Modern Statistical Methods

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Course webpage:
http://www.statslab.cam.ac.uk/~sb2116/modern_stat_methods.html

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Over the last 25 years, the sorts of datasets that statisticians have been challenged to study have changed greatly. Where in the past, we were used to datasets with many observations with a few carefully chosen variables, we are now seeing datasets where the number of variables can run into the thousands and greatly exceed the number of observations. For example, with microarray data, we typically have gene expression values measured for several thousands of genes, but only for a few hundred tissue samples. The classical statistical methods are often simply not applicable in these "high-dimensional" situations.

The course is divided into 4 chapters (of unequal size). Our first chapter will start by introducing ridge regression, a simple generalisation of ordinary least squares. Our study of this will lead us to some beautiful connections with functional analysis and ultimately one of the most successful and flexible classes of learning algorithms: kernel machines.

The second chapter concerns the Lasso and its extensions. The Lasso has been at the centre of much of the developments that have occurred in high-dimensional statistics, and will allow us to perform regression in the seemingly hopeless situation when the number of parameters we are trying to estimate is larger than the number of observations.

In the third chapter, we will study the estimation of covariance matrices from i.i.d. random vectors. The sample covariance is our main estimator and bounding its error in the operator norm requires understanding the spectrum of random matrices, which will give us a taste of an exciting area of probability theory. Principal components analysis (PCA) is a classical technique for dimensionality reduction based on projecting the data on the dominant eigenspace of the covariance matrix. We will see that PCA is inconsistent in truly high-dimensional problems where the dimension of the samples is larger than the number of samples, and we will study Sparse PCA as an answer to this problem.

Statistics is not only about developing methods that can predict well in the presence of noise, but also about assessing the uncertainty in our predictions and estimates. In the final chapter we will tackle the problem of how to handle performing thousands of hypothesis tests at the same time and more generally the task of quantifying uncertainty in high-dimensional settings.

Before we begin the course proper, we will briefly review two key classical statistical methods: ordinary least squares and maximum likelihood estimation. This will help to set

the scene and provide a warm-up for the modern methods to come later.

Classical statistics

Ordinary least squares

Imagine data are available in the form of observations $(Y_i, x_i) \in \mathbb{R} \times \mathbb{R}^p$, $i = 1, \ldots, n$, and the aim is to infer a simple *regression function* relating the average value of a *response*, Y_i, and a collection of *predictors* or *variables*, x_i. This is an example of regression analysis, one of the most important tasks in statistics.

A *linear model* for the data assumes that it is generated according to

$$Y = X\beta^0 + \varepsilon, \tag{0.0.1}$$

where $Y \in \mathbb{R}^n$ is the vector of responses; $X \in \mathbb{R}^{n \times p}$ is the predictor matrix (or design matrix) with ith row x_i^T; $\varepsilon \in \mathbb{R}^n$ represents random error; and $\beta^0 \in \mathbb{R}^p$ is the unknown vector of coefficients.

Provided $p \ll n$, a sensible way to estimate β is by ordinary least squares (OLS). This yields an estimator $\hat{\beta}^{\mathrm{OLS}}$ with

$$\hat{\beta}^{\mathrm{OLS}} := \underset{\beta \in \mathbb{R}^p}{\arg\min} \, \|Y - X\beta\|_2^2 = (X^T X)^{-1} X^T Y, \tag{0.0.2}$$

provided X has full column rank.

Under the assumptions that (i) $\mathbb{E}(\varepsilon_i) = 0$ and (ii) $\mathrm{Var}(\varepsilon) = \sigma^2 I$, we have that:

- $\mathbb{E}_{\beta^0, \sigma^2}(\hat{\beta}^{\mathrm{OLS}}) = \mathbb{E}\{(X^T X)^{-1} X^T (X\beta^0 + \varepsilon)\} = \beta^0$.
- $\mathrm{Var}_{\beta^0, \sigma^2}(\hat{\beta}^{\mathrm{OLS}}) = (X^T X)^{-1} X^T \mathrm{Var}(\varepsilon) X (X^T X)^{-1} = \sigma^2 (X^T X)^{-1}$.

The Gauss–Markov theorem states that OLS is the best linear unbiased estimator in our setting: for any other estimator $\tilde{\beta}$ that is linear in Y (so $\tilde{\beta} = AY$ for some fixed matrix A), we have

$$\mathrm{Var}_{\beta^0, \sigma^2}(\tilde{\beta}) - \mathrm{Var}_{\beta^0, \sigma^2}(\hat{\beta}^{\mathrm{OLS}})$$

is positive semi-definite.

Maximum likelihood estimation

The method of least squares is just one way to construct as estimator. A more general technique is that of maximum likelihood estimation. Here given data $y \in \mathbb{R}^n$ that we take as a realisation of a random variable Y, we specify its density $f(y; \theta)$ up to some unknown vector of parameters $\theta \in \Theta \subseteq \mathbb{R}^d$, where Θ is the parameter space. The likelihood function is a function of θ for each fixed y given by

$$L(\theta) := L(\theta; y) = c(y) f(y; \theta),$$

where $c(y)$ is an arbitrary constant of proportionality. The maximum likelihood estimate of θ maximises the likelihood, or equivalently it maximises the log-likelihood

$$\ell(\theta) := \ell(\theta; y) = \log f(y; \theta) + \log(c(y)).$$

A very useful quantity in the context of maximum likelihood estimation is the *Fisher information* matrix with jkth ($1 \leq j, k \leq d$) entry

$$i_{jk}(\theta) := -\mathbb{E}_\theta \left\{ \frac{\partial^2}{\partial\theta_j \partial\theta_k} \ell(\theta) \right\}.$$

It can be thought of as a measure of how hard it is to estimate θ when it is the true parameter value. The Cramér–Rao lower bound states that if $\tilde{\theta}$ is an unbiased estimator of θ, then under regularity conditions,

$$\mathrm{Var}_\theta(\tilde{\theta}) - i^{-1}(\theta)$$

is positive semi-definite.

A remarkable fact about maximum likelihood estimators (MLEs) is that (under quite general conditions) they are asymptotically normally distributed, asymptotically unbiased and asymptotically achieve the Cramér–Rao lower bound.

Assume that the Fisher information matrix when there are n observations, $i^{(n)}(\theta)$ (where we have made the dependence on n explicit) satisfies $i^{(n)}(\theta)/n \to I(\theta)$ for some positive definite matrix I. Then denoting the maximum likelihood estimator of θ when there are n observations by $\hat{\theta}^{(n)}$, under regularity conditions, as the number of observations $n \to \infty$ we have

$$\sqrt{n}(\hat{\theta}^{(n)} - \theta) \xrightarrow{d} N_d(0, I^{-1}(\theta)).$$

Returning to our linear model, if we assume in addition that $\varepsilon_i \sim N(0, \sigma^2)$, then the log-likelihood for (β, σ^2) is

$$\ell(\beta, \sigma^2) = -\frac{n}{2}\log(\sigma^2) - \frac{1}{2\sigma^2}\sum_{i=1}^{n}(y_i - x_i^T\beta)^2.$$

We see that the maximum likelihood estimate of β and OLS coincide. It is easy to check that

$$i(\beta, \sigma^2) = \begin{pmatrix} \sigma^{-2}X^TX & 0 \\ 0 & n\sigma^{-4}/2 \end{pmatrix}.$$

The general theory for MLEs would suggest that approximately $\sqrt{n}(\hat{\beta}-\beta) \sim N_p(0, n\sigma^2(X^TX)^{-1})$; in fact it is straight-forward to show that this distributional result is exact.

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Chapter 1

Kernel machines

Let us revisit the linear model with

$$Y_i = x_i^T \beta^0 + \varepsilon_i.$$

For unbiased estimators of β^0, their variance gives a way of comparing their quality in terms of squared error loss. For a potentially biased estimator, $\tilde{\beta}$, the relevant quantity is

$$\begin{aligned}\mathbb{E}_{\beta^0,\sigma^2}\{(\tilde{\beta}-\beta^0)(\tilde{\beta}-\beta^0)^T\} &= \mathbb{E}[\{\tilde{\beta}-\mathbb{E}(\tilde{\beta})+\mathbb{E}(\tilde{\beta})-\beta^0\}\{\tilde{\beta}-\mathbb{E}(\tilde{\beta})+\mathbb{E}(\tilde{\beta})-\beta^0\}^T] \\ &= \mathrm{Var}(\tilde{\beta}) + \{\mathbb{E}(\tilde{\beta}-\beta^0)\}\{\mathbb{E}(\tilde{\beta}-\beta^0)\}^T,\end{aligned}$$

a sum of squared bias and variance terms. A crucial part of the optimality arguments for OLS and MLEs was *unbiasedness*. Do there exist biased methods whose variance is is reduced compared to OLS such that their overall prediction error is lower? Yes!—in fact the use of biased estimators is essential in dealing with settings where the number of parameters to be estimated is large compared to the number of observations. In the first two chapters we'll explore two important methods for variance reduction based on different forms of penalisation: rather than forming estimators via optimising a least squares or log-likelihood term, we will introduce an additional penalty term that encourages estimates to be shrunk towards 0 in some sense. This will allow us to produce reliable estimators that work well when classical MLEs are infeasible, and in other situations can greatly out-perform the classical approaches.

1.1 Ridge regression

One way to reduce the variance of $\hat{\beta}^{\mathrm{OLS}}$ is to shrink the estimated coefficients towards 0. *Ridge regression* [Hoerl and Kennard, 1970] does this by solving the following optimisation problem

$$(\hat{\mu}_\lambda^{\mathrm{R}}, \hat{\beta}_\lambda^{\mathrm{R}}) = \underset{(\mu,\beta)\in\mathbb{R}\times\mathbb{R}^p}{\arg\min}\ \{\|Y-\mu\mathbf{1}-X\beta\|_2^2 + \lambda\|\beta\|_2^2\}.$$

Here $\mathbf{1}$ is an n-vector of 1's. We see that the usual OLS objective is penalised by an additional term proportional to $\|\beta\|_2^2$. The parameter $\lambda \geq 0$, which controls the severity of

the penalty and therefore the degree of the shrinkage towards 0, is known as a *regularisation parameter* or *tuning parameter*. We have explicitly included an intercept term which is not penalised. The reason for this is that were the variables to have their origins shifted so e.g. a variable representing temperature is given in units of Kelvin rather than Celsius, the fitted values would not change. However, $X\hat{beta}$ is not invariant under scale transformations of the variables so it is standard practice to centre each column of $\mathbf{X}$ (hence making them orthogonal to the intercept term) and then scale them to have ℓ_2-norm $\sqrt{n}$.

