq \frac{1}{2\gamma t} \|\theta_0 - \theta\|_2^2 + 4\gamma B^2 d^2 + 3d^{2/3} \gamma^{1/3} \sigma^{2/3} B^{2/3}.$$

To optimize the rate for large values of t , we can take $\gamma = \frac{1}{B^2 d^{1/2} t^{3/4}}$ for a final rate in

$$\frac{d^{1/2}}{2t^{1/4}} \left(B^2 \|\theta_0 - \theta\|_2^2 + 6\sigma^{2/3} \right) + 4 \frac{d^{3/2}}{t^{3/4}}.$$

Regret minimization. If we aim at minimizing regret by computing the loss function at the point we query, the situation becomes significantly more complicated. The simplest case (optimization of a linear function on the simplex is the classical multi-armed-bandit problem), with the usual exploration/exploitation trade-off we will consider next. For more general cases, see Hazan (2022).

13.3 Multi-armed bandits

The aim of this section is to provide the simplest results for multi-armed stochastic bandits. There is an extensive and rich literature; see Bubeck and Cesa-Bianchi (2012); Lattimore and Szepesvári (2020); Slivkins (2019) for a more detailed account.

Multi-armed bandits are the simplest model of sequential decision problems where information is gathered as decisions are made and losses incurred, where the “exploration-exploitation” dilemma occurs. Beyond being a stepping stone for many more complex models, it directly applies to clinical trials or routing in networks.

We consider k potential “arms” with associated means $\mu^{(1)}, \dots, \mu^{(k)} \in \mathbb{R}$. Every time we select the arm i , we receive a reward sampled independently of all other rewards and the previous arm choices from a sub-Gaussian distribution with mean $\mu^{(i)}$, and sub-Gaussian parameter σ . At time s , we select the arm i_s based on the information \mathcal{F}_{s-1} up to time $s-1$ (that is, the rewards received before time $s-1$) and receive the reward r_s .

Our criterion is the expected regret (adapted to the *maximization* of rewards), equal to

$$R_t = t \cdot \max_{i \in \{1, \dots, k\}} \mu^{(i)} - \sum_{s=1}^t \mathbb{E}[r_s].$$



As opposed to online learning in the previous section, here we are not dividing by t the regret.

Denoting $\Delta^{(j)} = \max_{i \in \{1, \dots, k\}} \mu^{(i)} - \mu^{(j)} \geqslant$ the difference between the mean of the best arm and the mean of arm j , and $n_t^{(j)}$ the number of times the arm j was selected in the first t iterations, we can express the regret as

$$R_t = \sum_{j=1}^k \Delta^{(j)} \mathbb{E}[n_t^{(j)}]. \quad (13.11)$$

Thus, the regret is a direct function of the number of times each arm is selected. For all algorithms, we consider the natural unbiased estimate of the arm means at time s , that is,

$$\hat{\mu}_t^{(j)} = \frac{1}{n_t^{(j)}} \sum_{s=1}^t r_s \mathbf{1}_{i_s=j} = \frac{1}{n_t^{(j)}} \sum_{a=1}^{n_t^{(j)}} x_a^{(j)},$$

where we imagine we select rewards from a sequence of i.i.d. samples $x_a^{(i)}$ with mean $\mu^{(i)}$ from each arm. This implies that as we select some arms multiple times, we get a more accurate estimate of $\mu^{(i)}$ as the expected squared distance between $\hat{\mu}_t^{(j)}$ and $\mu^{(i)}$ is proportional to $\frac{1}{n_t^{(j)}}$.

To simplify the exposition, we ignore the equality cases among the various estimated $\hat{\mu}_t^{(j)}$, which is safe as long as the distributions of the arm values are absolutely continuous with respect to the Lebesgue measure.

13.3.1 Need for an exploration-exploitation trade-off

We can now consider two extreme algorithms, highlighting the need to both “explore” and “exploit”.

Pure exploration. If we select a random arm at each step, then, from Eq. (13.11) and $\mathbb{E}[n_t^{(j)}] = \frac{t}{k}$, the expected regret is $t \cdot \frac{1}{k} \sum_{j=1}^k \Delta^{(j)}$ and depends linearly in t , that is, we have a “linear regret”. At time step t , we get a reasonable estimate of the best arm, but this incurs a strong loss along the iterations.

Pure exploitation. The previous strategy was ignoring the online estimates $\hat{\mu}_t^{(j)}$. The pure exploitation strategy does the opposite by only selecting the arm with the current largest estimate, assuming that the first k steps are dedicated to selecting each arm only once. This has linear regret because there is a non-zero probability that the best arm is never selected again.

Exercise 13.5 *Provide a lower bound on the regret of the pure exploitation strategy.*

13.3.2 “Explore-then-commit”

If we consider mk steps where we select exactly each arm m times, we can build the m estimates $\hat{\mu}^{(1)}, \dots, \hat{\mu}^{(k)}$, which are all independent random variables, with means $\mu^{(1)}, \dots, \mu^{(k)}$ and with sub-Gaussian parameters σ^2/m . Let i_* be the optimal arm.

We then select the arm with maximal $\hat{\mu}_{mk}^{(j)}$ for all remaining $t - km$ steps. The regret for this algorithm is then equal to, using Eq. (13.11), for $t > mk$:

$$R_t = m \sum_{j=1}^k \Delta^{(j)} + (t - mk) \sum_{j=1}^k \Delta^{(j)} \mathbb{P}(\hat{\mu}_{mk}^{(j)} \geq \hat{\mu}_{mk}^{(i)}, \forall i \neq j),$$

where the first term corresponds to the first m steps, for which this is the exact contribution of the regret, and the second term corresponds to the other $(t - mk)$ steps, where the arm j is selected if $\hat{\mu}_{mk}^{(i)}$ is maximized for $i = j$.

We can now upper-bound the second term by only imposing that an arm j is selected if $\hat{\mu}_{mk}^{(j)} \geq \hat{\mu}_{mk}^{(i_*)}$:

$$\begin{aligned} R_t &\leq m \sum_{j=1}^k \Delta^{(j)} + (t - mk) \sum_{j=1}^k \Delta^{(j)} \mathbb{P}(\hat{\mu}_{mk}^{(j)} \geq \hat{\mu}_{mk}^{(i_*)}) \\ &\leq m \sum_{j \neq i_*} \Delta^{(j)} + t \sum_{j \neq i_*} \Delta^{(j)} \exp\left(-\frac{(\Delta^{(j)})^2 m}{\sigma^2}\right), \end{aligned}$$

by using sub-Gaussian tail bounds (see Section 1.2.1) on the difference of the m arm values between j and i_* .

Two arms ($k = 2$). For $k = 2$ arms, then the upper-bound is, with $\Delta = \Delta^{(i)}$ for $i \neq i_*$:

$$m\Delta + t\Delta \exp\left(-\frac{\Delta^2 m}{\sigma^2}\right),$$

and we can minimize approximately with respect to m by taking the gradient with respect to m (assuming for a moment it is not restricted to be an integer): $\Delta = t\Delta \frac{\Delta^2}{\sigma^2} \exp\left(-\frac{\Delta^2 m}{\sigma^2}\right)$, that is, we consider the candidate $m^* = \lfloor \frac{\sigma^2}{\Delta^2} \log \frac{\Delta^2 t}{\sigma^2} \rfloor$.

If $t > \frac{\sigma^2}{\Delta^2} \exp(\sigma^2/\Delta^2)$, then $m^* \geq 1$, while it is always less than $t/2$. We then have a regret less than (using $\log \alpha \leq \alpha - 1$):

$$\begin{aligned} \frac{\sigma^2}{\Delta} \log \frac{\Delta^2 t}{\sigma^2} + t\Delta \exp\left[-\frac{\Delta^2}{\sigma^2} \left(\frac{\sigma^2}{\Delta^2} \log \frac{\Delta^2 t}{\sigma^2} - 1\right)\right] &= \frac{\sigma^2}{\Delta} \left[\exp(\Delta^2/\sigma^2) + 2 \log \frac{\Delta \sqrt{t}}{\sigma} \right] \\ &\leq \frac{\sigma^2}{\Delta} \left(\exp(\Delta^2/\sigma^2) - 2 + 2 \frac{\Delta \sqrt{t}}{\sigma} \right), \end{aligned}$$

which is less than a constant plus $2\sigma\sqrt{t}$. As shown below, this simple algorithm will achieve the lower bound (up to constant factors) for all possible algorithms. However, this requires knowing Δ and t in advance, to select m^* appropriately.

More than two arms ($k \geq 2$). We consider the event $\mathcal{A} = \{\forall i \neq i_*, \hat{\mu}^{(i)} - \mu^{(i)} \leq \frac{r}{\sqrt{m}}, \hat{\mu}^{(i_*)} - \mu^{(i_*)} \geq -\frac{r}{\sqrt{m}}\}$, where r is a constant to be determined later. This event is true if suboptimal arms are not too overestimated while the optimal arm is not too underestimated. If the event \mathcal{A} is true, then the loss in rewards for the last $t - mk$ steps is less than $2\frac{r}{\sqrt{m}}$ (since only arms with means that are less than $2\frac{r}{\sqrt{m}}$ away from the optimal one can be selected), while it is less than $\delta = \max_{i \neq i_*} \Delta^i$ otherwise. Moreover, using sub-Gaussian tail bounds and the union bound, $\mathbb{P}(\mathcal{A}^c) \leq k \exp(-\frac{r^2}{2\sigma^2})$.

Thus the regret is less than

$$R_t \leq mk\delta + 2\frac{rt}{\sqrt{m}} + \delta kt \exp\left(-\frac{r^2}{2\sigma^2}\right),$$

where the first term corresponds to the explore phase and the last two terms to the commit phase.

With $m^{3/2} \approx rt/(k\delta)$, we can minimize the first two terms and get

$$R_t \leq 3(rt)^{2/3}(k\delta)^{1/3} + \delta kt \exp\left(-\frac{r^2}{2\sigma^2}\right).$$

With $r = \sigma\sqrt{2\log(kt)}$, we then get $R_t \leq \delta + 3t^{2/3}k^{1/3}\delta^{1/3}\sigma^{2/3}(2\log(kt))^{1/3}$, which grows as $t^{2/3}$ and does not achieve the lower bound (see a better algorithm in Section 13.3.3).

ε -greedy. We can mix exploration and exploitation with the “ ε -greedy” strategy, which will update estimates $\hat{\mu}^{(i)}$ but spread the exploration phase over iterations by selecting with some positive probability a random arm. The final regret is similar to explore-and-commit (Auer et al., 2002).

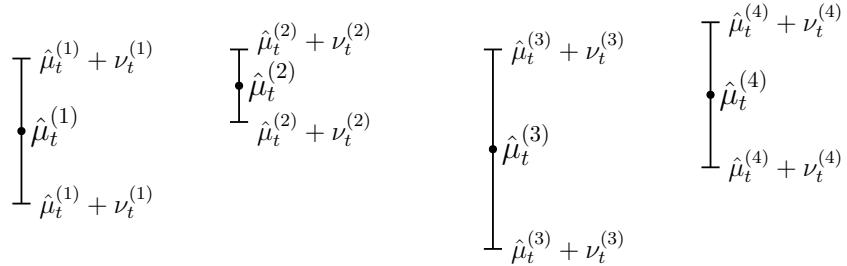
13.3.3 Optimism in the face of uncertainty (♦)

We consider the classical “upper confidence bound” (UCB) algorithm (Auer et al., 2002), whose principle is simple. As arms are being selected, confidence intervals for the values of each arm are maintained as $[\hat{\mu}_t^{(i)} - \nu_t^{(i)}, \hat{\mu}_t^{(i)} + \nu_t^{(i)}]$. The arm which is selected is the one with maximal upper-confidence bound $\hat{\mu}_t^{(i)} + \nu_t^{(i)}$. This is one instance of the general principle of optimism in the face of uncertainty (Munos et al., 2014).

The precise algorithm is as follows (assuming that σ is known):

- For the first k rounds, select each arm exactly once, and form $\hat{\mu}_k^{(i)}$ as the reward received for arm i , with $\nu_k^{(i)} = \sqrt{2\rho\sigma^2}$, with $\rho > 0$ to be determined later.
- For all other $t > k$, select the arm i which maximizes $\hat{\mu}_{t-1}^{(i)} + \nu_{t-1}^{(i)}$, and defined $\hat{\mu}_t^{(i)}$ as the average reward received for arm i , with $\nu_t^{(i)} = \sqrt{\frac{2\rho\sigma^2}{n_t^{(i)}}}$.

Thus, as illustrated below for $k = 4$, we have k confidence intervals, and we select the arm with the largest upper confidence bound (here $i = 4$).



The analysis consists in upper-bounding $\mathbb{E}[n_t^{(i)}]$ for $i \neq i_*$, following Lattimore and Szepesvári (2020). For simplicity, we assume that there is a single arm i_* with maximal mean.

We know that $n_t^{(i)} \leq t$ almost surely (since there are only t rounds). We consider some positive integer u_i 's (to be determined later) and the event, for t fixed:

$$\mathcal{A}_i = \left\{ \mu^{(i_*)} < \min_{s \in \{1, \dots, t\}} \{\hat{\mu}_s^{(i_*)} + \nu_s^{(i_*)}\} \right\} \cap \left\{ \frac{1}{u_i} \sum_{a=1}^{u_i} x_a^{(i)} + \sqrt{\frac{2\rho\sigma^2}{u_i}} < \mu^{(i_*)} \right\}.$$

This event corresponds to (a) the upper confidence bound of the best arm is always larger than the true mean for all time $s \leq t$, and (b) the upper confidence bound for the i -th arm for u_i observations is less than the value of the best arm. If \mathcal{A}_i is true, then we must have $n_t^{(i)} \leq u_i$, since if we have $n_t^{(i)} > u_i$, we must have one s such that i selected at time s , with $n_{s-1}^{(i)} = u_i$, which is impossible.

Moreover, we can upper bound the probability of \mathcal{A}_i^c by the union bound as

$$\mathbb{P}(\mathcal{A}_i^c) \leq \mathbb{P}\left(\mu^{(i_*)} \geq \min_{s \in \{1, \dots, t\}} \hat{\mu}_s^{(i_*)} + \nu_s^{(i_*)}\right) + \mathbb{P}\left(\frac{1}{u_i} \sum_{a=1}^{u_i} x_a^{(i)} + \sqrt{\frac{2\rho\sigma^2}{u_i}} \geq \mu^{(i_*)}\right).$$

By the union bound, the first probability is less than the sum of the probabilities for each $s \in \{1, \dots, t\}$, $\mathbb{P}\left(\mu^{(i_*)} \geq \frac{1}{s} \sum_{a=1}^s x_a^{(i_*)} + \sqrt{\frac{2\rho\sigma^2}{s}}\right)$, which are less than $\exp(-\rho)$ (by sub-Gaussian tail bounds). Here, $x_a^{(i_*)}$ denotes the a -th trial of arm i_* . Thus the first probability is less than $t \exp(-\rho)$.

For the second probability, this is equal to the probability that $\frac{1}{u_i} \sum_{a=1}^{u_i} x_a^{(i)} \geq \mu^{(i)} + \Delta^{(i)} - \sqrt{\frac{2\rho\sigma^2}{u_i}}$. If $\Delta^{(i)} - \sqrt{\frac{2\rho\sigma^2}{u_i}} \geq 0$, by sub-Gaussian tail bounds, it is less than $\exp\left(-\frac{u_i}{2\sigma^2}(\Delta^{(i)} - \sqrt{\frac{2\rho\sigma^2}{u_i}})^2\right)$. Otherwise, the probability is less than one. Thus, combining both cases, we get a bound $\exp\left(-\frac{u_i}{2\sigma^2}(\Delta^{(i)} - \sqrt{\frac{2\rho\sigma^2}{u_i}})^2\right)_+$.

Thus, we have

$$\begin{aligned} \mathbb{E}[n_t^{(i)}] &\leq \mathbb{E}[1_{\mathcal{A}_i} u_i] + \mathbb{E}[1_{\mathcal{A}_i^c} t] \\ &\leq u_i + t^2 \exp(-\rho) + t \exp\left(-\frac{u_i}{2\sigma^2}(\Delta^{(i)} - \sqrt{\frac{2\rho\sigma^2}{u_i}})^2\right)_+. \end{aligned}$$

It will make sense to consider $\sqrt{u_i \frac{\Delta^{(i)}}{\sigma^2}} = \sqrt{2\rho} + \sqrt{2\alpha}$, for a certain $\alpha \geq 0$, leading to a probability

$$\mathbb{E}[n_t^{(i)}] \leq u_i + t^2 \exp(-\rho) + t \exp(-\alpha) \leq \frac{\sigma^2}{(\Delta^{(i)})^2} (\sqrt{2\rho} + \sqrt{2\alpha})^2 + t^2 \exp(-\rho) + t \exp(-\alpha).$$

With $\rho = \alpha = \log(t^2)$, we get: $\mathbb{E}[n_t^{(i)}] \leq 2 + \frac{\sigma^2}{(\Delta^{(i)})^2} 16 \log t$. This leads to a regret

$$R_t \leq \sum_{i \neq i_*} \Delta^{(i)} \left(2 + \frac{\sigma^2}{(\Delta^{(i)})^2} 16 \log t \right),$$

which happens to achieve the lower bound (up to constants, see below). We can also obtain a regret which does not blow up when $\Delta^{(i)}$ goes to zero. Indeed, we always have $\sum_{i=1}^k n_t^{(i)} \leq t$, leading to

$$\begin{aligned} R_t &= \sum_{i, \Delta^{(i)} < \Delta} \Delta^{(i)} \mathbb{E}[n_t^{(i)}] + \sum_{i, \Delta^{(i)} > \Delta} \Delta^{(i)} \mathbb{E}[n_t^{(i)}] \text{ for a certain } \Delta, \\ &\leq t\Delta + \sum_{i, \Delta^{(i)} \geq \Delta} \Delta^{(i)} \left(2 + \frac{\sigma^2}{(\Delta^{(i)})^2} 16 \log t \right) \\ &\leq t\Delta + 2 \sum_i \Delta^{(i)} + k \frac{\sigma^2}{\Delta} 16 \log t \leq 2 \sum_i \Delta^{(i)} + 8\sigma \sqrt{kt \log t}, \end{aligned}$$

by optimizing over Δ , which is also optimal up to logarithmic terms (see below).

Lower bounds. It turns out that with k arms, the best that can be achieved is a regret of order $\sigma\sqrt{kt}$, and for the instance-dependent problem, of order $\log(t) \sum_{i \neq i_*} \frac{\sigma^2}{\Delta^{(i)}}$ (see, e.g., [Bubeck and Cesa-Bianchi, 2012](#)).

Illustration. In Figure 13.2, we plot the performance of the UCB algorithm with $k = 10$ arms. In particular, the right plot highlights the fact that the upper confidence bounds for all arms tend to be equal.

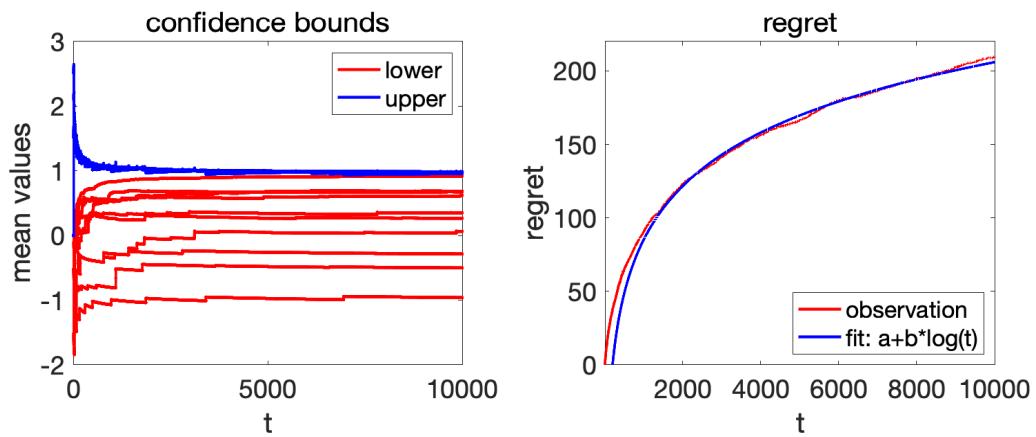


Figure 13.2: Upper-confidence bounds for $k = 10$ Bernoulli arms with random means: plot of upper and lower bounds as a function of time t (left), and regret (right).

Chapter 14

Probabilistic methods

Chapter summary

-Probabilistic models can give intuitive but sometimes misleading interpretations. In particular, maximum a posteriori (MAP) estimation does *not* work best when the parameters are generated from the prior distribution. Minimum mean-square estimation (MMSE) is preferable.

-Generative models (such as linear discriminant analysis) that explicitly tries to model the input data with simple models can lead to biased but efficient estimators in large dimensions compared to their discriminative counterparts (such as logistic regression).

-Bayesian inference can be used naturally for model selection using the marginal likelihood, both for model selection among a finite number of choices or with Gaussian processes.

-PAC-Bayesian analysis: aggregating estimators provide natural statistically efficient estimators with an elegant link with Bayesian inference.

In this chapter, we consider probabilistic modeling interpretations of several learning methods, focusing primarily on identifying losses and priors with log-densities but drawing clear distinctions between what this analogy brings and what it does not.

14.1 From empirical risks to log-likelihoods

Many methods in machine learning may be given a probabilistic interpretation through maximum likelihood or “maximum a posteriori” (MAP) estimation. For example, consider

the regularized empirical risk as:

$$\hat{\mathcal{R}}(\theta) = \frac{1}{n} \sum_{i=1}^n \ell(y_i, f_\theta(x_i)) + \lambda \Omega(\theta),$$

multiply by $-n$ and take the exponential to get:

$$\begin{aligned} \exp(-n\hat{\mathcal{R}}(\theta)) &= \exp\left(-\sum_{i=1}^n \ell(y_i, f_\theta(x_i)) - n\lambda\Omega(\theta)\right) \\ &= \prod_{i=1}^n \exp[-\ell(y_i, f_\theta(x_i))] \cdot \exp[-n\lambda\Omega(\theta)]. \end{aligned} \quad (14.1)$$

We can give a probabilistic interpretation by considering a *likelihood*, that is, a density (with respect to a well-defined base measure),

$$p(y_i|x_i, \theta) \propto \exp[-\ell(y_i, f_\theta(x_i))],$$

and a *prior* density

$$p(\theta) \propto \exp[-n\lambda\Omega(\theta)],$$

so that we have:

$$\exp(-n\hat{\mathcal{R}}(\theta)) \propto \prod_{i=1}^n p(y_i|x_i, \theta) \cdot p(\theta),$$

which is exactly the (conditional) likelihood for the model where θ is a parameter and where given θ , all pairs (x_i, y_i) are independent and identically distributed.

 Overloading of notations for probability densities, where the symbol p is used for all random variables.

 Note the difference between conditional likelihood and likelihood.

 There is more to probabilistic interpretation than simply taking the exponential, e.g., generative models, Bayesian inference for hyperparameter learning (as done in later sections), dealing with missing data through EM, etc.

 We only scratch the surface here, and from a learning theory point of view. See [Murphy \(2012\)](#); [Bishop \(2006\)](#) for many more details.

In this section, we primarily focus on the formulation in Eq. (14.1) and now look at specific examples for data likelihoods and priors.

14.1.1 Conditional likelihoods

For logistic regression where $\mathcal{Y} \in \{-1, 1\}$, we can interpret the loss as the conditional log-likelihood of the model where

$$\mathbb{P}(y_i = 1|x_i) = \frac{1}{1 + \exp(-f_\theta(x_i))},$$

which can be put in a compact way as $p(y_i|x_i) = \frac{1}{1+\exp(-y_if_\theta(x_i))} = \sigma(y_if_\theta(x_i))$.



To apply logistic regression, there is no need to assume that the model is well-specified, that is, there exists a θ_* so that the data are actually generated from the model above. For the non-parametric analysis, this is often assumed.

For least-squares regression, we can interpret the loss as a Gaussian model with mean $f_\theta(x_i)$ and variance 1. We can also estimate a more general variance parameter that is uniform across all x (homoscedastic regression) or depends on x (heteroscedastic regression).



No need to have Gaussian noise! Simply zero mean and bounded variance are enough for the analysis.

Exercise 14.1 Show that the negative log-density of the Gaussian distribution with mean μ and variance σ^2 , that is, $-\log p(y|\mu, \sigma) = \frac{1}{2\sigma^2}(x - \mu)^2 + \frac{1}{2}\log(2\pi) + \frac{1}{2}\log\sigma^2$ is not convex in (μ, σ^2) , but is jointly convex in $(\mu/\sigma^2, \sigma^{-2})$.

14.1.2 Classical priors

We can interpret classical regularizers that we have already encountered in previous chapters. For the squared ℓ_2 -norm with $\Omega(\theta) = \frac{\lambda}{2}\|\theta\|_2^2$, this corresponds to a Gaussian distribution with mean zero and covariance matrix $\lambda^{-1}I$.

For the ℓ_1 -norm with $\Omega(\theta) = \lambda\|\theta\|_1$, this is the so-called Laplace (or double exponential) prior:

$$p(\theta) = \prod_{j=1}^d \frac{\lambda}{2} \exp(-\lambda|\theta_j|).$$

Exercise 14.2 Show that the variance of a Laplace-distributed random variable is equal to $\frac{2}{\lambda^2}$.