It is straightforward to show that after this standardisation of X, $\hat{\mu}_\lambda^{\mathrm{R}} = \bar{Y} := \sum_{i=1}^n Y_i/n$, so we may assume that $\sum_{i=1}^n Y_i = 0$ by replacing Y_i by $Y_i - \bar{Y}$ and then we can remove μ from our objective function. In this case

$$\hat{\beta}_\lambda^{\mathrm{R}} = (X^T X + \lambda I)^{-1} X^T Y.$$

In this form, we can see how the addition of the λI term helps to stabilise the estimator. Note that when X does not have full column rank (such as in high-dimensional situations), we can still compute this estimator. On the other hand, when X does have full column rank, we have the following theorem.

Theorem 1. *For λ sufficiently small (depending on β^0 and σ^2),*

$$\mathbb{E}(\hat{\beta}^{\mathrm{OLS}} - \beta^0)(\hat{\beta}^{\mathrm{OLS}} - \beta^0)^T - \mathbb{E}(\hat{\beta}_\lambda^{\mathrm{R}} - \beta^0)(\hat{\beta}_\lambda^{\mathrm{R}} - \beta^0)^T$$

is positive definite.

Proof. First we compute the bias of $\hat{\beta}_\lambda^{\mathrm{R}}$. We drop the subscript λ and superscript R for convenience.

$$\begin{aligned}
\mathbb{E}(\hat{\beta}) - \beta^0 &= (X^T X + \lambda I)^{-1} X^T X \beta^0 - \beta^0 \\
&= (X^T X + \lambda I)^{-1} (X^T X + \lambda I - \lambda I)\beta^0 - \beta^0 \\
&= -\lambda (X^T X + \lambda I)^{-1} \beta^0.
\end{aligned}$$

Now we look at the variance of $\hat{\beta}$.

$$\begin{aligned}
\mathrm{Var}(\hat{\beta}) &= \mathbb{E}\{(X^T X + \lambda I)^{-1} X^T \varepsilon\}\{(X^T X + \lambda I)^{-1} X^T \varepsilon\}^T \\
&= \sigma^2 (X^T X + \lambda I)^{-1} X^T X (X^T X + \lambda I)^{-1}.
\end{aligned}$$

Thus $\mathbb{E}(\hat{\beta}^{\mathrm{OLS}} - \beta^0)(\hat{\beta}^{\mathrm{OLS}} - \beta^0)^T - \mathbb{E}(\hat{\beta} - \beta^0)(\hat{\beta} - \beta^0)^T$ is equal to

$$\sigma^2 (X^T X)^{-1} - \sigma^2 (X^T X + \lambda I)^{-1} X^T X (X^T X + \lambda I)^{-1} - \lambda^2 (X^T X + \lambda I)^{-1} \beta^0 {\beta^0}^T (X^T X + \lambda I)^{-1}.$$

After some simplification, we see that this is equal to

$$\lambda (X^T X + \lambda I)^{-1} [\sigma^2 \{2I + \lambda (X^T X)^{-1}\} - \lambda \beta^0 {\beta^0}^T] (X^T X + \lambda I)^{-1}.$$

Thus $\mathbb{E}(\hat{\beta}^{\mathrm{OLS}} - \beta^0)(\hat{\beta}^{\mathrm{OLS}} - \beta^0)^T - \mathbb{E}(\hat{\beta} - \beta^0)(\hat{\beta} - \beta^0)^T$ is positive definite for $\lambda > 0$ if and only if

$$\sigma^2 \{2I + \lambda (X^T X)^{-1}\} - \lambda \beta^0 {\beta^0}^T$$

is positive definite, which is true for $\lambda > 0$ sufficiently small (we can take $0 < \lambda < 2\sigma^2 / \|\beta^0\|_2^2$). □

The theorem says that $\hat{\beta}_\lambda^{\mathrm{R}}$ outperforms $\hat{\beta}^{\mathrm{OLS}}$ provided λ is chosen appropriately. To be able to use ridge regression effectively, we need a way of selecting a good λ—we will come to this very shortly. What the theorem doesn't really tell us is in what situations we expect ridge regression to perform well. To understand that, we will turn to one of the key matrix decompositions used in statistics, the singular value decomposition (SVD).

1.1.1 The singular value decomposition and principal components analysis

The singular value decomposition (SVD) is a generalisation of an eigendecomposition of a square matrix. We can factorise any $X \in \mathbb{R}^{n\times p}$ into its SVD

$$X = UDV^T.$$

Here the $U \in \mathbb{R}^{n\times n}$ and $V \in \mathbb{R}^{p\times p}$ are orthogonal matrices and $D \in \mathbb{R}^{n\times p}$ has $D_{11} \geq D_{22} \geq \cdots \geq D_{mm} \geq 0$ where $m := \min(n, p)$ and all other entries of D are zero. To compute such a decomposition requires $O(np\min(n, p))$ operations. The rth columns of U and V are known as the rth left and right singular vectors of X respectively, and D_{rr} is the rth singular value.

When $n > p$, we can replace U by its first p columns and D by its first p rows to produce another version of the SVD (sometimes known as the thin SVD). Then $X = UDV^T$ where $U \in \mathbb{R}^{n\times p}$ has orthonormal columns (but is no longer square) and D is square and diagonal. There is an equivalent version for when $p > n$.

Let us take $X \in \mathbb{R}^{n\times p}$ as our matrix of predictors and suppose $n \geq p$. Using the (thin) SVD we may write the fitted values from ridge regression as follows.

$$\begin{aligned} X\hat{\beta}_\lambda^{\mathrm{R}} &= X(X^TX + \lambda I)^{-1}X^TY \\ &= UDV^T(VD^2V^T + \lambda I)^{-1}VDU^TY \\ &= UD(D^2 + \lambda I)^{-1}DU^TY \\ &= \sum_{j=1}^{p} U_j \frac{D_{jj}^2}{D_{jj}^2 + \lambda} U_j^TY. \end{aligned}$$

Here we have used the notation (that we shall use throughout the course) that U_j is the jth column of U. For comparison, the fitted values from OLS (when X has full column rank) are

$$X\hat{\beta}^{\mathrm{OLS}} = X(X^TX)^{-1}X^TY = UU^TY.$$

Both OLS and ridge regression compute the coordinates of Y with respect to the columns of U. Ridge regression then shrinks these coordinates by the factors $D_{jj}^2/(D_{jj}^2 + \lambda)$; if D_{jj} is small, the amount of shrinkage will be larger.

To interpret this further, note that the SVD is intimately connected with Principal Components Analysis (PCA). Consider $v \in \mathbb{R}^p$ with $\|v\|_2 = 1$. Since the columns of X

have had their means subtracted, the sample variance of $Xv \in \mathbb{R}^n$, is

$$\frac{1}{n} v^T X^T X v = \frac{1}{n} v^T V D^2 V^T v.$$

Writing $a = V^T v$, so $\|a\|_2 = 1$, we have

$$\frac{1}{n} v^T V D^2 V^T v = \frac{1}{n} a^T D^2 a = \frac{1}{n} \sum_j a_j^2 D_{jj}^2 \leq \frac{1}{n} D_{11} \sum_j a_j^2 = \frac{1}{n} D_{11}^2.$$

As $\|XV_1\|_2^2/n = D_{11}^2/n$, V_1 determines the linear combination of the columns of X which has the largest sample variance, when the coefficients of the linear combination are constrained to have ℓ_2-norm 1. $XV_1 = D_{11}U_1$ is known as the first principal component of X. Subsequent principal components $D_{22}U_2, \ldots, D_{pp}U_p$ have maximum variance D_{jj}^2/n, subject to being orthogonal to all earlier ones—see example sheet 1 for details.

Returning to ridge regression, we see that it shrinks Y most in the smaller principal components of X. Thus it will work well when most of the signal is in the large principal components of X. We now turn to the problem of choosing λ.

1.2 v-fold cross-validation

Cross-validation is a general technique for selecting a good regression method from among several competing regression methods. We illustrate the principle with ridge regression, where we have a family of regression methods given by different λ values.

So far, we have considered the matrix of predictors X as fixed and non-random. However, in many cases, it makes sense to think of it as random. Let us assume that our data are i.i.d. pairs (x_i, Y_i), $i = 1, \ldots, n$. Then ideally, we might want to pick a λ value such that

$$\mathbb{E}\{(Y^* - x^{*T}\hat{\beta}_\lambda^{\mathrm{R}}(X, Y))^2 | X, Y\} \tag{1.2.1}$$

is minimised. Here $(x^*, Y^*) \in \mathbb{R}^p \times \mathbb{R}$ is independent of (X, Y) and has the same distribution as (x_1, Y_1), and we have made the dependence of $\hat{\beta}_\lambda^{\mathrm{R}}$ on the training data (X, Y) explicit. This λ is such that conditional on the original *training* data, it minimises the expected prediction error on a new observation drawn from the same distribution as the training data.

A less ambitious goal is to find a λ value to minimise the expected prediction error,

$$\mathbb{E}[\mathbb{E}\{(Y^* - x^{*T}\hat{\beta}_\lambda^{\mathrm{R}}(X, Y))^2 | X, Y\}] \tag{1.2.2}$$

where compared with (1.2.1), we have taken a further expectation over the training set.

We still have no way of computing (1.2.2) directly, but we can attempt to estimate it. The idea of v-fold cross-validation is to split the data into v groups or folds of roughly equal size: $(X^{(1)}, Y^{(1)}), \ldots, (X^{(v)}, Y^{(v)})$. Let $(X^{(-k)}, Y^{(-k)})$ be all the data except that in the kth fold. For each λ on a grid of values, we compute $\hat{\beta}_\lambda^{\mathrm{R}}(X^{(-k)}, Y^{(-k)})$: the ridge regression

estimate based on all the data except the kth fold. Writing $\kappa(i)$ for the fold to which (x_i, Y_i) belongs, we choose the value of λ that minimises

$$\mathrm{CV}(\lambda) = \frac{1}{n}\sum_{i=1}^{n}\{Y_i - x_i^T\hat{\beta}^{\mathrm{R}}_{\lambda}(X^{(-\kappa(i))}, Y^{(-\kappa(i))})\}^2. \tag{1.2.3}$$

Writing λ_{CV} for the minimiser, our final estimate of β^0 can then be $\hat{\beta}^{R}_{\lambda_{\mathrm{CV}}}(X, Y)$.

Note that for each i,

$$\mathbb{E}\{Y_i - x_i^T\hat{\beta}^{\mathrm{R}}_{\lambda}(X^{(-\kappa(i))}, Y^{(-\kappa(i))})\}^2 = \mathbb{E}[\mathbb{E}\{Y_i - x_i^T\hat{\beta}^{\mathrm{R}}_{\lambda}(X^{(-\kappa(i))}, Y^{(-\kappa(i))})\}^2 | X^{(-\kappa(i))}, Y^{(-\kappa(i))}]. \tag{1.2.4}$$

This is precisely the expected prediction error in (1.2.2) but with the training data X, Y replaced with a training data set of smaller size. If all the folds have the same size, then $\mathrm{CV}(\lambda)$ is an average of n identically distributed quantities, each with expected value as in (1.2.4). However, the quantities being averaged are not independent as they share the same data.

Thus cross-validation gives a biased estimate of the expected prediction error. The amount of the bias depends on the size of the folds, the case when the $v = n$ giving the least bias—this is known as leave-one-out cross-validation. The quality of the estimate, though, may be worse as the quantities being averaged in (1.2.3) will be highly positively correlated. Typical choices of v are 5 or 10.

Cross-validation aims to allow us to choose the single best λ (or more generally regression procedure); we could instead aim to find the best weighted combination of regression procedures. Returning to our ridge regression example, suppose λ is restricted to a grid of values $\lambda_1 > \lambda_2 > \cdots > \lambda_L$. We can then minimise

$$\frac{1}{n}\sum_{i=1}^{n}\left\{Y_i - \sum_{l=1}^{L} w_l x_i^T\hat{\beta}^{\mathrm{R}}_{\lambda_l}(X^{(-\kappa(i))}, Y^{(-\kappa(i))})\right\}^2$$

over $w \in \mathbb{R}^L$ subject to $w_l \geq 0$ for all l. This is a non-negative least-squares optimisation, for which efficient algorithms are available. This is known as *stacking* [Wolpert, 1992, Breiman, 1996] and it can often outperform cross-validation.

1.3 The kernel trick

The fitted values from ridge regression are

$$X(X^TX + \lambda I)^{-1}X^TY. \tag{1.3.1}$$

An alternative way of writing this is suggested by the following

$$\begin{aligned} X^T(XX^T + \lambda I) &= (X^TX + \lambda I)X^T \\ (X^TX + \lambda I)^{-1}X^T &= X^T(XX^T + \lambda I)^{-1} \\ X(X^TX + \lambda I)^{-1}X^TY &= XX^T(XX^T + \lambda I)^{-1}Y. \end{aligned} \tag{1.3.2}$$

Two remarks are in order:

- Note while X^TX is $p \times p$, XX^T is $n \times n$. Computing fitted values using (1.3.1) would require roughly $O(np^2 + p^3)$ operations. If $p \gg n$ this could be extremely costly. However, our alternative formulation would only require roughly $O(n^2p + n^3)$ operations, which could be substantially smaller.

- We see that the fitted values of ridge regression depend only on inner products $K = XX^T$ between observations (note $K_{ij} = x_i^T x_j$).

Now suppose that we believe the signal depends quadratically on the predictors:

$$Y_i = x_i^T \beta + \sum_{k,l} x_{ik} x_{il} \theta_{kl} + \varepsilon_i.$$

We can still use ridge regression provided we work with an enlarged set of predictors

$$x_{i1}, \ldots, x_{ip}, x_{i1}x_{i1}, \ldots, x_{i1}x_{ip}, x_{i2}x_{i1}, \ldots, x_{i2}x_{ip}, \ldots, x_{ip}x_{ip}.$$

This will give us $O(p^2)$ predictors. Our new approach to computing fitted values would therefore have complexity $O(n^2p^2 + n^3)$, which could be rather costly if p is large.

However, rather than first creating all the additional predictors and then computing the new K matrix, we can attempt to directly compute K. To this end consider

$$\begin{aligned}(1 + x_i^T x_j)^2 &= \left(1 + \sum_k x_{ik} x_{jk}\right)^2 \\ &= 1 + 2\sum_k x_{ik} x_{jk} + \sum_{k,l} x_{ik} x_{il} x_{jk} x_{jl}.\end{aligned}$$

Observe this amounts to an inner product between vectors of the form

$$(1, \sqrt{2}x_{i1}, \ldots, \sqrt{2}x_{ip}, x_{i1}x_{i1}, \ldots, x_{i1}x_{ip}, x_{i2}x_{i1}, \ldots, x_{i2}x_{ip}, \ldots, x_{ip}x_{ip})^T. \tag{1.3.3}$$

Thus if we set

$$K_{ij} = (1 + x_i^T x_j)^2 \tag{1.3.4}$$

and plug this into the formula for the fitted values, it is *exactly* as if we had performed ridge regression on an enlarged set of variables given by (1.3.3). Now computing K using (1.3.4) would require only p operations per entry, so $O(n^2p)$ operations in total. It thus seems we have improved things by a factor of p using our new approach. This is a nice computational trick, but more importantly for us it serves to illustrate some general points.

- Since ridge regression only depends on inner products between observations, rather than fitting non-linear models by first mapping the original data $x_i \in \mathbb{R}^p$ to $\phi(x_i) \in \mathbb{R}^d$ (say) using some *feature map* ϕ (which could, for example introduce quadratic effects), we can instead try to directly compute $k(x_i, x_j) = \langle \phi(x_i), \phi(x_j) \rangle$.

- In fact rather than thinking in terms of feature maps, we can instead try to think about an appropriate measure of similarity $k(x_i, x_j)$ between observations. Modelling in this fashion is sometimes much easier.

We will now formalise and extend what we have learnt with this example.

1.4 Kernels

We have seen how a model with quadratic effects can be fitted very efficiently by replacing the inner product matrix (known as the *Gram matrix*) XX^T in (1.3.2) with the matrix in (1.3.4). It is then natural to ask what other non-linear models can be fitted efficiently using this sort of approach.

We won't answer this question directly, but instead we will try to understand the sorts of similarity measures k that can be represented as inner products between transformations of the original data.

That is, we will study the similarity measures $k : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$ from the input space $\mathcal{X}$ to $\mathbb{R}$ for which there exists a *feature map* $\phi : \mathcal{X} \to \mathcal{H}$ where $\mathcal{H}$ is some (real) inner product space with

$$k(x, x') = \langle \phi(x), \phi(x') \rangle. \tag{1.4.1}$$

Recall that an inner product space is a real vector space $\mathcal{H}$ endowed with a map $\langle \cdot, \cdot \rangle : \mathcal{H} \times \mathcal{H} \to \mathbb{R}$ that obeys the following properties.

(i) Symmetry: $\langle u, v \rangle = \langle v, u \rangle$.

(ii) Linearity: for $a, b \in \mathbb{R}$ $\langle au + bw, v \rangle = a\langle u, v \rangle + b\langle w, v \rangle$.

(iii) Positive-definiteness: $\langle u, u \rangle \geq 0$ with equality if and only if $u = 0$.

Definition 1. A *positive definite kernel* or more simply a *kernel* (for brevity) k is a symmetric map $k : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$ for which for all $n \in \mathbb{N}$ and all $x_1, \ldots, x_n \in \mathcal{X}$, the matrix K with entries

$$K_{ij} = k(x_i, x_j)$$

is positive semi-definite.

A kernel is a little like an inner product, but need not be bilinear in general. However, a form of the Cauchy–Schwarz inequality does hold for kernels.

Proposition 2.

$$k(x, x')^2 \leq k(x, x)k(x', x').$$

Proof. The matrix

$$\begin{pmatrix} k(x, x) & k(x, x') \\ k(x', x) & k(x', x') \end{pmatrix}$$

must be positive semi-definite so in particular its determinant must be non-negative. □

First we show that any inner product of feature maps will give rise to a kernel.

Proposition 3. *k defined by $k(x, x') = \langle \phi(x), \phi(x') \rangle$ is a kernel.*

Proof. Let $x_1, \dots, x_n \in \mathcal{X}$, $\alpha_1, \dots, \alpha_n \in \mathbb{R}$ and consider

$$\begin{aligned}\sum_{i,j} \alpha_i k(x_i, x_j) \alpha_j &= \sum_{i,j} \alpha_i \langle \phi(x_i), \phi(x_j) \rangle \alpha_j \\ &= \left\langle \sum_i \alpha_i \phi(x_i), \sum_j \alpha_j \phi(x_j) \right\rangle \geq 0.\end{aligned}$$

□

Showing that every kernel admits a representation of the form (1.4.1) is slightly more involved, and we delay this until after we have studied some examples.

1.4.1 Examples of kernels

Proposition 4. *Suppose $k_1, k_2, \dots$ are kernels.*

(i) If $\alpha_1, \alpha_2 \geq 0$ then $\alpha_1 k_1 + \alpha_2 k_2$ is a kernel. If $\lim_{m\to\infty} k_m(x, x') =: k(x, x')$ exists for all $x, x' \in \mathcal{X}$, then k is a kernel.

(ii) The pointwise product $k = k_1 k_2$ is a kernel.

Linear kernel. $k(x, x') = x^T x'$.