The interactions between regularization terms and priors can go both ways, and we can consider other classical priors. One which will be useful later in the Bayesian setting is the

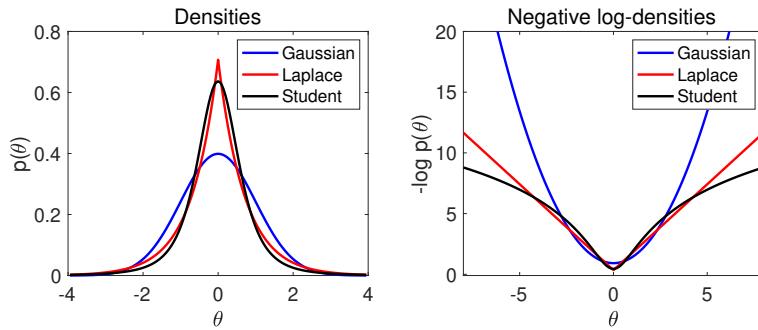


Figure 14.1: Classical priors in one dimension: (left) densities, (right) negative log-densities.

multivariate Student distribution (often used marginally for independent components):

$$p(\theta) \propto \left(\beta + \frac{1}{2} \|\theta\|_2^2 \right)^{-\alpha-d/2},$$

leading to the regularizer $(\alpha + d/2) \log(\beta + \frac{1}{2} \|\theta\|_2^2)$, which is not convex. This will be used within sparse priors in the next section.

Exercise 14.3 (♦) We consider a random vector θ which is Gaussian with mean zero and covariance matrix ηI , with $1/\eta$ being distributed as a Gamma random variable with parameters α and β , that is, η with density $p(\eta) = \frac{\beta^\alpha}{\Gamma(\alpha)} (1/\eta)^{\alpha+1} \exp(-\beta/\eta)$. Show that the marginal density of θ is the Student distribution $p(\theta) = \frac{1}{(2\pi)^{d/2}} \frac{\beta^\alpha \Gamma(\alpha+d/2)}{\Gamma(\alpha)} \frac{1}{(\beta + \frac{1}{2} \|\theta\|_2^2)^{\alpha+d/2}}$, and that $\mathbb{E}[\theta\theta^\top] = \frac{\beta}{\alpha-1} I$ if $\alpha > 1$.



This can be misleading as even when the target function is sampled from the prior, MAP estimation may not work. See Section 14.1.4.

The expression of regularizers as log-densities may lead to the impression that MAP estimation is particularly well suited when (1) the conditional model is well-specified, that is, there exists θ_* such that $p(y|x)$ is indeed proportional to $\exp(-\ell(y, f_{\theta_*}))$ and (2) the optimal θ_* is sampled from the prior distribution proportional to $\exp(-\lambda\Omega(\theta))$. This is not the case *at all*, as we now explain.

14.1.3 Sparse priors

As we will show in the next section, the Laplace prior is not a good prior for sparse data. We consider the following ones instead. For each one-dimensional component, we consider:

- Generalized Gaussians: $p(\theta) = \frac{\alpha}{2} \frac{\lambda^{1/\alpha}}{\Gamma(1/\alpha)} \exp(-\lambda|\theta|^\alpha)$, with variance $\lambda^{-2/\alpha} \frac{\Gamma(3/\alpha)}{\Gamma(1/\alpha)}$.

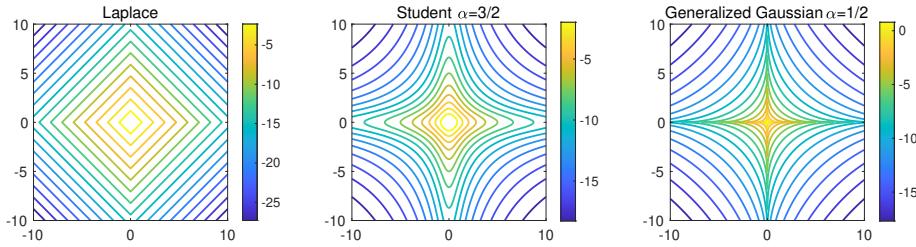


Figure 14.2: Sparse priors

- Student: $p(\theta) = \frac{1}{(2\pi)^{1/2}} \frac{\beta^\alpha \Gamma(\alpha+1/2)}{\Gamma(\alpha)} \frac{1}{(\beta + \frac{1}{2}\theta^2)^{\alpha+1/2}}$, with variance $\frac{\beta}{\alpha-1}$ if $\alpha > 1$.
- Mixture of two Gaussians: $p(\theta) = \alpha \mathcal{N}(\theta|0, \sigma_0^2) + (1-\alpha) \mathcal{N}(\theta|0, \tau^2)$, with variance $\alpha \sigma_0^2 + (1-\alpha) \tau^2$.

It turns out that all of these examples happen to be “scale mixtures of Gaussians”, that is, they can be seen as the (potentially continuous) mixtures of Gaussian distributions with zero mean but different variances:

$$p(\theta) = \int_0^{+\infty} \frac{1}{\sqrt{2\pi\eta}} e^{-\frac{1}{2}\frac{\theta^2}{\eta}} dq(\eta),$$

where q is a probability measure on \mathbb{R}_+ . For the third example, this is straightforward, with q being a weighted sum of two Diracs at σ_0^2 and τ^2 . For the Laplace distribution (generalized Gaussians with $\alpha = 1$), one can check by direct integration that we can take q to be an exponential distribution, that is, with density $q(\eta) = \frac{\lambda^2}{2} \exp(-\eta\lambda^2/2)$, while for the Student distribution, q has an inverse Gamma distribution, with density $q(\eta) = \frac{\beta^\alpha}{\Gamma(\alpha)} \eta^{-\alpha-1} e^{-\beta/\eta}$ (see exercise 14.3).

As we show in Section 14.3.2, this hierarchical model can be used with marginal likelihood maximization, leading to reweighted least-squares algorithms that are close to the “ η -trick” from Section 8.3.1, and thus provides a Bayesian interpretation.

Exercise 14.4 A density $p(\theta)$ on \mathbb{R} is said super-Gaussian if $\log p(\theta)$ is convex in θ^2 and non-increasing. Show that scale mixtures of Gaussians are super-Gaussian.¹

14.1.4 On the relationship between MAP and MMSE (\blacklozenge)

In this section, following Gribonval (2011), we consider a very simple conditional model of the form

$$y = \theta + \varepsilon, \tag{14.2}$$

¹The converse is not true, see Palmer et al. (2005).

where ε is normal with zero mean and covariance matrix $\sigma^2 I$, assuming σ^2 is known. We have prior knowledge on θ in the form of a prior density $q(\theta)$. Given the observation of y , our goal is to obtain an estimator of θ with the most favorable properties, which we define here as the minimum squared error (this estimator will be generalized in Section 14.3).

That is, given an estimator $\hat{\theta}(y)$, we consider the criterion:

$$J(\hat{\theta}) = \int_{\mathbb{R}^d} q(\theta) \|\theta - \hat{\theta}(y)\|_2^2 d\theta.$$

As shown in Section 2.2.3, the optimal estimator (i.e., function) $\hat{\theta} : \mathbb{R}^d \rightarrow \mathbb{R}^d$ is the *a posteriori mean*, that is

$$\hat{\theta}_{\text{MMSE}}(y) = \mathbb{E}[\theta|y],$$

assuming that θ is sampled according to $q(\theta)$ and y follows the model in Eq. (14.2). Here, MMSE stands for “minimum mean-square error”. We now want to compare it with the maximum a posteriori parameter

$$\hat{\theta}_{\text{MAP}}(y) \in \arg \max_{\theta \in \mathbb{R}^d} p(\theta|y) = \arg \max_{\theta \in \mathbb{R}^d} q(\theta)p(y|\theta).$$

Gaussian prior. When q is a Gaussian distribution with mean zero and covariance matrix $\tau^2 I$, then, (θ, y) is a Gaussian vector and from conditioning results presented in Section 1.1.3, we have

$$\hat{\theta}_{\text{MMSE}}(y) = \mathbb{E}[\theta|y] = \frac{\tau^2}{\tau^2 + \sigma^2} y,$$

while the MAP estimate is also equal to $\frac{\tau^2}{\tau^2 + \sigma^2} y$ because, for Gaussians, the mean and the mode are the same, but, as we will show later, Gaussian priors are the only ones for which these two are equal.

Simple expression of the MMSE. We denote by $p(y)$ the density of y , that is,

$$\begin{aligned} p(y) &= \int_{\mathbb{R}^d} p(y, \theta) d\theta = \int_{\mathbb{R}^d} p(\theta)p(y|\theta) d\theta \\ &= \int_{\mathbb{R}^d} q(\theta) \frac{1}{(2\pi\sigma^2)^{d/2}} \exp\left(-\frac{1}{2\sigma^2}\|\theta - y\|_2^2\right) d\theta. \end{aligned}$$

We can now express the a posteriori mean as:

$$\begin{aligned}
\hat{\theta}_{\text{MMSE}}(y) &= \mathbb{E}[\theta|y] = \int_{\mathbb{R}^d} \frac{p(\theta, y)}{p(y)} \theta d\theta \\
&= y + \sigma^2 \int_{\mathbb{R}^d} \frac{p(y|\theta)p(\theta)}{p(y)} \frac{1}{\sigma^2} (\theta - y) d\theta \\
&= y + \frac{\sigma^2}{p(y)} \int_{\mathbb{R}^d} q(\theta) \frac{1}{(2\pi\sigma^2)^{d/2}} \exp\left(-\frac{1}{2\sigma^2}\|\theta - y\|_2^2\right) \frac{1}{\sigma^2} (\theta - y) d\theta \\
&= y - \frac{1}{(2\pi\sigma^2)^{d/2}} \frac{\sigma^2}{p(y)} \int_{\mathbb{R}^d} q(\theta) \frac{\partial}{\partial\theta} \left[\exp\left(-\frac{1}{2\sigma^2}\|\theta - y\|_2^2\right) \right] d\theta.
\end{aligned}$$

Thus, using integration by parts, we get:

$$\begin{aligned}
\hat{\theta}_{\text{MMSE}}(y) &= y + \frac{1}{(2\pi\sigma^2)^{d/2}} \frac{\sigma^2}{p(y)} \int_{\mathbb{R}^d} q'(\theta) \exp\left(-\frac{1}{2\sigma^2}\|\theta - y\|_2^2\right) d\theta \\
&= y + \frac{1}{(2\pi\sigma^2)^{d/2}} \frac{\sigma^2}{p(y)} \int_{\mathbb{R}^d} q'(y - \eta) \exp\left(-\frac{1}{2\sigma^2}\|\eta\|_2^2\right) d\eta \\
&= y + \frac{\sigma^2}{p(y)} p'(y) = y + \sigma^2 \frac{d}{dy} (\log p(y)). \tag{14.3}
\end{aligned}$$

We thus get an explicit expression of the minimum means square error estimate. Note that for a Gaussian prior, y is (marginally) normally distributed; hence, the gradient of $\log p(y)$ is a linear function, and the MMSE is affine in y if and only if the prior is Gaussian.

Exercise 14.5 (♦) Show that the posterior covariance matrix can be expressed as $\text{var}(\theta|y) = \sigma^2 I + \sigma^4 \frac{d^2}{dy dy^\top} (\log p(y))$.

Expression of the MAP estimate. If $q(\theta) = \exp(-h(\theta))$, then the MAP estimate is

$$\hat{\theta}_{\text{MAP}}(y) \in \arg \max_{\theta \in \mathbb{R}^d} \frac{1}{2\sigma^2} \|\theta - y\|_2^2 + h(\theta),$$

with optimality condition, for differentiable h , $\theta - y - \sigma^2 \frac{d}{d\theta} (\log q(\theta)) = 0$, thus we have:

$$\hat{\theta}_{\text{MAP}}(y) = y + \sigma^2 \frac{d}{dy} (\log q)[\hat{\theta}_{\text{MAP}}(y)]. \tag{14.4}$$

Exercise 14.6 (♦♦) We denote by $f(y) = -\log p(y)$. Show that the MMSE estimator $\hat{\theta}_{\text{MMSE}}(y) = y - \sigma^2 f'(y)$ defined in Eq. (14.3) is the MAP estimator for the negative log-prior g that satisfies $g(\hat{\theta}_{\text{MMSE}}(y)) = f(y) - \frac{\sigma^2}{2} \|f'(y)\|_2^2$ for all $y \in \mathbb{R}^d$.