Polynomial kernel. $k(x, x') = (1 + x^T x')^d$. To show this is a kernel, we can simply note that $1 + x^T x'$ gives a kernel owing to the fact that 1 is a kernel and (i) of Proposition 4. Next (ii) and induction shows that k as defined above is a kernel.

Gaussian kernel. The highly popular Gaussian kernel is defined by

$$k(x, x') = \exp\left(- \frac{\|x - x'\|_2^2}{2\sigma^2} \right).$$

For x close to x' it is large whilst for x far from x' the kernel quickly decays towards 0. The additional parameter σ^2 known as the *bandwidth* controls the speed of the decay to zero. Note it is less clear how one might find a corresponding feature map and indeed any feature map that represents this must be infinite dimensional.

To show that it is a kernel first decompose $\|x - x'\|_2^2 = \|x\|_2^2 + \|x'\|_2^2 - 2x^T x'$. Note that by Proposition 3,

$$k_1(x, x') = \exp\left(- \frac{\|x\|_2^2}{2\sigma^2} \right) \exp\left(- \frac{\|x'\|_2^2}{2\sigma^2} \right)$$

is a kernel. Next writing

$$k_2(x, x') = \exp(x^T x'/\sigma^2) = \sum_{r=0}^{\infty} \frac{(x^T x'/\sigma^2)^r}{r!}$$

and using (i) of Proposition 4 shows that k_2 is a kernel. Finally observing that $k = k_1 k_2$ and using (ii) shows that the Gaussian kernel is indeed a kernel.

Sobolev kernel. Take $\mathcal{X}$ to be $[0,1]$ and let $k(x,x') = \min(x,x')$. Note this is the covariance function of Brownian motion so it must be positive definite.

Jaccard similarity kernel. Take $\mathcal{X}$ to be the set of all subsets of $\{1,\dots,p\}$. For $x, x' \in \mathcal{X}$ with $x \cup x' \neq \emptyset$ define

$$k(x,x') = \frac{|x \cap x'|}{|x \cup x'|}$$

and if $x \cup x' = \emptyset$ then set $k(x,x') = 1$. Showing that this is a kernel is left to the example sheet.

1.4.2 Reproducing kernel Hilbert spaces

Theorem 5. *For every kernel k there exists a feature map ϕ taking values in some inner product space $\mathcal{H}$ such that*

$$k(x,x') = \langle \phi(x), \phi(x') \rangle. \tag{1.4.2}$$

Proof. We will take $\mathcal{H}$ to be the vector space of functions of the form

$$f(\cdot) = \sum_{i=1}^{n} \alpha_i k(\cdot, x_i), \tag{1.4.3}$$

where $n \in \mathbb{N}$, $x_i \in \mathcal{X}$ and $\alpha_i \in \mathbb{R}$. Our feature map $\phi : \mathcal{X} \to \mathcal{H}$ will be

$$\phi(x) = k(\cdot, x). \tag{1.4.4}$$

We now define an inner product on $\mathcal{H}$. If f is given by (1.4.3) and

$$g(\cdot) = \sum_{j=1}^{m} \beta_j k(\cdot, x'_j) \tag{1.4.5}$$

we define their inner product to be

$$\langle f, g \rangle = \sum_{i=1}^{n} \sum_{j=1}^{m} \alpha_i \beta_j k(x_i, x'_j). \tag{1.4.6}$$

We need to check this is well-defined as the representations of f and g in (1.4.3) and (1.4.5) need not be unique. To this end, note that

$$\sum_{i=1}^{n} \sum_{j=1}^{m} \alpha_i \beta_j k(x_i, x'_j) = \sum_{i=1}^{n} \alpha_i g(x_i) = \sum_{j=1}^{m} \beta_j f(x'_j). \tag{1.4.7}$$

The first equality shows that the inner product does not depend on the particular expansion of g whilst the second equality shows that it also does not depend on the expansion of f. Thus the inner product is well-defined.

First we check that with ϕ defined as in (1.4.4) we do have relationship (1.4.2). Observe that

$$\langle k(\cdot, x), f\rangle = \sum_{i=1}^{n} \alpha_i k(x_i, x) = f(x), \tag{1.4.8}$$

so in particular we have

$$\langle \phi(x), \phi(x')\rangle = \langle k(\cdot, x), k(\cdot, x')\rangle = k(x, x').$$

It remains to show that it is indeed an inner product. It is clearly symmetric and (1.4.7) shows linearity. We now need to show positive definiteness.

First note that

$$\langle f, f\rangle = \sum_{i,j} \alpha_i k(x_i, x_j)\alpha_j \geq 0 \tag{1.4.9}$$

by positive definiteness of the kernel. Now from (1.4.8),

$$f(x)^2 = (\langle k(\cdot, x), f\rangle)^2.$$

If we could use the Cauchy–Schwarz inequality on the right-hand side, we would have

$$f(x)^2 \leq \langle k(\cdot, x), k(\cdot, x)\rangle\langle f, f\rangle, \tag{1.4.10}$$

which would show that if $\langle f, f\rangle = 0$ then necessarily $f = 0$; the final property we need to show that $\langle \cdot, \cdot\rangle$ is an inner product. However, in order to use the traditional Cauchy–Schwarz inequality we need to first know we're dealing with an inner product, which is precisely what we're trying to show!

Although we haven't shown that $\langle \cdot, \cdot\rangle$ is an inner product, we do have enough information to show that it is itself a kernel. We may then appeal to Proposition 2 to obtain (1.4.10). With this in mind, we argue as follows. Given functions $f_1, \ldots, f_m$ and coefficients $\gamma_1, \ldots, \gamma_m \in \mathbb{R}$, we have

$$\sum_{i,j} \gamma_i \langle f_i, f_j\rangle \gamma_j = \left\langle \sum_i \gamma_i f_i, \sum_j \gamma_j f_j \right\rangle \geq 0$$

where we have used linearity and (1.4.9), showing that it is a kernel. □

To further discuss the space $\mathcal{H}$ we recall some facts from analysis. Any inner product space $\mathcal{B}$ is also a normed space: for $f \in \mathcal{B}$ we may define $\|f\|_{\mathcal{B}}^2 := \langle f, f\rangle_{\mathcal{B}}$. Recall that a Cauchy sequence $(f_m)_{m=1}^{\infty}$ in $\mathcal{B}$ has $\|f_m - f_n\|_{\mathcal{B}} \to 0$ as $n, m \to \infty$. A normed space where every Cauchy sequence has a limit (in the space) is called *complete*, and a complete inner product space is called a *Hilbert space*.

Hilbert spaces may be thought of as the (potentially) infinite-dimensional analogues of finite-dimensional Euclidean spaces. For later use we note that if V is a closed subspace of a Hilbert space $\mathcal{B}$, then any $f \in \mathcal{B}$ has a decomposition $f = u + v$ with $u \in V$ and

$$v \in V^{\perp} := \{v \in \mathcal{B} : \langle v, u\rangle_{\mathcal{B}} = 0 \text{ for all } u \in V\}.$$

By adding the limits of Cauchy sequences to $\mathcal{H}$ (from Theorem 5) we can make $\mathcal{H}$ a Hilbert space. Indeed, note that if $(f_m)_{m=1}^{\infty} \in \mathcal{H}$ is Cauchy then since by (1.4.10) we have

$$|f_m(x) - f_n(x)| \leq \sqrt{k(x,x)}\|f_m - f_n\|_{\mathcal{H}},$$

we may define function $f^* : \mathcal{X} \to \mathbb{R}$ by $f^*(x) = \lim_{m\to\infty} f_m(x)$. We can check that all such f^* can be added to $\mathcal{H}$ to create a Hilbert space.

In fact, the completion of $\mathcal{H}$ is a special type of Hilbert space known as a *reproducing kernel Hilbert space* (RKHS).

Definition 2. A Hilbert space $\mathcal{B}$ of functions $f : \mathcal{X} \to \mathbb{R}$ is a *reproducing kernel Hilbert space* (RKHS) if for all $x \in \mathcal{X}$, there exists $k_x \in \mathcal{B}$ such that

$$f(x) = \langle k_x, f\rangle \qquad \text{for all } f \in \mathcal{B}.$$

The function

$$\begin{aligned} k : \mathcal{X} \times \mathcal{X} &\to \mathbb{R} \\ (x, x') &\mapsto \langle k_x, k_{x'}\rangle = k_{x'}(x) \end{aligned}$$

is known as the *reproducing kernel* of $\mathcal{B}$.

By Proposition 3 the reproducing kernel of any RKHS is a (positive definite) kernel, and Theorem 5 shows that to any kernel k is associated a (unique) RKHS that has reproducing kernel k.

Examples

Linear kernel. Here $\mathcal{H} = \{f : f(x) = \beta^T x,\, \beta \in \mathbb{R}^p\}$ and if $f(x) = \beta^T x$ then $\|f\|_{\mathcal{H}}^2 = \|\beta\|_2^2$.

Sobolev kernel. It can be shown that $\mathcal{H}$ is roughly the space of continuous functions $f : [0,1] \to \mathbb{R}$ with $f(0) = 0$ that are differentiable almost everywhere, and for which $\int_0^1 f'(x)^2 dx < \infty$. It contains the class of Lipschitz functions (functions $f : [0,1] \to \mathbb{R}$ for which there exists some L with $|f(x) - f(y)| \leq L|x - y|$ for all $x, y \in [0,1]$) that are 0 at the origin. The norm is

$$\left(\int_0^1 f'(x)^2 dx\right)^{1/2}.$$

Though the construction of the RKHS from a kernel is explicit, it can be challenging to understand precisely the space and the form of the norm.

1.4.3 The representer theorem

To recap, what we have shown so far is that replacing the matrix XX^T in the definition of an algorithm by K derived form a positive definite kernel is essentially equivalent to running the same algorithm on some mapping of the original data, though with the modification that instances of $x_i^T x_j$ become $\langle \phi(x_i), \phi(x_j) \rangle$.