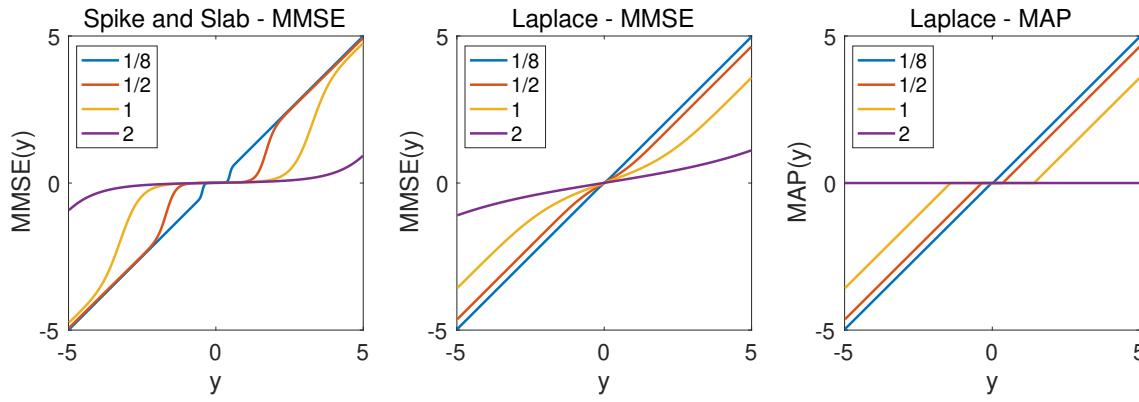


Figure 14.3: Comparison of MMSE and MAP for the spike-and-slab and Laplace priors: MMSE for the spike-and-slab prior (left), MMSE for the Laplace prior (middle), MAP for the Laplace prior (right).

Differences between MMSE and MAP. Given the expressions in Eq. (14.3) and Eq. (14.4), we can now study how the two estimators differ for the various sparse priors that we have described above, where we consider the one-dimensional case for simplicity (which extends to independent marginal priors in the multi-dimensional case) (see plots in Figure 14.3):

- Spike-and-slab: this is the model essentially used in the analysis of the Lasso in Chapter 8, for which MAP with the Laplace prior (that is, the Lasso) is shown to work well. We consider the prior, which is the mixture of a Dirac at zero (with weight α) and a Gaussian with mean zero and variance τ^2 . The variance is then equal to $(1 - \alpha)\tau^2$, and $p(y)$ is the mixture of two Gaussian distributions, centered in zero, with variances σ^2 and $\sigma^2 + \tau^2$.

Exercise 14.7 Show that the marginal density $p(y)$ for the spike-and-slab prior is equal to $p(y) = \alpha \frac{1}{(2\pi\sigma^2)^{1/2}} \exp\left(-\frac{y^2}{2\sigma^2}\right) + (1 - \alpha) \frac{1}{(2\pi(\sigma^2 + \tau^2))^{1/2}} \exp\left(-\frac{y^2}{2(\sigma^2 + \tau^2)}\right)$. Provide an expression of $\hat{\theta}_{\text{MMSE}}(y)$ and of $\hat{\theta}_{\text{MAP}}(y)$.

- Laplace: this is the model for which the MAP estimation leads to the Lasso method. For $q(\theta) = \frac{2}{\lambda} \exp(-\lambda|\theta|)$, the variance is equal to $2/\lambda^2$. We can compute the MMSE by explicitly computing $p(y)$ by integrating separately over positive et negative numbers (see the exercise below). We see in Figure 14.3 that the MMSE is very far from the soft-thresholding operator from Section 8.3.1. In other words, the Lasso is not adapted to signals which are sampled from the Laplace distribution, but rather to signals sampled from the spike-and-slab prior.

Exercise 14.8 Show that the marginal density $p(y)$ for the Laplace prior can be expressed using the Gauss error function $\text{erf}(\alpha) = \frac{2}{\sqrt{\pi}} \int_0^\alpha \exp(-t^2) dt$, as: $p(y) = \frac{\lambda}{4} \exp\left(\frac{\lambda^2 \sigma^2}{2} - \lambda y\right) \left[1 - \text{erf}\left(\frac{\lambda \sigma - \frac{y}{\sigma}}{\sqrt{2}}\right)\right] + \frac{\lambda}{4} \exp\left(\frac{\lambda^2 \sigma^2}{2} + \lambda y\right) \left[1 - \text{erf}\left(\frac{\lambda \sigma + \frac{y}{\sigma}}{\sqrt{2}}\right)\right]$. Provide an expression of $\hat{\theta}_{\text{MMSE}}(y)$ and of $\hat{\theta}_{\text{MAP}}(y)$.

Exercise 14.9 When q is a Gaussian distribution with mean zero and covariance matrix C , provide an expression of the MMSE and MAP estimates.

Exercise 14.10 (♦) Provide a closed-form expression for the marginal density $p(y)$ for the Student prior.

14.2 Discriminative vs. generative models

We consider a traditional supervised learning set-up, with $(x, y) \in \mathcal{X} \times \mathcal{Y}$. The goal is for any $x \in \mathcal{X}$ to obtain a good conditional predictive model of y given x , that is, to get a good model for $p(y|x)$.

We can first directly model $p(y|x)$ with a parameterized conditional model (like done for least-squares or logistic regression). This will be called the *discriminative* approach.

We can also consider a joint density $p(x, y)$, and obtain $p(y|x) = \frac{p(x, y)}{p(x)} \propto p(x, y)$ using Bayes rule. Most often (in particular for classification problems), the joint model is obtained by modeling y and $x|y$, that is, the conditional model of the inputs given the outputs, with a particularly simple model. This will be called the *generative* approach.

14.2.1 Linear discriminant analysis and softmax regression

We consider a generative model with Gaussian class-conditional densities with a common covariance matrix, with $x \in \mathbb{R}^d$ and $y \in \{1, \dots, k\}$:

$$\begin{aligned} y &\sim \text{multinomial}(\pi) \\ x|y = i &\sim \text{Gaussian}(\mu_i, \Sigma). \end{aligned}$$

We can then compute the distribution of y given x as (removing all parts that are independent of i):

$$\begin{aligned} \mathbb{P}(y = i|x) &\propto \mathbb{P}(y = i, x) = \pi_i \exp\left[-\frac{1}{2}(x - \mu_i)^\top \Sigma^{-1}(x - \mu_i)\right] \\ &\propto \pi_i \exp\left[-\frac{1}{2}\mu_i^\top \Sigma^{-1}\mu_i\right] \exp(\mu_i^\top \Sigma^{-1}x). \end{aligned}$$

This implies that, defining the softmax function $\text{softmax} : \mathbb{R}^k \rightarrow \mathbb{R}^k$ through $\text{softmax}(v)_j = \frac{e^{v_j}}{\sum_{i=1}^k e^{v_i}}$:

$$\mathbb{P}(y = i|x) = \text{softmax}\left[(\mu_i^\top \Sigma^{-1} x + \log \pi_i - \frac{1}{2} \mu_i^\top \Sigma^{-1} \mu_i)_i\right] = \text{softmax}\left[(w_i^\top x + b_i)_i\right],$$

that is, the conditional model is the softmax function of a linear model, which is exactly the definition of softmax regression, with $w_i = \Sigma^{-1} \mu_i$, and $b_i = \log \pi_i - \frac{1}{2} \mu_i^\top \Sigma^{-1} \mu_i$. The availability of a generative model will lead to alternative parameter estimation algorithms (see below). Note that (a) for $k = 2$, we recover logistic regression, and that (b) we can apply the softmax regression model for any set of k prediction functions f_1, \dots, f_k beyond affine functions.

Note finally that the common covariance matrix is often restricted to be diagonal.

Exercise 14.11 Assume that the class-conditional covariance matrices are different for each class. Show that the conditional model is still a softmax function, but now of “affine + quadratic” functions of x .

14.2.2 Naive Bayes

We consider discrete data, that is $x \in \{1, \dots, m\}^d$ and $y \in \{1, \dots, k\}$, and the following generative model

$$\begin{aligned} y &\sim \text{multinomial}(\pi) \\ x|y = i &\sim \prod_{j=1}^d \text{multinomial}(x_j|\theta_{ji}), \end{aligned}$$

where $\pi \in \mathbb{R}^k$, and each θ_{ji} is in \mathbb{R}^m . In other words, given y , the d components x_1, \dots, x_d are independent.

Using the usual “one-hot” encoding of discrete distribution, we see each x_j in \mathbb{R}^m as one of the canonical basis vectors so that the probability of $x_j|y = i$ is equal to $\prod_{a=1}^m \theta_{jia}^{x_{ja}}$. We can then compute

$$\begin{aligned} \mathbb{P}(y = i|x) &\propto \mathbb{P}(y = i, x) = \prod_{i=1}^k \pi_i^{y_i} \prod_{i=1}^k \prod_{j=1}^d \prod_{a=1}^m \theta_{jia}^{x_{ja} y_i} \\ \log \mathbb{P}(y = i|x) &\propto \sum_{i=1}^k y_i \left(\log \pi_i + \sum_{j=1}^d \sum_{a=1}^m (\log \theta_{jia}) x_{ja} \right). \end{aligned}$$

Like for linear discriminant analysis, we thus also get a softmax model $\text{softmax}\left[(w_i^\top x + b_i)_i\right]$, with $b_i = \log \pi_i$, and w_i with components $\log \theta_{jia}$.

14.2.3 Maximum likelihood estimations

As shown above, for linear discriminant analysis and naive Bayes, we obtain conditional models corresponding to softmax regression, for which we can use optimization algorithms to get the relevant parameters (this is the discriminative approach).

However, we can also use the generative models to estimate parameters in closed form. For example, for linear discriminant analysis, the maximum likelihood estimates for the class proportions are the empirical class proportions $\hat{\pi}_i$, the means are the empirical means, and $\hat{\Sigma} = \sum_{i=1}^k \hat{\pi}_i \hat{\Sigma}_i$, which allows us to compute \hat{w}_i and \hat{b}_i , through the formula above, instead of having to solve a convex problem. The key question is: which one is better?

Discriminative vs. generative learning. When making an even simpler assumption of Σ diagonal, we can study the potential benefits of the discriminative and the generative set-up, following [Ng and Jordan \(2001\)](#): the generative approach has a stronger bias but potentially a lower variance.

For both linear discriminant analysis in Section 14.2.1 and Naive Bayes in Section 14.2.2, if we use the conditional log-likelihood as a criterion, the discriminative approaches in the population case optimize directly the correct criterion, and thus must lead to better or equal performance. However, in the unregularized case, to approach the population case for logistic regression, we need a number of samples proportional to d (e.g., by considering our bounds on Rademacher complexities in Section 4.5 with data with equal variance in all directions). For LDA or Naive Bayes, we need to estimate d separate quantities simultaneously, and, when using concentration inequalities and the union bound, we should expect to have n larger than a constant times $\log d$ to attain the population performance. We thus get a larger bias with generative approaches but significantly less variability. See the experiments in Figure 14.4, more details by [Ng and Jordan \(2001\)](#), and a similar approach to variable selection in regression ([Fan and Lv, 2008](#)).

14.3 Bayesian inference

For simplicity, in this section, we consider random observations $z \in \mathcal{Z}$ that could be the traditional pair $(x, y) \in \mathcal{X} \times \mathcal{Y}$ in supervised learning, but we note that Bayesian inference applies much more generally. See more details by [Robert \(2007\)](#).

We assume that we have a set of probability distributions over z , with densities with respect to some base measure, which are parameterized by some vector $\theta \in \Theta$ (a subset of a vector space), and which we denote $p(z|\theta)$, and refer to as the *likelihood function*. We assume some *prior distribution* with density $q(\theta)$ with respect to the Lebesgue measure. In

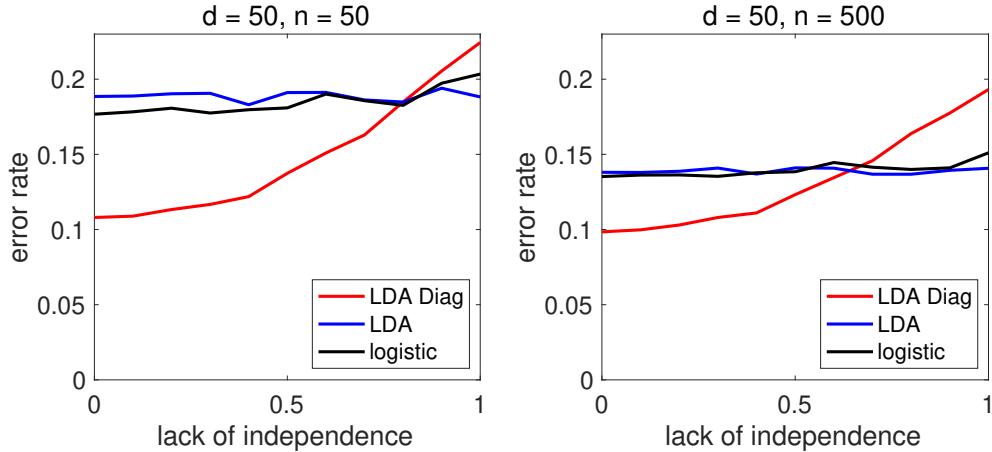


Figure 14.4: Comparison of LDA with full covariance matrix, LDA with diagonal covariance matrix, and logistic regression, on a well-specified binary classification problem (Gaussian class-conditional densities with same covariance matrix), with independent components and non-independent components (with a smooth transition, which is linear in the matrix logarithm). For independent components (left parts of the plots), linear discriminant analysis with the independence assumptions leads to better performance.

the Bayesian methodology, we assume that θ is sampled once from the prior distribution and that we obtain *i.i.d.* observations $z_1, \dots, z_n \in \mathcal{Z}$ sampled from $p(z|\theta)$.