But what exactly is the optimisation problem we are solving when performing kernel ridge regression? Clearly it is determined by the kernel or equivalently by the RKHS. Note we know that an alternative way of writing the usual ridge regression optimisation is

$$\arg\min_{f \in \mathcal{H}} \left\{ \sum_{i=1}^{n} \{Y_i - f(x_i)\}^2 + \lambda \|f\|_{\mathcal{H}}^2 \right\} \tag{1.4.11}$$

where $\mathcal{H}$ is the RKHS corresponding to the linear kernel. The following theorem shows in particular that kernel ridge regression (i.e. ridge regression replacing XX^T with K) with kernel k is equivalent to the above with $\mathcal{H}$ now being the RKHS corresponding to k.

Theorem 6 (Representer theorem, [Kimeldorf and Wahba, 1970, Schölkopf et al., 2001])**.** *Let $c : \mathbb{R}^n \times \mathcal{X}^n \times \mathbb{R}^n \to \mathbb{R}$ be an arbitrary loss function, and let $J : [0, \infty) \to \mathbb{R}$ be strictly increasing. Let $x_1, \ldots, x_n \in \mathcal{X}$, $Y \in \mathbb{R}^n$. Finally, let $f \in \mathcal{H}$ where $\mathcal{H}$ is an RKHS with reproducing kernel k, and let $K_{ij} = k(x_i, x_j)$ $i, j = 1, \ldots, n$. Then $\hat{f}$ minimises*

$$Q_1(f) := c(Y, x_1, \ldots, x_n, f(x_1), \ldots, f(x_n)) + J(\|f\|_{\mathcal{H}}^2)$$

over $f \in \mathcal{H}$ iff. $\hat{f}(\cdot) = \sum_{i=1}^n \hat{\alpha}_i k(\cdot, x_i)$ and $\hat{\alpha} \in \mathbb{R}^n$ minimises Q_2 over $\alpha \in \mathbb{R}^n$ where

$$Q_2(\alpha) = c(Y, x_1, \ldots, x_n, K\alpha) + J(\alpha^T K \alpha).$$

Proof. Suppose $\hat{f}$ minimises Q_1. We may write $\hat{f} = u + v$ where $u \in V := \text{span}\{k(\cdot, x_1), \ldots, k(\cdot, x_n)\}$ and $v \in V^\perp$. Then

$$\hat{f}(x_i) = \langle k(\cdot, x_i), u + v \rangle = \langle k(\cdot, x_i), u \rangle = u(x_i).$$

Meanwhile, by Pythagoras' theorem we have $J(\|\hat{f}\|_{\mathcal{H}}^2) = J(\|u\|_{\mathcal{H}}^2 + \|v\|_{\mathcal{H}}^2) \geq J(\|u\|_{\mathcal{H}}^2)$ with equality iff. $v = 0$. Thus by optimality of $\hat{f}$, $v = 0$, so $\hat{f}(\cdot) = \sum_{i=1}^n \alpha_i k(\cdot, x_i)$ for $\alpha \in \mathbb{R}^n$. Now observe that if $\hat{f}$ takes this form, then $\|\hat{f}\|_{\mathcal{H}}^2 = \alpha^T K \alpha$, so $Q_1(\hat{f}) = Q_2(\alpha)$. Then by optimality of $\hat{f}$, we have that α must minimise Q_2.

Now suppose $\hat{\alpha}$ minimises Q_2 and $\hat{f}(\cdot) = \sum_{i=1}^n \hat{\alpha}_i k(\cdot, x_i)$. Note that $Q_1(\hat{f}) = Q_2(\hat{\alpha})$. If $\tilde{f} \in \mathcal{H}$ has $Q_1(\tilde{f}) \leq Q_1(\hat{f})$, by the argument above, writing $\tilde{f} = u + v$ with $u \in V$, $v \in V^\perp$, we know that $Q_1(u) \leq Q_1(\tilde{f})$. But by optimality of $\hat{\alpha}$ we have $Q_1(\hat{f}) \leq Q_1(u)$, so $Q_1(\hat{f}) = Q_1(\tilde{f})$. □

Consider the result specialised the ridge regression objective. We see that (1.4.11) is essentially equivalent to minimising

$$\|Y - K\alpha\|_2^2 + \lambda \alpha^T K \alpha,$$

and you may check (see example sheet 1) that the minimiser $\hat{\alpha}$ satisfies $K\hat{\alpha} = K(K + \lambda I)^{-1}Y$. Thus (1.4.11) is indeed an alternative way of expressing kernel ridge regression.

Viewing the result in the opposite direction gives a more "sensational" perspective. If you had set out trying to minimise Q_1, it might appear completely hopeless as $\mathcal{H}$ could be infinite-dimensional. However, somewhat remarkably we see that this reduces to finding the coefficients $\hat{\alpha}_i$ which solve the simple(r) optimisation problem Q_2.

The result also tells us how to form predictions: given a new observation x, our prediction for $f(x)$ is

$$\hat{f}(x) = \sum_{i=1}^{n} \hat{\alpha}_i k(x, x_i).$$

1.5 Kernel ridge regression

We have seen how the kernel trick allows us to solve a potentially infinite-dimensional version of ridge regression. This may seem impressive, but ultimately we should judge kernel ridge regression on its statistical properties e.g. predictive performance. Consider a setting where

$$Y_i = f^0(x_i) + \varepsilon_i, \qquad \mathbb{E}(\varepsilon) = 0,\ \mathrm{Var}(\varepsilon) = \sigma^2 I.$$

We shall assume that $f^0 \in \mathcal{H}$ where $\mathcal{H}$ is an RKHS with reproducing kernel k. By scaling σ^2, we may assume $\|f^0\|_{\mathcal{H}} \leq 1$. Let K be the kernel matrix $K_{ij} = k(x_i, x_j)$ with eigenvalues $d_1 \geq d_2 \geq \cdots \geq d_n \geq 0$. We will see that the predictive performance depends delicately on these eigenvalues.

Let $\hat{f}_\lambda$ be the estimated regression function from kernel ridge regression with kernel k:

$$\hat{f}_\lambda = \operatorname*{arg\,min}_{f \in \mathcal{H}} \left\{ \sum_{i=1}^{n} \{Y_i - f(x_i)\}^2 + \lambda \|f\|_{\mathcal{H}}^2 \right\}.$$

Theorem 7. *The mean squared prediction error (MSPE) may be bounded above in the following way:*

$$\begin{aligned} \frac{1}{n}\mathbb{E}\left\{ \sum_{i=1}^{n} \{f^0(x_i) - \hat{f}_\lambda(x_i)\}^2 \right\} &\leq \frac{\sigma^2}{n} \sum_{i=1}^{n} \frac{d_i^2}{(d_i + \lambda)^2} + \frac{\lambda}{4n} \\ &\leq \frac{\sigma^2}{n} \frac{1}{\lambda} \sum_{i=1}^{n} \min(d_i/4, \lambda) + \frac{\lambda}{4n}. \end{aligned} \tag{1.5.1}$$

Proof. We know from the representer theorem that

$$\left(\hat{f}_\lambda(x_1), \ldots, \hat{f}_\lambda(x_n)\right)^T = K(K + \lambda I)^{-1} Y.$$

You will show on the example sheet that

$$\left(f^0(x_1), \ldots, f^0(x_n)\right)^T = K\alpha,$$

for some $\alpha \in \mathbb{R}^n$, and moreover that $\|f^0\|_{\mathcal{H}}^2 \geq \alpha^T K \alpha$. Let the eigendecomposition of K be given by $K = UDU^T$ with $D_{ii} = d_i$ and define $\theta = U^T K \alpha$. We see that n times the LHS of (1.5.1) is

$$\begin{aligned}\mathbb{E}\|K(K+\lambda I)^{-1}(U\theta+\varepsilon) - U\theta\|_2^2 &= \mathbb{E}\|DU^T(UDU^T+\lambda I)^{-1}(U\theta+\varepsilon) - \theta\|_2^2 \\ &= \mathbb{E}\|D(D+\lambda I)^{-1}(\theta + U^T\varepsilon) - \theta\|_2^2 \\ &= \|\{D(D+\lambda I)^{-1} - I\}\theta\|_2^2 + \mathbb{E}\|D(D+\lambda I)^{-1}U^T\varepsilon\|_2^2.\end{aligned}$$

To compute the second term, we use the 'trace trick':

$$\begin{aligned}\mathbb{E}\|D(D+\lambda I)^{-1}U^T\varepsilon\|_2^2 &= \mathbb{E}[\{D(D+\lambda I)^{-1}U^T\varepsilon\}^T D(D+\lambda I)^{-1}U^T\varepsilon] \\ &= \mathbb{E}[\mathrm{tr}\{D(D+\lambda I)^{-1}U^T\varepsilon\varepsilon^T UD(D+\lambda I)^{-1}\}] \\ &= \sigma^2 \mathrm{tr}\{D(D+\lambda I)^{-1}D(D+\lambda I)^{-1}\} \\ &= \sigma^2 \sum_{i=1}^n \frac{d_i^2}{(d_i+\lambda)^2}.\end{aligned}$$

For the first term, we have

$$\|\{D(D+\lambda I)^{-1} - I\}\theta\|_2^2 = \sum_{i=1}^n \frac{\lambda^2\theta_i^2}{(d_i+\lambda)^2}.$$

Now as $\theta = DU^T\alpha$ note that $\theta_i = 0$ when $d_i = 0$. Let D^+ be the diagonal matrix with ith diagonal entry equal to D_{ii}^{-1} if $D_{ii} > 0$ and 0 otherwise. Then

$$\sum_{i:d_i>0} \frac{\theta_i^2}{d_i} = \|\sqrt{D^+}\theta\|_2^2 = \alpha^T KUD^+U^TK\alpha = \alpha^T UDD^+DU^T\alpha = \alpha^T K\alpha \leq 1.$$

By Hölder's inequality we have

$$\sum_{i=1}^n \frac{\theta_i^2}{d_i}\frac{d_i\lambda^2}{(d_i+\lambda)^2} \leq \max_{i=1,\ldots,n} \frac{d_i\lambda^2}{(d_i+\lambda)^2} \leq \lambda/4,$$

using the inequality $(a+b)^2 \geq 4ab$ in the final line. Finally note that

$$\frac{d_i^2}{(d_i+\lambda)^2} \leq \min\{1, d_i^2/(4d_i\lambda)\} = \min(\lambda, d_i/4)/\lambda. \qquad \square$$

To interpret this result further, it will be helpful to express it in terms of $\hat{\mu}_i := d_i/n$ (the eigenvalues of K/n) and $\lambda_n := \lambda/n$. We have

$$\frac{1}{n}\mathbb{E}\Big\{\sum_{i=1}^n \{f^0(x_i) - \hat{f}_\lambda(x_i)\}^2\Big\} \leq \frac{\sigma^2}{\lambda_n}\frac{1}{n}\sum_{i=1}^n \min(\hat{\mu}_i/4, \lambda_n) + \lambda_n/4 =: \delta_n(\lambda_n). \qquad (1.5.2)$$

Here we have treated the x_i as fixed, but we could equally well think of them as random. Consider a setup where the x_i are i.i.d. and independent of ε. If we take a further expectation on the RHS of (1.5.2), our result still holds true (the $\hat{\mu}_i$ are random in this setting). Ideally we would like to then replace $\mathbb{E}\min(\hat{\mu}_i/4, \lambda_n)$ with a quantity more directly related to the kernel k.