By independence and identical distributions, the overall joint distribution of the data and θ is

$$p(z_1, \dots, z_n, \theta) = q(\theta) \prod_{i=1}^n p(z_i|\theta).$$

We can then obtain the *posterior distribution* of θ given the data (z_1, \dots, z_n) , which is proportional to $p(z_1, \dots, z_n, \theta)$, and with density:

$$p(\theta|z_1, \dots, z_n) = \frac{q(\theta) \prod_{i=1}^n p(z_i|\theta)}{\int_{\Theta} q(\eta) \prod_{i=1}^n p(z_i|\eta) d\eta}.$$

As already noted, the mode of the posterior distribution is the “maximum a posteriori” (MAP) estimate, which is rarely used within Bayesian inference (see some reasons in Section 14.1.4). Other estimates or estimation procedures are preferred, all using the posterior distribution as the main source. Thus being able to characterize this posterior distribution is the computational tool (see below).

Posterior mean. A good summary of the posterior distribution is the posterior mean $\int_{\Theta} \theta p(\theta|z_1, \dots, z_n) d\theta$ and is traditionally associated with parameter estimation with the square loss. This was called the MMSE in Section 14.1.4.

Bayesian model averaging. Given the multiple models characterized by the posterior distribution, we can consider performing inference on unseen data through the mixture distribution

$$\int_{\Theta} p(z|\theta)p(\theta|z_1, \dots, z_n)d\theta.$$

Thus, overall, Bayesian inference naturally leads to parameter estimation procedures that can be studied both from a computational perspective (see Section 14.3.1) and a statistical perspective, as part of the “PAC-Bayes” framework described in Section 14.4. But it can also be used for model selection, as described in Section 14.3.2.

14.3.1 Computational handling of posterior distributions

In this section, only a brief account of algorithms to characterize posterior distributions is given. See many more details by [Gelman et al. \(1995\)](#); [Robert \(2007\)](#).

Conjugate priors. In rare instances, the posterior distribution has a simple form. Two classic examples are the Gaussian prior on the mean parameter of a Gaussian variable and the Dirichlet prior on the parameters of a multinomial distribution.

Gaussian approximation (Laplace method). When the number of observations gets large, then the integral defining the normalizing factor of the posterior distribution can be written as:

$$\int_{\Theta} q(\eta) \prod_{i=1}^n p(z_i|\eta)d\eta = \int_{\Theta} \exp \left[n \times \left(\frac{1}{n} \log q(\eta) + \frac{1}{n} \sum_{i=1}^n \log p(z_i|\eta)d\eta \right) \right],$$

and thus as $\int_{\Theta} \exp(nh(\theta))d\theta$ for a certain function h . The Laplace method is a traditional approximation technique for approximating integrals of that form when the function h has a global maximum within the interior of Θ .² This maximizer is exactly the MAP estimate $\hat{\theta}_{\text{MAP}}$, and the approximation is exactly equivalent to modeling the posterior density as a Gaussian with mean $\hat{\theta}_{\text{MAP}}$ and covariance matrix $\frac{1}{n}h''(\hat{\theta}_{\text{MAP}})^{-1}$.

Sampling. Obtaining independent samples from the posterior distribution is often enough for inference purposes, and many algorithms exist, such as Markov chain Monte Carlo methods ([Robert and Casella, 2005](#)).

²See <https://francisbach.com/laplace-method/> for details.

Variational inference. An alternative to sampling is to approximate the posterior distribution by a family of simple tractable distributions that are made to fit the posterior as closely as possible. See Blei et al. (2017) and references therein.

14.3.2 Model selection through marginal likelihood

Probabilistic models are often naturally defined hierarchically, with prior distributions that have themselves parameters (which we can call hyperparameters), themselves with their own prior distribution (often called hyperprior distribution). For example, using the above notations, the prior distribution is $q(\theta|\lambda)$ with a hyperprior $r(\lambda)$, with often a data distribution that depends on both θ and λ .

While we could still treat λ as a random variable on which Bayesian inference is performed, it is common to perform maximum-likelihood estimation on λ , or more generally, maximum a posteriori estimation. This is sometimes referred to as “type II maximum likelihood” or “empirical Bayes”. This leads to a form of hyperparameter selection for λ . More precisely, we maximize

$$\begin{aligned} p(\lambda|z_1, \dots, z_n) &\propto p(\lambda, z_1, \dots, z_n) = \int_{\Theta} p(\lambda, \theta, z_1, \dots, z_n) d\theta \\ &\propto r(\lambda) \int_{\Theta} \prod_{i=1}^n p(z_i|\theta, \lambda) q(\theta|\lambda) d\theta. \end{aligned}$$

The quantity $\int_{\Theta} \prod_{i=1}^n p(z_i|\theta) q(\theta|\lambda) d\theta$ is referred to as the *marginal likelihood*, and its maximization is a generic tool for hyperparameter selection, with many applications. We present briefly two of them below.

Selection among finitely many models. A classical application of marginal likelihood maximization is to consider m different models, that is, m different distribution $p_j(z|\theta_j)$, with potentially parameters $\theta_j \in \Theta_j$ living in different spaces, with prior distribution $q_j(\theta_j)$. With a uniform distribution on the models, model selection is performed by maximizing with respect to $j \in \{1, \dots, m\}$:

$$\int_{\Theta_j} \prod_{i=1}^n p_j(z_i|\theta_j) q_j(\theta_j) d\theta_j.$$

If we consider the Gaussian approximation obtained from Laplace approximation, then one can show that we obtain penalized maximum log-likelihood with a penalty equal to $\frac{d_j}{2} \log n$, where d_j is the dimension of Θ_j , leading to the Bayesian information criterion (BIC) (see Robert, 2007, Chapter 7).

Sparsity with automatic relevance determination. As mentioned in Section 14.1.3, we consider a prior distribution $q(\theta|\eta)$ which is Gaussian with mean zero and covariance matrix ηI . Maximizing the penalized marginal likelihood ends up being similar to the “ η -trick” from Section 8.3.1. Indeed, when we consider regression with Gaussian noise, that is, when y given θ is normal with mean $\Phi\theta$ and covariance matrix $\sigma^2 I$, then y given η is Gaussian with mean $\Phi \text{Diag}(\eta)\Phi^\top + \sigma^2 I$, and thus we can compute the log-likelihood in closed form.

Gaussian processes. The example above may be extended to kernel methods presented in Chapter 7. Indeed, it is possible to define a probabilistic model of random function from a set \mathcal{X} to \mathbb{R} such that the marginal distribution of $f(x_1), \dots, f(x_n)$ is Gaussian with mean zero and covariance matrix $K \in \mathbb{R}^{n \times n}$ where $K_{ij} = k(x_i, x_j)$, where k is a positive definite kernel function. This allows us to combine Bayesian inference with non-parametric kernel learning. See more details by [Rasmussen and Williams \(2006\)](#).

14.4 PAC-Bayesian analysis

In this section, we briefly review a generic framework to obtain generalization guarantees for randomized or averaged predictors like the ones coming from Bayesian inference. For more details, see [Alquier \(2021\)](#) and the many references therein.

14.4.1 Set-up

We consider the classical supervised learning framework that we have been following throughout the book, namely, with n pairs of i.i.d. observations (x_i, y_i) from a distribution p on $\mathcal{X} \times \mathcal{Y}$, a loss function $\ell : \mathcal{Y} \times \mathbb{R} \rightarrow \mathbb{R}$. We assume that we have a family of prediction functions $f_\theta : \mathcal{X} \rightarrow \mathbb{R}$, parameterized by $\theta \in \Theta$ (which is a subset of a vector space equipped with the Lebesgue measure).

We consider predictors that are not based on selecting a single $\theta \in \Theta$, but a probability distribution ρ over θ . Given that probability distribution, we can consider:

- (a) a randomized predictor f_θ , where θ is sampled from ρ . Then the generalization performance will be considered with this extra randomness (on top of the randomness of the training data),
- (b) the posterior mean $x \mapsto \int_\Theta f_\theta(x) d\rho(\theta)$ which is a function from \mathcal{X} to \mathbb{R} and then only the randomness of the training data need to be considered. Note that in this situation, the final prediction function is not in the set of all f_θ , $\theta \in \Theta$, and is often called an “aggregated predictor”.

The generalization bounds that will be presented will be valid for *all* potential probability distributions ρ , including ones that depend on the data, which implies that we can then optimize the bounds over the distribution, leading to a candidate which is very close to the Bayesian posterior distribution (but with an added temperature). Like in Bayesian inference, we consider a fixed probability distribution q on Θ , which we will refer to as the prior.

We use the notation $\mathcal{R}(\theta) = \mathbb{E}[\ell(y, f_\theta(x))]$ for the expected risk (a deterministic function of θ), and $\widehat{\mathcal{R}}(\theta) = \frac{1}{n} \sum_{i=1}^n \ell(y_i, f_\theta(x_i))$ for the empirical risk (which is a random function of θ with expectation \mathcal{R}).

14.4.2 Uniformly bounded loss functions

We assume that almost surely, for all $\theta \in \Theta$, we have: $\ell(y, f_\theta(x)) \in [0, \ell_\infty]$ (for example, with the 0-1 loss for binary classification, or with bounded predictors for regression). Following the exposition of Alquier (2021); Catoni (2003), in the proof of Hoeffding's inequality in Section 1.2.1, we saw that for all $\theta \in \Theta$ and $s \in \mathbb{R}_+$, we have:

$$\mathbb{E}[\exp(s(\mathcal{R}(\theta) - \widehat{\mathcal{R}}(\theta)))] \leq \exp\left(\frac{s^2 \ell_\infty^2}{8n}\right).$$

Integrating over θ , we get

$$\int_{\Theta} \mathbb{E}[\exp(s(\mathcal{R}(\theta) - \widehat{\mathcal{R}}(\theta)))] dq(\theta) \leq \exp\left(\frac{s^2 \ell_\infty^2}{8n}\right).$$

We now use the variational formulation of the log-partition function (also known as the Donsker-Varadhan formula), with $h(\theta) = s(\mathcal{R}(\theta) - \widehat{\mathcal{R}}(\theta))$.

$$\log \int_{\Theta} \exp(h(\theta)) dq(\theta) = \sup_{\rho \in \mathcal{P}(\theta)} \int_{\Theta} h(\theta) d\rho(\theta) - D(\rho \| q),$$

with $\mathcal{P}(\theta)$ the set of probability distribution on Θ and $D(\rho \| q)$ the Kullback-Leibler divergence between ρ and q , defined as (see also Section 12.1.3):

$$D(\rho \| q) = \int_{\Theta} \log\left(\frac{d\rho}{dq}(\theta)\right) d\rho(\theta).$$

This leads to

$$\mathbb{E}\left[\exp\left(\sup_{\rho \in \mathcal{P}(\theta)} \int_{\Theta} s(\mathcal{R}(\theta) - \widehat{\mathcal{R}}(\theta)) d\rho(\theta) - D(\rho \| q)\right)\right] \leq \exp\left(\frac{s^2 \ell_\infty^2}{8n}\right). \quad (14.5)$$

Thus, using Chernoff bound,³ we obtain that with probability greater than $1 - \delta$,

$$\sup_{\rho \in \mathcal{P}(\theta)} \int_{\Theta} s(\mathcal{R}(\theta) - \widehat{\mathcal{R}}(\theta)) d\rho(\theta) - D(\rho \| q) \leq \frac{s^2 \ell_\infty^2}{8n} + \log \frac{1}{\delta},$$

³See https://en.wikipedia.org/wiki/Chernoff_bound.

or, in other words, for all $\rho \in \mathcal{P}(\theta)$,

$$\int_{\Theta} \mathcal{R}(\theta) d\rho(\theta) \leq \int_{\Theta} \widehat{\mathcal{R}}(\theta) d\rho(\theta) + \frac{1}{s} D(\rho \| q) + \frac{1}{s} \log \frac{1}{\delta} + \frac{s\ell_{\infty}^2}{8n}.$$

We thus get a bound on the average generalization error based on the average empirical error. The bound can be empirically computed for any ρ , and minimized, with the optimal distribution being proportional to $\exp(-s\widehat{\mathcal{R}}(\theta))dq(\theta)$, which is often called the Gibbs posterior distribution. With $s = n$, this is exactly the Bayesian posterior distribution. Denoting $\hat{\rho}_s$ this distribution, we get with probability greater than $1 - \delta$, that

$$\int_{\Theta} \mathcal{R}(\theta) d\hat{\rho}_s(\theta) \leq \inf_{\rho \in \mathcal{P}(\Theta)} \int_{\Theta} \widehat{\mathcal{R}}(\theta) d\rho(\theta) + \frac{1}{s} D(\rho \| q) + \frac{1}{s} \log \frac{1}{\delta} + \frac{s\ell_{\infty}^2}{8n}.$$

Beyond integrated risks. For convex loss functions, by Jensen's inequality, the risk of the posterior mean $x \mapsto \int_{\Theta} f_{\theta}(x) d\rho(\theta)$ is less than the integrated risk, so the bound applies.