Mercer's theorem is helpful in this regard. This guarantees (under some mild conditions) an eigendecomposition for kernels, which are somewhat like infinite-dimensional analogues of symmetric positive semi-definite matrices. Under certain technical conditions, we may write

$$k(x, x') = \sum_{j=1}^{\infty} \mu_j e_j(x) e_j(x')$$

where given some density $p(x)$ on $\mathcal{X}$, the eigenfunctions e_j and corresponding eigenvalues μ_j obey the integral equation

$$\mu_j e_j(x') = \int_{\mathcal{X}} k(x, x') e_j(x) p(x) dx,$$

and the e_j form an orthonormal basis of $\mathcal{H}$ in the sense that

$$\int_{\mathcal{X}} e_i(x) e_j(x) p(x) dx = \mathbb{1}_{\{i=j\}}.$$

One can further show that (ignoring a multiplicative constant)

$$\mathbb{E}\left(\frac{1}{n}\sum_{i=1}^{n} \min(\hat{\mu}_i/4, \lambda_n)\right) \leq \frac{1}{n}\sum_{i=1}^{\infty} \min(\mu_i/4, \lambda_n).$$

When k is the Sobolev kernel and $p(x)$ is the uniform density on $[0, 1]$, we find the eigenvalues satisfy

$$\mu_j/4 = \frac{1}{\pi^2(2j-1)^2}.$$

Thus

$$\begin{aligned}\sum_{i=1}^{\infty} \min(\mu_i/4, \lambda_n) &\leq \frac{\lambda_n}{2}\left(\frac{1}{\sqrt{\pi^2\lambda_n}} + 1\right) + \frac{1}{\pi^2}\int_{\{(\pi^2\lambda_n)^{-1/2}+1\}/2}^{\infty} \frac{1}{(2x-1)^2} dx \\ &= \sqrt{\lambda_n}/\pi + \lambda_n/2 = O(\sqrt{\lambda_n})\end{aligned}$$

as $\lambda_n \to 0$. Putting things together, we see that

$$\mathbb{E}(\delta_n(\lambda_n)) = O\left(\frac{\sigma^2}{n\lambda_n^{1/2}} + \lambda_n\right).$$

Thus an optimal $\lambda_n \sim (\sigma^2/n)^{2/3}$ gives an error rate of order $(\sigma^2/n)^{2/3}$.

In fact, one can show that this is the best error rate one can achieve with any estimator in this problem. More generally Yang et al. [2015] shows that for essentially any RKHS $\mathcal{H}$ we have

$$\inf_{\hat{f}} \sup_{f^0:\|f^0\|_{\mathcal{H}}\leq 1} \mathbb{E}\left\{\frac{1}{n}\sum_{i=1}^{n}\{f^0(x_i) - \hat{f}(x_i)\}^2\right\} \geq c \inf_{\lambda_n} \delta_n(\lambda_n)$$

where $c > 0$ is a constant and $\hat{f}$ is allowed to range over all (measurable) functions of the data Y, X. The conclusion is that kernel ridge regression is the optimal regression procedure up to a constant factor in terms of MSPE when the true signal f^0 is from an RKHS.

1.6 Other kernel machines

Thus far we have we have only considered applying the kernel trick to ridge regression, which as we have seen has attractive theoretical properties as a regression method. However the kernel trick and the representer theorem are much more generally applicable. In settings where the Y_i are not continuous but are in $\{-1, 1\}$ (e.g. labels for spam and ham, fraud and not fraud etc.), popular approaches include kernel logistic regression and the support vector machine (SVM) [Cortes and Vapnik, 1995].

1.6.1 The support vector machine

Consider first the simple case where the data in the two classes $\{x_i\}_{i:Y_i=1}$ and $\{x_i\}_{i:Y_i=-1}$ are separable by a hyperplane through the origin, so there exists $\beta \in \mathbb{R}^p$ with $\|\beta\|_2 = 1$ such that $Y_i\beta^T x_i > 0$ for all i. Note β would then be a unit normal vector to a plane that separates the two classes.

There may be an infinite number of planes that separate the classes, in which case it seems sensible to use the plane that maximises the margin between the two classes. Consider therefore the following optimisation problem.

$$\max_{\beta \in \mathbb{R}^p, M \geq 0} M$$
$$\text{subject to } Y_i x_i^T \beta / \|\beta\|_2 \geq M,\ i = 1, \ldots, n.$$

Note that by normalising β above we need not impose the constraint that $\|\beta\|_2 = 1$.

Suppose now that the classes are not separable. One way to handle this is to replace the constraint $Y_i x_i^T \beta / \|\beta\|_2 \geq M$ with a penalty for how far over the margin boundary x_i is. This penalty should be zero if x_i is on the correct side of the boundary (i.e. when $Y_i x_i^T \beta / \|\beta\|_2 \geq M$), and should be equal to the distance over the boundary, $M - Y_i x_i^T \beta / \|\beta\|_2$ otherwise. It will in fact be more convenient to penalise according to $1 - Y_i x_i^T \beta / (\|\beta\|_2 M)$ in the latter case, which is the distance measured in units of M. This penalty is invariant to β undergoing any positive scaling, so we may set $\|\beta\|_2 = 1/M$, thus eliminating M from the objective function. Switching $\max 1/\|\beta\|_2$ with $\min \|\beta\|_2^2$ and adding the penalty we arrive at

$$\arg\min_{\beta \in \mathbb{R}^p} \|\beta\|_2^2 + \lambda \sum_{i=1}^n (1 - Y_i x_i^T \beta)_+,$$

where $(\cdot)_+$ denotes the positive part. Replacing λ with $1/\lambda$ we can write the objective in the more familiar-looking form

$$\arg\min_{\beta \in \mathbb{R}^p} \sum_{i=1}^n (1 - Y_i x_i^T \beta)_+ + \lambda \|\beta\|_2^2.$$

Thus far we have restricted ourselves to hyperplanes through the origin but we would more generally want to consider any translate of these i.e. any hyperplane. This can be achieved by allowing ourselves to translate the x_i by an arbitrary vector b, giving

$$\arg\min_{\beta \in \mathbb{R}^p, b \in \mathbb{R}^p} \sum_{i=1}^n (1 - Y_i (x_i - b)^T \beta)_+ + \lambda \|\beta\|_2^2,$$

or equivalently

$$(\hat{\mu}, \hat{\beta}) = \arg\min_{(\mu, \beta) \in \mathbb{R} \times \mathbb{R}^p} \sum_{i=1}^n \{1 - Y_i (x_i^T \beta + \mu)\}_+ + \lambda \|\beta\|_2^2. \tag{1.6.1}$$

This final objective defines the *support vector classifier*; given a new observation x predictions are obtained via $\text{sgn}(\hat{\mu} + x^T \hat{\beta})$.

Note that the objective in (1.6.1) may be re-written as

$$(\hat{\mu}, \hat{f}) = \arg\min_{(\mu, f) \in \mathbb{R} \times \mathcal{H}} \sum_{i=1}^n [1 - Y_i \{f(x_i) + \mu\}]_+ + \lambda \|f\|_{\mathcal{H}}^2, \tag{1.6.2}$$

where $\mathcal{H}$ is the RKHS corresponding to the linear kernel. The representer theorem (more specifically the variant in question 10 of example sheet 1) shows that (1.6.2) for an arbitrary RKHS with kernel k and kernel matrix K is equivalent to the *support vector machine*

$$(\hat{\mu}, \hat{\alpha}) = \underset{(\mu,\alpha)\in\mathbb{R}\times\mathbb{R}^n}{\arg\min} \sum_{i=1}^{n} [1 - Y_i\{K_i^T\alpha + \mu\}]_+ + \lambda\alpha^T K\alpha.$$

Predictions at a new x are given by

$$\operatorname{sgn}\left(\hat{\mu} + \sum_{i=1}^{n} \hat{\alpha}_i k(x, x_i)\right).$$

1.6.2 Logistic regression

Recall that standard logistic regression may be motivated by assuming

$$\log\left(\frac{\mathbb{P}(Y_i = 1)}{\mathbb{P}(Y_i = -1)}\right) = x_i^T\beta^0$$

and picking $\hat{\beta}$ to maximise the log-likelihood. This leads to (see example sheet) the following optimisation problem:

$$\underset{\beta\in\mathbb{R}^p}{\arg\min} \sum_{i=1}^{n} \log\{1 + \exp(-Y_i x_i^T\beta)\}.$$

The 'kernelised' version is given by

$$\underset{f\in\mathcal{H}}{\arg\min} \left\{ \sum_{i=1}^{n} \log[1 + \exp\{-Y_i f(x_i)\}] + \lambda\|f\|_{\mathcal{H}}^2 \right\},$$

where $\mathcal{H}$ is an RKHS. As in the case of the SVM, the representer theorem gives a finite-dimensional optimisation that is equivalent to the above.

1.7 Large-scale kernel machines

We introduced the kernel trick as a computational device that avoided performing calculations in a high or infinite dimensional feature space and, in the case of kernel ridge regression reduced computation down to forming the $n \times n$ matrix K and then inverting $K + \lambda I$. This can be a huge saving, but when n is very large, this can present serious computational difficulties. Even if p is small, the $O(n^3)$ cost of inverting $K + \lambda I$ may cause problems. What's worse, the fitted regression function is a sum over n terms:

$$\hat{f}(\cdot) = \sum_{i=1}^{n} \hat{\alpha}_i k(x_i, \cdot).$$

Even to evaluate a prediction at a single new observation requires $O(n)$ computations unless $\hat{\alpha}$ is sparse.

In recent years, there has been great interest in speeding up computations for kernel machines. We will discuss one exciting approach based on random feature expansions. Given a kernel k, the key idea is to develop a random map

$$\hat{\phi} : \mathcal{X} \to \mathbb{R}^b$$

with b small such that $\mathbb{E}\{\hat{\phi}(x)^T \hat{\phi}(x')\} = k(x, x')$. In a sense we are trying to reverse the kernel trick by approximating the kernel using a random feature map. To increase the quality of the approximation of the kernel, we can consider

$$x \mapsto \frac{1}{\sqrt{L}}(\hat{\phi}_1(x), \ldots, \hat{\phi}_L(x)) \in \mathbb{R}^{Lb}$$

with each $(\hat{\phi}_l(x))_{l=1}^L$ being i.i.d. for each x. Let Φ be the matrix with ith row given by $(\hat{\phi}_1(x_i), \ldots, \hat{\phi}_L(x_i))/\sqrt{L}$. We may then run our learning algorithm replacing the initial matrix of predictors X with Φ. For example, when performing ridge regression, we can compute

$$(\Phi^T \Phi + \lambda I)^{-1} \Phi^T Y,$$

which would require $O(nL^2b^2 + L^3b^3)$ operations: a cost linear in n. Predicting a new observation would cost $O(Lb)$.

The work of Rahimi and Recht [2007] proposes a construction of such a random mapping $\hat{\phi}$ for shift-invariant kernels, that is kernels for which there exists a function h with $k(x, x') = h(x - x')$ for all $x, x' \in \mathcal{X} = \mathbb{R}^p$. A useful property of such kernels is given by Bochner's theorem.

Theorem 8 (Bochner's theorem)**.** *Let $k : \mathbb{R}^p \times \mathbb{R}^p \to \mathbb{R}$ be a continuous kernel. Then k is shift-invariant if and only if there exists some $c > 0$ and distribution F on $\mathbb{R}^p$ such that when $W \sim F$*

$$k(x, x') = c\mathbb{E}e^{i(x-x')^T W} = c\mathbb{E}\cos((x - x')^T W).$$

To make use of this theorem, first observe the following. Let $u \sim U[-\pi, \pi]$, $x, y \in \mathbb{R}$. Then

$$2\mathbb{E}\cos(x+u)\cos(y+u) = 2\mathbb{E}\{(\cos x \cos u - \sin x \sin u)(\cos y \cos u - \sin y \sin u)\}.$$

Now as $u \stackrel{d}{=} -u$, $\mathbb{E}\cos u \sin u = \mathbb{E}\cos(-u)\sin(-u) = -\mathbb{E}\cos u \sin u = 0$. Also of course $\cos^2 u + \sin^2 u = 1$ so $\mathbb{E}\cos^2 u = \mathbb{E}\sin^2 u = 1/2$. Thus

$$2\mathbb{E}\cos(x+u)\cos(y+u) = \cos x \cos y + \sin x \sin y = \cos(x-y).$$

Given a shift-invariant kernel k with associated distribution F, suppose $W \sim F$ and let $u \sim U[-\pi, \pi]$ independently. Define

$$\hat{\phi}(x) = \sqrt{2c}\cos(W^T x + u).$$

Then

$$\begin{aligned}\mathbb{E}\hat{\phi}(x)\hat{\phi}(x') &= 2c\mathbb{E}[\mathbb{E}\{\cos(W^T x + u)\cos(W^T x' + u)|W\}] \\ &= c\mathbb{E}\cos((x-x')^T W) = k(x, x').\end{aligned}$$

As a concrete example of this approach, let us take the Gaussian kernel $k(x, x') = \exp\{-\|x - x'\|_2^2/(2\sigma^2)\}$. Note that if $W \sim N(0, \sigma^{-2}I)$, it has characteristic function $\mathbb{E}(e^{it^T W}) = e^{-\|t\|_2^2/(2\sigma^2)}$ so we may take $\hat{\phi}(x) = \sqrt{2}\cos(W^T x + u)$.

Chapter 2

The Lasso and beyond

2.1 Model selection

Let us revisit the linear model $Y = X\beta^0 + \varepsilon$ where $\mathbb{E}(\varepsilon) = 0$, $\mathrm{Var}(\varepsilon) = \sigma^2 I$. In many modern datasets, there are reasons to believe there are many more variables present than are necessary to explain the response. Let S be the set $S = \{k : \beta_k^0 \neq 0\}$ and suppose $s := |S| \ll p$.

The MSPE of OLS is

$$\begin{aligned}\frac{1}{n}\mathbb{E}\|X\beta^0 - X\hat{\beta}^{\mathrm{OLS}}\|_2^2 &= \frac{1}{n}\mathbb{E}\{(\beta^0 - \hat{\beta}^{\mathrm{OLS}})^T X^T X(\beta^0 - \hat{\beta}^{\mathrm{OLS}})\} \\ &= \frac{1}{n}\mathbb{E}[\mathrm{tr}\{(\beta^0 - \hat{\beta}^{\mathrm{OLS}})(\beta^0 - \hat{\beta}^{\mathrm{OLS}})^T X^T X\}] \\ &= \frac{1}{n}\mathrm{tr}[\mathbb{E}\{(\beta^0 - \hat{\beta}^{\mathrm{OLS}})(\beta^0 - \hat{\beta}^{\mathrm{OLS}})^T\} X^T X] \\ &= \frac{1}{n}\mathrm{tr}(\mathrm{Var}(\hat{\beta}^{\mathrm{OLS}}) X^T X) = \frac{p}{n}\sigma^2.\end{aligned}$$

If we could identify S and then fit a linear model using just these variables, we'd obtain an MSPE of $\sigma^2 s/n$ which could be substantially smaller than $\sigma^2 p/n$. Furthermore, it can be shown that parameter estimates from the reduced model are more accurate. The smaller model would also be easier to interpret.

We now briefly review some classical model selection strategies.

Best subset regression

A natural approach to finding S is to consider all 2^p possible regression procedures each involving regressing the response on a different sets of explanatory variables X_M where M is a subset of $\{1, \ldots, p\}$. We can then pick the best regression procedure using cross-validation (say). For general design matrices, this involves an exhaustive search over all subsets, so this is not really feasible for $p > 50$.

Forward selection

This can be seen as a greedy way of performing best subsets regression. Given a target model size m (the tuning parameter), this works as follows.

1. Start by fitting an intercept only model.
2. Add to the current model the predictor variable that reduces the residual sum of squares the most.
3. Continue step 2 until m predictor variables have been selected.

2.2 The Lasso estimator

The ***L**east **a**bsolute **s**hrinkage and **s**election **o**perator (Lasso)* [Tibshirani, 1996] estimates β^0 by $\hat{\beta}^{\mathrm{L}}_\lambda$, where $(\hat{\mu}^{\mathrm{L}}, \hat{\beta}^{\mathrm{L}}_\lambda)$ minimise

$$\frac{1}{2n}\|Y - \mu\mathbf{1} - X\beta\|_2^2 + \lambda\|\beta\|_1 \tag{2.2.1}$$

over $(\mu, \beta) \in \mathbb{R} \times \mathbb{R}^p$. Here $\|\beta\|_1$ is the ℓ_1-norm of β: $\|\beta\|_1 = \sum_{k=1}^p |\beta_k|$.

Like ridge regression, $\hat{\beta}^{\mathrm{L}}_\lambda$ shrinks the OLS estimate towards the origin, but there is an important difference. The ℓ_1 penalty can force some of the estimated coefficients to be exactly 0. In this way the Lasso can perform simultaneous variable selection and parameter estimation. As we did with ridge regression, we can centre and scale the X matrix, and also centre Y and thus remove μ from the objective. Define

$$Q_\lambda(\beta) = \frac{1}{2n}\|Y - X\beta\|_2^2 + \lambda\|\beta\|_1. \tag{2.2.2}$$

Now the minimiser(s) of $Q_\lambda(\beta)$ will also be the minimiser(s) of

$$\|Y - X\beta\|_2^2 \text{ subject to } \|\beta\|_1 \leq \|\hat{\beta}^{\mathrm{L}}_\lambda\|_1.$$

Similarly, with the Ridge regression objective, we know that $\hat{\beta}^{\mathrm{R}}_\lambda$ minimises $\|Y - X\beta\|_2^2$ subject to $\|\beta\|_2 \leq \|\hat{\beta}^{\mathrm{R}}_\lambda\|_2$.

Now the contours of the OLS objective $\|Y - X\beta\|_2^2$ are ellipsoids centred at $\hat{\beta}^{\mathrm{OLS}}$, while the contours of $\|\beta\|_2^2$ are spheres centred at the origin, and the contours of $\|\beta\|_1$ are 'diamonds' centred at 0.

The important point to note is that the ℓ_1 ball $\{\beta \in \mathbb{R}^p : \|\beta\|_1 \leq \|\hat{\beta}^{\mathrm{L}}_\lambda\|_1\}$ has corners where some of the components are zero, and it is likely that the OLS contours will intersect the ℓ_1 ball at such a corner.

2.2.1 Prediction error of the Lasso with no assumptions on the design

A remarkable property of the Lasso is that even when $p \gg n$, it can still perform well in terms of prediction error. Suppose the columns of X have been centred and scaled (as we will always assume from now on unless stated otherwise) and assume the normal linear model (where we have already centred Y),

$$Y = X\beta^0 + \varepsilon - \bar{\varepsilon}\mathbf{1} \tag{2.2.3}$$

where $\varepsilon \sim N_n(0, \sigma^2 I)$.