Moreover, by applying Jensen's inequality to Eq. (14.5), we can get a bound in expectation as for all $\rho \in \mathcal{P}(\theta)$ (again ρ may depend on the data):

$$\mathbb{E} \left[\int_{\Theta} \mathcal{R}(\theta) d\rho(\theta) \right] \leq \mathbb{E} \left[\int_{\Theta} \widehat{\mathcal{R}}(\theta) d\rho(\theta) + \frac{1}{s} D(\rho \| q) + \frac{s\ell_{\infty}^2}{8n} \right].$$

Moreover, for the Gibbs posterior, by applying Jensen's inequality, we get:

$$\mathbb{E} \left[\int_{\Theta} \mathcal{R}(\theta) d\hat{\rho}_s(\theta) \right] \leq \inf_{\rho \in \mathcal{P}(\Theta)} \int_{\Theta} \mathcal{R}(\theta) d\rho(\theta) + \frac{1}{s} D(\rho \| q) + \frac{s\ell_{\infty}^2}{8n}. \quad (14.6)$$

Finite set of models. We consider m prediction functions $\hat{f}_1, \dots, \hat{f}_n$. By considering all Diracs in Eq. (14.6), we get that

$$\mathbb{E} \left[\int_{\Theta} \mathcal{R}(\theta) d\hat{\rho}_s(\theta) \right] \leq \inf_{\theta \in \Theta} \mathcal{R}(\theta) + \frac{1}{s} \log \frac{1}{q(\theta)} + \frac{s\ell_{\infty}^2}{8n}.$$

With $q(\theta) = 1/m$ and optimizing over s , we get the usual $\ell_{\infty} \sqrt{\frac{\log m}{n}}$ like we obtained for empirical risk minimization in Section 4.4.3.

Lipschitz-continuous losses, linear predictions, and Gaussian priors. See Alquier (2021) to recover rates similar to ones that can be obtained with Rademacher complexities in Chapter 4.

Application to sparse regression. PAC-Bayesian analysis can be considered in many settings, including the sparse linear regression problems as dealt with in Chapter 8. For example, [Alquier and Lounici \(2011\)](#); [Rigollet and Tsybakov \(2011\)](#) consider the combination of all least-squares predictors with supports restricted to a set $A \subset \{1, \dots, d\}$ for all such sets A . The combination is performed with exponential weights, and the estimator is shown to exhibit the same performance as the ℓ_0 -penalty from Section 8.2.2, but now requires sampling as an estimation algorithm instead of combinatorial optimization.

Chapter 15

Structured prediction

Chapter summary

- With appropriate modifications, we can design convex surrogates for output spaces that are arbitrarily complex and with generic loss functions.
- Like for binary classification, these convex surrogates lead to efficient algorithms which predict optimally given infinite amounts of data (Fisher consistency).
- Quadratic surrogates that extend the square loss lead to simple, intuitive consistent estimation procedures with well-defined decoding steps once a score function has been learned. They can be extended to smooth surrogates.
- Non-smooth surrogates can be defined in the general structured prediction framework, that extend the support vector machine.

In most of this book on supervised learning, we have focused on regression or binary classification, which led to estimating real-valued prediction functions directly when predicting a real-valued output (least-squares regression) or indirectly through convex surrogates (support vector machine or logistic regression) where the binary output in $\{-1, 1\}$ was obtained by taking the sign function. As shown in Section 4.1, the use of convex surrogates comes from strong theoretical guarantees in terms of achieving the Bayes error (that is, the optimal performance on unseen data).

In this chapter, we tackle arbitrary output spaces \mathcal{Y} , with arbitrary loss functions, which are ubiquitous in practice (see examples in Section 15.1). Most developments from Section 4.1 will extend with appropriate modifications.

15.1 General set-up and examples

We consider the same general set-up presented earlier in Section 2.2, that is, we want to predict a variable $y \in \mathcal{Y}$ from some $x \in \mathcal{X}$, and given a prediction $z \in \mathcal{Y}$, we incur the loss $\ell(y, z)$, with the loss function $\ell : \mathcal{Y} \times \mathcal{Y} \rightarrow \mathbb{R}$.

Like in Section 2.2, given a test distribution p on $\mathcal{X} \times \mathcal{Y}$, we can define the Bayes predictor

$$f^*(x) \in \arg \min_{z \in \mathcal{Y}} \int_{\mathcal{Y}} \ell(y, z) dp(y|x) \quad (15.1)$$

in the usual way. While it led to simple closed-form formulas for the 0–1 loss and binary classification, this will not always be the case. Nevertheless, our goal will still be to achieve its (optimal) performance at a reasonable computational cost.

15.1.1 Examples

We now consider classic examples with their applicative motivations in natural language processing, biology, or computer vision—see more examples by [Nowak et al. \(2019\)](#) and [Ciliberto et al. \(2020\)](#):

- **Multi-category classification:** $\mathcal{Y} = \{1, \dots, k\}$ and a loss matrix $L \in \mathbb{R}^{k \times k}$, with $\ell(i, j) = L_{ij}$. The usual 0–1 loss corresponds to $L_{ij} = 1_{i \neq j}$, but in most applications, errors do not have the same cost (for example, in spam prediction, classifying a legitimate email as spam costs much more than the opposite).
- **Robust regression:** $\mathcal{Y} = \mathbb{R}$, with $\ell(y, z) = \rho(y - z)$ and typically ρ non convex. When ρ is convex, such as $\rho(\delta) = |\delta|$ or $\rho(\delta) = \delta^2$, there is no need for a surrogate framework, but then regression may be non-robust to strong outlier perturbations. Having a non-convex ρ , such as, $\rho(\delta) = 1 - \exp(-\delta^2)$ leads to robust regression.
- **Ordinal regression:** this is a particular case of the situation above, where the loss matrix has a particular structure where the loss L_{ij} is increasing in $|i - j|$. This is common when using a rating system with a few discrete levels. One possibility is to ignore the discrete structure of the loss and use least-squares regression together with rounding, but this does not lead to optimal predictions.
- **Multiple labels:** $\mathcal{Y} = \{-1, 1\}^k$, with cardinality 2^k , with the traditional Hamming loss $\ell(y, z) = \frac{1}{2}\|y - z\|_1 = \frac{1}{4}\|y - z\|_2^2$, which counts the number of mistakes and which will be a running example in this chapter. Other scores, such as precision/recall or “F-scores”, are typically used (and may not be symmetric) and can be treated as well with the frameworks presented in this chapter. Multiple label prediction is common in multimedia applications, where there are potentially k objects in a document, and one wants to predict which ones are present.

- **Permutations:** \mathcal{Y} is the set of permutations among m elements, that is, y a bijection from $\{1, \dots, m\}$ to $\{1, \dots, m\}$. We have then $|\mathcal{Y}| = m!$. A common loss function is the “pairwise disagreement”, equal to $\ell(y, z) = \sum_{i,j=1}^m 1_{y(i)>y(j)} 1_{z(i)<z(j)}$, but other losses such as the discounted cumulative gain can be used. Predicting permutations occurs in information retrieval and ranking problems where the permutation encodes a user’s preferences over a set of m items. This is typically used in ranking problems.
- **Sequences:** \mathcal{Y} is the set of sequences of potentially arbitrary lengths over some alphabet; this has applications in natural language processing (e.g., translation from one language to another), computational biology (DNA basis or amino-acid sequences), or econometrics/finance (prediction of time series, where the alphabet is usually not finite). The cardinality of y is thus large (or infinite), and the Hamming loss is commonly used.
- **Trees, graphs:** \mathcal{Y} is set of potentially labelled graphs over some vertices. Classic examples include the prediction of molecules (which can be represented as graphs) or the grammatical analysis of sentences in natural language processing.

Why is it difficult? Structured prediction is challenging for two reasons:

- Computationally: we need to predict large structured (often discrete) objects from real-valued outputs.
- Statistically: there is a potential curse of dimensionality in both k (the underlying dimension of the problem, to be defined later precisely) *and* the input d , in addition to a complicated combinatorial structure.

Our goal is to obtain polynomial-time algorithms in k , n , and d to attain the optimal prediction, that is, we aim to obtain:

1. Computational tractability by introducing convex surrogates (to use convex optimization) and efficient decoding steps (often dedicated algorithms).
2. Fisher consistency (excess risk goes to zero in the population case) and calibration (sub-optimality for the convex surrogate leads to sub-optimality for the true risk).

Following the rest of the book, we will always go through vector-space valued prediction functions. Thus, there will always be two components:

1. Learning some scores from data, implicitly and explicitly, in a Hilbert space \mathcal{H} or \mathbb{R}^k , where k is the (potentially implicit) “affine dimension” of \mathcal{Y} .
2. Decoding step to go from score functions to predictions (obvious and somewhat overlooked in the binary classification case).

15.1.2 Structure encoding loss functions

To achieve some guaranteed predictive performance, we will need to impose some low-dimensional vectorial structure, which in turn imposes some specific structure within \mathcal{Y} , hence the name “structured prediction”. More precisely, we will assume that we have two embeddings of the label space \mathcal{Y} into the same Hilbert space \mathcal{H} , that is, two maps $\varphi, \psi : \mathcal{Y} \rightarrow \mathcal{H}$ and a constant $c \in \mathbb{R}$, such that

$$\forall (y, z) \in \mathcal{Y} \times \mathcal{Y}, \ell(y, z) = c + \langle \varphi(z), \psi(y) \rangle. \quad (15.2)$$

This assumption is referred to as “structure encoding loss function” (SELF) (Ciliberto et al., 2020). This can be an implicit or explicit embedding (see examples below). Note that the representation is not unique as given a pair (φ, ψ) , any pair $(V\varphi, V^{-*}\psi)$ is valid for any invertible operator.

Bayes predictor. With the assumption in Eq. (15.2) above, we can now express the optimal predictor in Eq. (15.1) as:

$$f^*(x) \in \arg \min_{z \in \mathcal{Y}} \left\langle \varphi(z), \int_{\mathcal{Y}} \psi(y) dp(y|x) \right\rangle. \quad (15.3)$$

Thus, to obtain Fisher consistency, it is sufficient to estimate well the conditional expectation $\int_{\mathcal{Y}} \psi(y) dp(y|x) \in \mathcal{H}$; this is what smooth surrogates will do in Section 15.3. However, what is only needed is in fact sufficient knowledge of this conditional expectation to perform the computation of $f^*(x)$ above. This will lead to non-smooth surrogates in Section 15.4.

Examples. We can now revisit the list of losses described in Section 15.1.1 to check if a SELF decomposition exists. In our analysis, we will need a bound on $R_\ell = \sup_{z \in \mathcal{Y}} \|\varphi(z)\|$, which we also provide here.

- **Binary classification**, with $\mathcal{Y} \in \{-1, 1\}$ and the 0-1 loss: $\mathcal{H} = \mathbb{R}$, $\varphi(y) = -y/2$ and $\psi(z) = z$, since $\ell(y, z) = 1_{y \neq z} = \frac{1}{2} - \frac{yz}{2}$.
- **Multi-category classification**: $\mathcal{Y} = \{1, \dots, k\}$ and a loss matrix $L \in \mathbb{R}^{k \times k}$, with $\ell(i, j) = L_{ij}$. This corresponds to the usual “one-hot” encoding of discrete distributions, where $\psi(i) \in \mathbb{R}^k$ is the i -th element of the canonical basis. We then have $\ell(i, j) = L_{ij} = \psi(i)^\top L \psi(j)$, that is, $\varphi(j) = L \psi(j)$. For this case, we have $R_\ell = \sup_{j \in \{1, \dots, k\}} \|L(:, j)\|_2$. In particular, for the 0-1 loss, we have $L_{ij} = 1_{i \neq j}$, and we can write $\ell(i, j) = 1 - \psi(i)^\top \psi(j)$, and we can take $\varphi(i) = -\psi(i)$.
- **Robust regression**: $\mathcal{Y} = \mathbb{R}$, with the loss $\ell(y, z) = 1 - \exp[-(y - z)^2]$, which can be written as, using the Fourier transform, $\ell(y, z) = 1 - \frac{1}{2\sqrt{\pi}} \int_{-\infty}^{\infty} \exp(-\omega^2/4) \cos \omega(x - z) d\omega$, which leads to the existence of an infinite-dimensional \mathcal{H} .

Indeed, we can select \mathcal{H} to be the set of square integrable functions from \mathbb{R} to \mathbb{R}^2 , with $\psi(y)(\omega) = e^{-\omega^2/8} \begin{pmatrix} \cos \omega y \\ \sin \omega y \end{pmatrix}$, and $\varphi(z)(\omega) = -\frac{1}{2\sqrt{\pi}} e^{-\omega^2/8} \begin{pmatrix} \cos \omega z \\ \sin \omega z \end{pmatrix}$, leading to $R_\ell^2 = \frac{1}{4\pi} \int_{-\infty}^{\infty} \exp(-\omega^2/4) = \frac{1}{2\sqrt{\pi}}$.

- **Multiple labels:** for $\mathcal{Y} = \{-1, 1\}^k$, the traditional Hamming loss can be rewritten as $\ell(y, z) = \frac{k}{2} - \frac{1}{2} y^\top z$. We then have, $\psi(y) = y$ and $\varphi(z) = -z/2$, and $R_\ell = \sqrt{m}$.
- **Permutations:** for the pairwise disagreement, we have directly $\mathcal{H} = \mathbb{R}^k$ with $k = m(m-1)$, with $\psi(y)_{ij} = 1_{y(i)>y(j)}$ and $\varphi(z)_{ij} = 1_{z(i)<z(j)}$ for $i \neq j$, and $R_\ell \leq m$.

 Like for binary classification or regression, the choice of the loss is independent of the function space which is considered (local averaging, kernels, neural nets).

15.2 Surrogate methods

In this section, our main concerns will be to obtain consistent convex surrogates, convex so that we can run efficient algorithms from Chapter 5, consistent so that we are sure that given sufficient amounts of data and sufficiently flexible models, predictions are optimal.

15.2.1 Score functions and decoding step

Binary classification. In this book, we have performed binary classification by learning a real-valued function $g : \mathcal{X} \rightarrow \mathbb{R}$, and then predicting with $f(x) = \text{sign}(g(x)) \in \{-1, 1\}$. In the language of this chapter, we have learned a real-valued score function and applied a specific decoding step from \mathbb{R} to $\{-1, 1\}$ (the sign function). We now present the general surrogate framework.

General surrogate framework. In this chapter, we will consider functions $f : \mathcal{X} \rightarrow \mathcal{Y}$ that can be written as:

$$f(x) = \text{dec} \circ g(x),$$

where

- $g : \mathcal{X} \rightarrow \mathcal{H}$ is a function with values in the vector space \mathcal{H} , referred to as a score function.¹

¹In statistics, the score function often refers to the gradient of the log-density with respect to parameters. There is no link between these two definitions.

- $\text{dec} : \mathcal{H} \rightarrow \mathcal{Y}$ is the decoding function.

We then need a surrogate loss $S : \mathcal{Y} \times \mathcal{H} \rightarrow \mathbb{R}$, that will be used to form empirical and expected surrogate risks:

$$\hat{\mathcal{R}}_S(g) = \frac{1}{n} \sum_{i=1}^n S(y_i, g(x_i)) \quad \text{and} \quad \mathcal{R}_S(g) = \mathbb{E}[S(y, g(x))].$$

For binary classification where $\mathcal{Y} = \{-1, 1\}$, we had $S(y, g(x)) = \Phi(yg(x))$ for Φ a convex function.

15.2.2 Fisher consistency and calibration functions

Following the same definition as in Section 4.1, we denote \mathcal{R}_S^* the minimum S -risk, that is the infimum over all functions from \mathcal{X} to \mathcal{H} of $\mathcal{R}_S(g) = \mathbb{E}[S(y, g(x))]$. It is equal to:

$$\mathcal{R}_S^* = \mathbb{E}\left[\inf_{h \in \mathcal{H}} \mathbb{E}[S(y, h)|x]\right].$$

The loss is said “Fisher-consistent” if we can get an arbitrary small excess risk $\mathcal{R}(f) - \mathcal{R}^*$ for $f = \text{dec} \circ g$, as soon as the excess S -risk of g is sufficiently small. In other words, perfectly minimizing the S -risk should lead to the Bayes predictor.

A stronger property that enables to transfer convergence rates for the excess S -risk to the excess risk is the existence of a *calibration function*, that is, an increasing function $H : \mathbb{R}_+ \rightarrow \mathbb{R}_+$ such that $\mathcal{R}(\text{dec} \circ g) - \mathcal{R}^* \leq H[\mathcal{R}_S(g) - \mathcal{R}_S^*]$.

15.2.3 Main surrogate frameworks

As described in Section 4.1, for binary classification, we saw two classes of convex surrogates:

- Smooth surrogates, where the predictor minimizing the expected surrogate risk led to a complete description of the conditional distribution of y given x , that is, since we had only two outcomes, knowledge of $\mathbb{E}[y|x]$. Classic examples were the square loss and the logistic loss. Then, when going from the excess surrogate risk to the true excess risk, the calibration function was the square root.
- Non-smooth surrogates, where the predictor minimizing the expected surrogate risk already provided a thresholded version, that is, $\text{sign}(\mathbb{E}[y|x])$. The calibration function, however, did not exhibit a square root behavior but rather a (better) linear behavior.

In this chapter, we will present extensions of these two sets of surrogates: (1) least-squares (or more generally smooth surrogates), (2) max-margin (non-smooth that estimates the discrete estimator directly), as they come with efficient algorithms and guarantees. But there are other related frameworks that we will not study (Osokin et al., 2017; Lee et al., 2004; Blondel et al., 2020). In particular, probabilistic graphical models in the form of conditional random fields are popular (Sutton et al., 2012).

15.3 Smooth/quadratic surrogates

We first look at a class of techniques that extends the square and logistic losses beyond binary classification for the whole class of structure encoding loss functions. We first start with quadratic surrogates, following Ciliberto et al. (2020), where the analysis is the simplest and most elegant.

15.3.1 Quadratic surrogate

Given the SELF decomposition in Eq. (15.2), we consider estimating a score function $g : \mathcal{X} \rightarrow \mathcal{H}$ with the following surrogate function:

$$S(y, g(x)) = \|\psi(y) - g(x)\|^2,$$

for the Hilbert norm $\|\cdot\|$. In other words, we aim at directly estimating $\mathbb{E}[\psi(y)|x]$ for every $x \in \mathcal{X}$. The decoding function is then naturally

$$\text{dec}(s) \in \arg \min_{z \in \mathcal{Y}} \langle \varphi(z), g(x) \rangle,$$

since, when $g(x) = \mathbb{E}[\psi(y)|x]$, it leads to $\arg \min_{z \in \mathcal{Y}} \mathbb{E}[\langle \varphi(z), \psi(y) \rangle | x] = \arg \min_{z \in \mathcal{Y}} \mathbb{E}[\ell(y, z) | x]$, which is the optimal predictor.

For the binary classification case, it leads to the square loss framework from Section 4.1.1, but in the general case, it extends to the many situations alluded to earlier. The decoding steps will be described in Section 15.3.3.

15.3.2 Theoretical guarantees

For the framework proposed above, we can prove a precise calibration result by leveraging the properties of the square loss. We first notice that

$$\mathcal{R}_S(g) - \mathcal{R}_S^* = \mathbb{E} \left[\|g(x) - \mathbb{E}[\psi(y)|x]\|^2 \right]. \quad (15.4)$$

Moreover, by construction, the function defined by $g^*(x) = \mathbb{E}[\psi(y)|x]$ is the minimizer of the expected S -risk, and the Bayes predictor is indeed $f^* = \text{dec} \circ g^*$.

We can then express the excess risk using the decomposition of the loss as:

$$\begin{aligned}
& \mathcal{R}(\text{dec} \circ g) - \mathcal{R}^* \\
&= \mathcal{R}(\text{dec} \circ g) - \mathcal{R}(\text{dec} \circ g^*) \\
&= \mathbb{E}\left[\mathbb{E}[\ell(y, \text{dec} \circ g(x)) - \ell(y, \text{dec} \circ g^*(x))|x]\right] \\
&= \mathbb{E}\left[\mathbb{E}[\langle \psi(y), \varphi(\text{dec} \circ g(x)) - \varphi(\text{dec} \circ g^*(x)) \rangle|x]\right] \text{ by the SELF decomposition,} \\
&= \mathbb{E}\left[\langle \mathbb{E}[\psi(y)|x], \varphi(\text{dec} \circ g(x)) - \varphi(\text{dec} \circ g^*(x)) \rangle\right] \text{ by moving expectations,} \\
&= \mathbb{E}\left[\langle \mathbb{E}[\psi(y)|x] - \mathbf{g}(x), \varphi(\text{dec} \circ g(x)) - \varphi(\text{dec} \circ g^*(x)) \rangle\right] \\
&\quad + \mathbb{E}\left[\langle \mathbf{g}(x), \varphi(\text{dec} \circ g(x)) - \varphi(\text{dec} \circ g^*(x)) \rangle\right],
\end{aligned}$$

by adding and subtracting $\mathbf{g}(x)$. The definition of the decoding function implies the negativity of the second term. Thus, we get:

$$\begin{aligned}
\mathcal{R}(\text{dec} \circ g) - \mathcal{R}^* &\leq \mathbb{E}\left[\langle \mathbb{E}[\psi(y)|x] - g(x), \varphi(\text{dec} \circ g(x)) - \varphi(\text{dec} \circ g^*(x)) \rangle\right] \\
&\leq 2 \sup_{z \in \mathcal{Y}} \|\varphi(z)\| \cdot \mathbb{E}\left[\|\mathbb{E}[\psi(y)|x] - g(x)\|\right] \text{ using Cauchy-Schwarz inequality,} \\
&\leq 2 \sup_{z \in \mathcal{Y}} \|\varphi(z)\| \cdot \sqrt{\mathbb{E}\left[\|\mathbb{E}[\psi(y)|x] - g(x)\|^2\right]} \text{ using Jensen's inequality,} \\
&= 2R_\ell \cdot \sqrt{\mathcal{R}_S(g) - \mathcal{R}_S^*} \text{ because of Eq. (15.4),}
\end{aligned}$$

which is exactly a calibration function result. A key feature of this result is that the constant R_ℓ typically does not explode, even for sets \mathcal{Y} with large cardinality (see examples in Section 15.1.2). To get a learning bound, we then need to use learning bounds for multivariate least-squares regression, which behave similarly to univariate least-squares regression. For example, if we assume that the target function $g^*(x) = \mathbb{E}[\psi(y)|x]$ from $\mathcal{X} \rightarrow \mathcal{H}$ is in the space of functions that we are using for learning, then penalized least-squares with the proper choice of regularization parameter will lead to explicit convergence rates. Otherwise, we need to let the parameter go to zero to obtain universal consistency. See Ciliberto et al. (2020) for more details.

15.3.3 Linear estimators and decoding steps

When the function g is linear in the observations $\psi(y_i)$, $i = 1, \dots, n$ (e.g., local averaging methods from Section 6.2.1, or kernel methods from Section 7.6.1), that is,

$$g(x) = \sum_{i=1}^n w_i(x) \psi(y_i),$$

for well-defined functions $w_i : \mathcal{X} \rightarrow \mathbb{R}$, we see that the decoding step is

$$\text{dec}(s) \in \arg \min_{z \in \mathcal{Y}} \left\langle \varphi(z), \sum_{i=1}^n w_i(x) \psi(y_i) \right\rangle = \arg \min_{z \in \mathcal{Y}} \sum_{i=1}^n w_i(x) \ell(y_i, z), \quad (15.5)$$

that is, there is no need to know the decomposition of the loss to run the algorithm. This makes the decoding step even easier, with the following examples:

- **Robust regression:** $\mathcal{Y} = \mathbb{R}$, with the loss $\ell(y, z) = 1 - \exp[-(y - z)^2]$. Eq. (15.5) then leads to

$$\arg \max_{z \in \mathbb{R}} \sum_{i=1}^n w_i(x) \exp[-(y_i - z)^2],$$

which is a one-dimensional optimization problem that can be solved by grid search.

- **Multi-category classification:** $\mathcal{Y} = \{1, \dots, k\}$ and a loss matrix $L \in \mathbb{R}^{k \times k}$, with $\ell(i, j) = L_{ij}$. Eq. (15.5) then leads to $\arg \max_{z \in \{1, \dots, k\}} \sum_{i=1}^n w_i(x) L_{iz}$.

- **Multiple labels:** $\mathcal{Y} = \{-1, 1\}^k$ with $\ell(y, z) = \frac{k}{2} - \frac{1}{2} y^\top z$. Eq. (15.5) then leads to $\arg \max_{z \in \{-1, 1\}^k} z^\top \sum_{i=1}^n w_i(x) y_i$, which leads to a closed-form formula for z .

- **Permutations:** for the pairwise disagreement, the optimization problem does not have a closed form anymore and is an instance of a hard combinatorial problem (“minimum weighted feedback arc set”), which can be solved for small m , and with simple approximation algorithms otherwise (see Ciliberto et al., 2020).

15.3.4 Smooth surrogates (♦)

Following Nowak-Vila et al. (2019) and as done in Section 4.1, we can also consider smooth surrogate functions of the form:

$$S(y, g(x)) = c(y) - 2\langle \psi(y), g(x) \rangle + 2a(g(x)),$$

where $a : \mathcal{H} \rightarrow \mathbb{R}$ is convex and β -smooth, that is, for any $h, h' \in \mathcal{H}$, $a(h') \leq a(h) + \langle a'(h), h' - h \rangle + \frac{\beta}{2} \|h - h'\|^2$. We also assume that $a(0) = 0$ and that the domain of its Fenchel conjugate includes all $\psi(y)$ for $y \in \mathcal{Y}$. The square loss corresponds to $a(h) = \frac{1}{2}\|h\|^2$ and $c(y) = \|\psi(y)\|^2$.

We consider the decoding function $\text{dec} : \mathcal{H} \rightarrow \mathcal{Y}$ equal to

$$\text{dec}(h) \in \arg \min_{z \in \mathcal{H}} \varphi(z)^\top a'(h).$$

For the square loss, we recover exactly the quadratic surrogate. We then have, by definition of the Fenchel-conjugate $a^*(u) = \sup_{h \in \mathcal{H}} \langle u, h \rangle - a(h)$:

$$\begin{aligned} \mathcal{R}_S(g) &= \mathbb{E}[\mathbb{E}[c(y)|x] - 2\langle \mathbb{E}[\psi(y)|y], g(x) \rangle + 2a(g(x))] \\ \mathcal{R}_S^* &= \mathbb{E}[\mathbb{E}[c(y)|x] + \inf_{h \in \mathcal{H}} -2\langle \mathbb{E}[\psi(y)|x], h \rangle + 2a(h)] \\ &= \mathbb{E}[\mathbb{E}[c(y)|x] - 2a^*(\mathbb{E}[\psi(y)|x])], \text{ by definition of } a^*, \end{aligned}$$

leading to a compact expression of the excess S -risk and a lower bound:

$$\begin{aligned} \mathcal{R}_S(g) - \mathcal{R}_S^* &= \mathbb{E}[-2\langle \mathbb{E}[\psi(y)|x], g(x) \rangle + 2a(g(x)) + 2a^*(\mathbb{E}[\psi(y)|x])] \\ &\geq \frac{1}{\beta} \mathbb{E}[\|\textcolor{red}{a}'(g(x)) - \mathbb{E}[\psi(y)|x]\|^2], \end{aligned}$$

where we have used the $(1/\beta)$ -strong-convexity of a^* .

Moreover, like in the previous section, we can express the excess risk as:

$$\begin{aligned} \mathcal{R}(\text{dec} \circ g) - \mathcal{R}^* &= \mathcal{R}(\text{dec} \circ g) - \mathcal{R}(\text{dec} \circ g^*) \\ &= \mathbb{E}[\mathbb{E}[\ell(y, \text{dec} \circ g(x)) - \ell(y, \text{dec} \circ g^*(x))|x]] \\ &= \mathbb{E}[\mathbb{E}[\langle \psi(y), \varphi(\text{dec} \circ g(x)) - \varphi(\text{dec} \circ g^*(x)) \rangle|x]] \\ &= \mathbb{E}[\langle \mathbb{E}[\psi(y)|x], \varphi(\text{dec} \circ g(x)) - \varphi(\text{dec} \circ g^*(x)) \rangle] \\ &= \mathbb{E}[\langle \mathbb{E}[\psi(y)|x] - \textcolor{red}{a}'(g(x)), \varphi(\text{dec} \circ g(x)) - \varphi(\text{dec} \circ g^*(x)) \rangle] \\ &\quad + \mathbb{E}[\langle \textcolor{red}{a}'(g(x)), \varphi(\text{dec} \circ g(x)) - \varphi(\text{dec} \circ g^*(x)) \rangle]. \end{aligned}$$

By definition of the decoding step, we get:

$$\begin{aligned} \mathcal{R}(\text{dec} \circ g) - \mathcal{R}^* &\leq \mathbb{E}[\langle \mathbb{E}[\psi(y)|x] - \textcolor{red}{a}'(g(x)), \varphi(\text{dec} \circ g(x)) - \varphi(\text{dec} \circ g^*(x)) \rangle] \\ &\leq 2 \sup_{z \in \mathcal{Y}} \|\varphi(z)\| \cdot \mathbb{E}[\|\mathbb{E}[\psi(y)|x] - \textcolor{red}{a}'(g(x))\|] \\ &\leq 2 \sup_{z \in \mathcal{Y}} \|\varphi(z)\| \cdot \sqrt{\mathbb{E}[\|\mathbb{E}[\psi(y)|x] - g(x)\|^2]} = 2\sqrt{\beta} R_\ell \cdot \sqrt{\mathcal{R}_S(g) - \mathcal{R}_S^*}, \end{aligned}$$

We thus have the same calibration function as for the quadratic surrogate but with an extra factor of $\sqrt{\beta}$. For example, this applies to softmax regression.

15.4 Max-margin formulations

Rather than extending the square or logistic loss from binary classification to structured prediction, we can also extend the hinge loss, leading to “max-margin formulations” in reference to the geometric interpretation from Section 4.1.2. In this section, we assume that for any $y \in \mathcal{Y}$, $z \mapsto \ell(z, y)$ is minimized at y , that is, the loss provides a measure of dissimilarity with y .

15.4.1 Structured SVM

Following Taskar et al. (2005); Tsochantaridis et al. (2005), we consider a traditional extension of the support vector machine with a simple interpretation.

We consider a score function which is a function of $x \in \mathcal{X}$ and $y \in \mathcal{Y}$, with the decoder $\arg \max_{z \in \mathcal{Y}} h(x, z)$. The score $S(y, h(x, \cdot))$ is defined as the minimal $\xi \in \mathbb{R}_+$ such that for all $z \in \mathcal{Y}$,

$$h(x, y) \geq h(x, z) + \ell(z, y) - \ell(y, y) - \xi.$$

The intuition behind this definition is that we aim at making $h(x, y)$ larger for the observed y than for the other $h(x, z)$, with a difference that is stronger when y and z are further apart, as measured by the loss.

If we take the particular form $h(x, z) = \langle \psi(z), g(x) \rangle$ for $g : \mathcal{X} \rightarrow \mathcal{H}$, then the constraint becomes

$$\langle \psi(y), g(x) \rangle \geq \langle \psi(z), g(x) \rangle + \langle \varphi(y), \psi(z) \rangle - \langle \varphi(y), \psi(y) \rangle - \xi,$$

which is equivalent to

$$\xi \geq \langle \psi(z) - \psi(y), \varphi(y) + g(x) \rangle,$$

and thus the score function is:

$$S(y, g(x)) = \max_{z \in \mathcal{Y}} \langle \psi(z) - \psi(y), \varphi(y) + g(x) \rangle. \quad (15.6)$$

For binary classification with the 0-1 loss, this recovers exactly the SVM. Moreover, this convex loss is computable as soon as we can maximize linear functions of $\varphi(z)$; thus, this applies to many combinatorial problems, in particular those described earlier.

However, this approach is not consistent; that is, even in the population case where the test distribution is known, it does not lead to the optimal predictor in general; note that there are subcases, such as multi-category classification with the 0-1 loss and a “majority class”, where the approach is consistent (Liu, 2007) (see exercise below).

Exercise 15.1 (♦) For the multi-category classification with the 0–1 loss, show that the structural SVM is Fisher-consistent if for all $x \in \mathcal{X}$, $\max_{j \in \{1, \dots, k\}} \mathbb{P}(y = j|x) > \frac{1}{2}$.

15.4.2 Max-min formulations (♦♦)

Following Fathony et al. (2016); Nowak-Vila et al. (2020), we can provide a non-smooth surrogate, which is both consistent and comes with a calibration function that does not have a square root.

We consider the convex function $a : \mathcal{H} \rightarrow \mathbb{R}$ defined through its Fenchel conjugate defined on the domain $\mathcal{M}(\psi)$ as:

$$a^*(\mu) = -\min_{y' \in \mathcal{Y}} \langle \varphi(y'), \mu \rangle,$$

where $\mathcal{M}(\psi) \subset \mathcal{H}$ is the closure of the convex hull of all $\psi(z), z \in \mathcal{Y}$.

The key property is that its subdifferential at $\mu \in \mathcal{M}(\psi) \subset \mathcal{H}$ is exactly the convex hull of all maximizers of $-\langle h, \mu \rangle$, for $h = \varphi(y') \in \mathcal{H}$ for some $y' \in \mathcal{Y}$.

We then consider the score function $S(y, g(x)) = a(g(x)) - \langle g(x), \psi(y) \rangle$, which can be expressed as, using Fenchel duality:

$$\begin{aligned} S(y, g(x)) &= \max_{\mu \in \mathcal{M}(\psi)} \langle g(x), \mu \rangle + \min_{y' \in \mathcal{Y}} \langle \varphi(y'), \mu \rangle - \langle g(x), \psi(y) \rangle \\ &= \max_{\mu \in \mathcal{M}(\psi)} \min_{y' \in \mathcal{Y}} \langle g(x) + \varphi(y'), \mu - \psi(y) \rangle + \ell(y, y'). \end{aligned}$$

Given this score function, we consider the decoder function

$$\text{dec} \circ g(x) \in \arg \max_{y' \in \mathcal{Y}} \psi(y')^\top g(x),$$

taking any arbitrary elements within maximizers.

Note the similarity with the maximum-margin SVM loss in Eq. (15.6), which considers $y' = y$ instead of the minimization with respect to $y' \in \mathcal{Y}$. This extra minimization makes the surrogate loss function more complicated to minimize (though it is still convex) but leads to a Fisher-consistent estimator.

Fisher consistency. We now prove that any minimizer g^* of $\mathbb{E}[S(y, g(x))]$ over all measurable functions from \mathcal{X} to \mathcal{H} leads to the optimal prediction, with

$$\text{dec} \circ g^*(x) = \arg \max_{y' \in \mathcal{Y}} \psi(y')^\top g^*(x) = f^*(x).$$

As in Section 15.3.4, for $x \in \mathcal{X}$, any minimizer g^* has a value $g^*(x)$ that minimizes

$$\mathbb{E}[S(y, g(x))|x] = a(g(x)) - \langle g(x), \mathbb{E}[\psi(y)|x] \rangle.$$

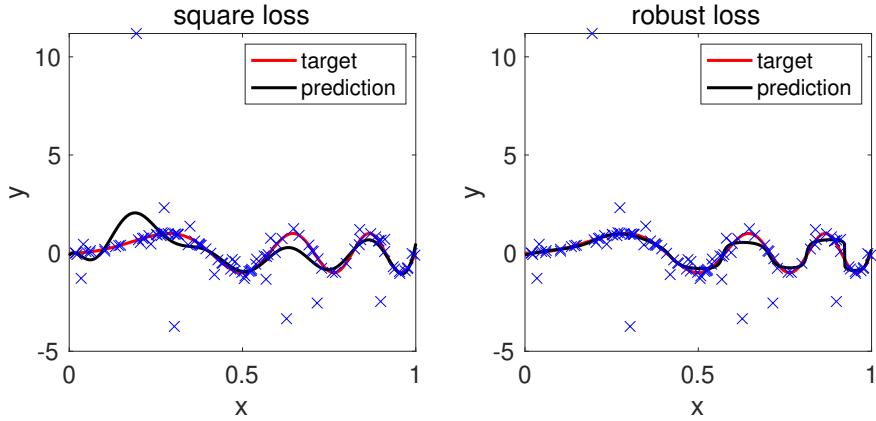


Figure 15.1: Robust regression in one dimension, with heavy-tail noise (fifth power of Gaussian noise): regular square loss (left), vs. robust loss (right).

By definition of a , $g^*(x)$ is a minimizer of $h \mapsto \langle h, \mathbb{E}[\psi(y)|x] \rangle$ over $h \in \mathcal{M}(\varphi)$. Thus, given the expression of the Bayes predictor in Eq. (15.3), we get $g^*(x) = \varphi(f^*(x)) \in \mathcal{H}$. This leads to $\text{dec} \circ g^*(x) = f^*(x)$ because of the assumption that $z \mapsto \ell(z, y)$ is minimized at y .

We can also get a linear calibration function in generic situations; see [Nowak-Vila et al. \(2020\)](#) for details.

Binary classification with the 0-1 loss. In this situation, we can compute $a^*(\mu) = \frac{1}{2}|\mu|$ with domain $[-1, 1]$, leading to $a(v) = (|v| - 1/2)_+$, and a formulation that is close to the binary SVM (but non-identical).

Exercise 15.2 Compute the function a^* and a for the multi-category classification problem with the 0-1 loss.

15.5 Experiments

We consider a toy robust regression problem to illustrate the use of the quadratic surrogates presented in Section 15.3.1. We use a simple one-dimensional robust regression problem, where we compare the square loss and the loss $\ell(y, z) = 1 - \exp(-(y - z)^2)$. We generate data with heavy-tail additive noise and plot below with best performance for kernel ridge regression with the Gaussian kernel, with the optimal regularization parameter (selected for test performance). See results in Figure 15.1.

15.6 Conclusion

In this chapter, we explored surrogate frameworks beyond binary classification, focusing on convex surrogates. These convex formulations can be used with any prediction functions (linear in the parameter or not) and come with guarantees for linear models. Alternative formulations based on smoothing directly non-convex losses exist (see, e.g., [Berthet et al., 2020](#), and references therein), but currently come with no guarantee.

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