Theorem 9. *Let $\hat{\beta}$ be the Lasso solution when*

$$\lambda = A\sigma\sqrt{\frac{\log(p)}{n}}.$$

With probability at least $1 - 2p^{-(A^2/2-1)}$

$$\frac{1}{n}\|X(\beta^0 - \hat{\beta})\|_2^2 \leq 4A\sigma\sqrt{\frac{\log(p)}{n}}\|\beta^0\|_1.$$

Proof. From the definition of $\hat{\beta}$ we have

$$\frac{1}{2n}\|Y - X\hat{\beta}\|_2^2 + \lambda\|\hat{\beta}\|_1 \leq \frac{1}{2n}\|Y - X\beta^0\|_2^2 + \lambda\|\beta^0\|_1.$$

Rearranging,

$$\frac{1}{2n}\|X(\beta^0 - \hat{\beta})\|_2^2 \leq \frac{1}{n}\varepsilon^T X(\hat{\beta} - \beta^0) + \lambda\|\beta^0\|_1 - \lambda\|\hat{\beta}\|_1.$$

Now $|\varepsilon^T X(\hat{\beta} - \beta^0)| \leq \|X^T\varepsilon\|_\infty\|\hat{\beta} - \beta^0\|_1$. Let $\Omega = \{\|X^T\varepsilon\|_\infty/n \leq \lambda\}$. Lemma 13 below shows that $\mathbb{P}(\Omega) \geq 1 - 2p^{-(A^2/2-1)}$. Working on the event Ω, we obtain

$$\begin{aligned}
&\frac{1}{2n}\|X(\beta^0 - \hat{\beta})\|_2^2 \leq \lambda\|\beta^0 - \hat{\beta}\|_1 + \lambda\|\beta^0\|_1 - \lambda\|\hat{\beta}\|_1, \\
&\frac{1}{n}\|X(\beta^0 - \hat{\beta})\|_2^2 \leq 4\lambda\|\beta^0\|_1, \qquad \text{by the triangle inequality.}
\end{aligned}$$

□

2.2.2 Basic concentration inequalities

The proof of Theorem 9 relies on a lower bound for the probability of the event Ω. A union bound gives

$$\begin{aligned}
\mathbb{P}(\|X^T\varepsilon\|_\infty/n > \lambda) &= \mathbb{P}(\cup_{j=1}^p |X_j^T\varepsilon|/n > \lambda) \\
&\leq \sum_{j=1}^p \mathbb{P}(|X_j^T\varepsilon|/n > \lambda).
\end{aligned}$$

Now $X_j^T\varepsilon/n \sim N(0, \sigma^2/n)$, so if we obtain a bound on the tail probabilities of normal distributions, the argument above will give a bound for $\mathbb{P}(\Omega)$.

Motivated by the need to bound normal tail probabilities, we will briefly discuss the topic of *concentration inequalities* that provide such bounds for much wider classes of random variables. Concentration inequalities are vital for the study of many modern algorithms and in our case here, they will reveal that the attractive properties of the Lasso presented in Theorem 9 hold true for a variety of non-normal errors.

We begin our discussion with the simplest tail bound, *Markov's inequality*, which states that given a non-negative random variable W,

$$\mathbb{P}(W \geq t) \leq \frac{\mathbb{E}(W)}{t}.$$

This immediately implies that given a strictly increasing function $\varphi : \mathbb{R} \to [0, \infty)$ and any random variable W,

$$\mathbb{P}(W \geq t) = \mathbb{P}\{\varphi(W) \geq \varphi(t)\} \leq \frac{\mathbb{E}(\varphi(W))}{\varphi(t)}.$$

Applying this with $\varphi(t) = e^{\alpha t}$ ($\alpha > 0$) yields the so-called *Chernoff bound*:

$$\mathbb{P}(W \geq t) \leq \inf_{\alpha > 0} e^{-\alpha t}\mathbb{E}e^{\alpha W}.$$

Consider the case when $W \sim N(0, \sigma^2)$. Recall that

$$\mathbb{E}e^{\alpha W} = e^{\alpha^2\sigma^2/2}. \tag{2.2.4}$$

Thus

$$\mathbb{P}(W \geq t) \leq \inf_{\alpha > 0} e^{\alpha^2\sigma^2/2 - \alpha t} = e^{-t^2/(2\sigma^2)}.$$

Note that to arrive at this bound, all we required was (an upper bound on) the moment generating function (mgf) of W (2.2.4).

Sub-Gaussian variables

Definition 3. We say a random variable W with mean $\mu = \mathbb{E}(W)$ is *sub-Gaussian* if there exists $\sigma > 0$ such that

$$\mathbb{E}e^{\alpha(W-\mu)} \leq e^{\alpha^2\sigma^2/2}$$

for all $\alpha \in \mathbb{R}$. We then say that W is *sub-Gaussian with parameter* σ.

Proposition 10 (Sub-Gaussian tail bound)**.** *If W is sub-Gaussian with parameter σ and $\mathbb{E}(W) = \mu$ then*

$$\mathbb{P}(W - \mu \geq t) \leq e^{-t^2/(2\sigma^2)}.$$

As well as Gaussian random variables, the sub-Gaussian class includes bounded random variables.

Lemma 11 (Hoeffding's lemma)**.** *If W is mean-zero and takes values in $[a, b]$, then W is sub-Gaussian with parameter $(b-a)/2$.*

The following proposition shows that analogously to how a linear combination of jointly Gaussian random variables is Gaussian, a linear combination of sub-Gaussian random variables is also sub-Gaussian.

Proposition 12. *Let $(W_i)_{i=1}^n$ be a sequence of independent mean-zero sub-Gaussian random variables with parameters $(\sigma_i)_{i=1}^n$ and let $\gamma \in \mathbb{R}^n$. Then $\gamma^T W$ is sub-Gaussian with parameter $\left(\sum_i \gamma_i^2 \sigma_i^2\right)^{1/2}$.*

Proof.

$$\begin{aligned}\mathbb{E}\exp\left(\alpha \sum_{i=1}^n \gamma_i W_i\right) &= \prod_{i=1}^n \mathbb{E}\exp(\alpha\gamma_i W_i) \\ &\leq \prod_{i=1}^n \exp(\alpha^2\gamma_i^2\sigma_i^2/2) \\ &= \exp\left(\alpha^2 \sum_{i=1}^n \gamma_i^2\sigma_i^2/2\right).\end{aligned}$$

□

We can now prove a more general version of the probability bound required for Theorem 9.

Lemma 13. *Suppose $(\varepsilon_i)_{i=1}^n$ are independent, mean-zero and sub-Gaussian with common parameter σ. Note that this includes $\varepsilon \sim N_n(0, \sigma^2 I)$. Let $\lambda = A\sigma\sqrt{\log(p)/n}$. Then*

$$\mathbb{P}(\|X^T\varepsilon\|_\infty/n \leq \lambda) \geq 1 - 2p^{-(A^2/2-1)}.$$

Proof.

$$\mathbb{P}(\|X^T\varepsilon\|_\infty/n > \lambda) \leq \sum_{j=1}^p \mathbb{P}(|X_j^T\varepsilon|/n > \lambda).$$

But $\pm X_j^T\varepsilon/n$ are both sub-Gaussian with parameter $(\sigma^2\|X_j\|_2^2/n^2)^{1/2} = \sigma/\sqrt{n}$. Thus the RHS is at most

$$2p\exp(-A^2\log(p)/2) = 2p^{1-A^2/2}.$$

□

When trying to understand the impact of the design matrix X on properties of the Lasso, it will be helpful to have a tail bound for a product of sub-Gaussian random variables. Bernstein's inequality, which applies to random variables satisfying the condition below, is helpful in this regard.

Definition 4 (Bernstein's condition)**.** We say that the random variable W with $\mathbb{E}W = \mu$ satisfies Bernstein's condition with parameter (σ, b) where $\sigma, b > 0$ if

$$\mathbb{E}(|W-\mu|^k) \le \frac{1}{2}k!\sigma^2 b^{k-2} \qquad \text{for } k = 2, 3, \ldots.$$

Proposition 14 (Bernstein's inequality)**.** *Let $W_1, W_2, \ldots$ be independent random variables with $\mathbb{E}(W_i) = \mu$. Suppose each W_i satisfies Bernstein's condition with parameter (σ, b). Then*

$$\mathbb{E}(e^{\alpha(W_i-\mu)}) \le \exp\left(\frac{\alpha^2\sigma^2/2}{1-b|\alpha|}\right) \qquad \textit{for all } |\alpha| < 1/b$$

$$\mathbb{P}\left(\frac{1}{n}\sum_{i=1}^n W_i - \mu \ge t\right) \le \exp\left(-\frac{nt^2}{2(\sigma^2+bt)}\right) \qquad \textit{for all } t \ge 0.$$

Proof. Fix i and let $W = W_i$. We have

$$\begin{aligned}
\mathbb{E}(e^{\alpha(W-\mu)}) &= 1 + \alpha\mathbb{E}(W-\mu) + \sum_{k=2}^{\infty}\alpha^k\frac{\mathbb{E}\{(W-\mu)^k\}}{k!} \\
&\le 1 + \frac{\sigma^2\alpha^2}{2}\sum_{k=2}^{\infty}|\alpha|^{k-2}b^{k-2} \\
&= 1 + \frac{\sigma^2\alpha^2}{2}\frac{1}{1-|\alpha|b} \le \exp\left(\frac{\alpha^2\sigma^2/2}{1-b|\alpha|}\right),
\end{aligned}$$

provided $|\alpha| < 1/b$ and using the inequality $e^u \ge 1+u$ in the final line. For the probability bound, first note that

$$\begin{aligned}
\mathbb{E}\exp\left(\sum_{i=1}^n \alpha(W_i-\mu)/n\right) &= \prod_{i=1}^n \mathbb{E}\exp\{\alpha(W_i-\mu)/n\} \\
&\le \exp\left(n\frac{(\alpha/n)^2\sigma^2/2}{1-b|\alpha/n|}\right)
\end{aligned}$$

for $|\alpha|/n < 1/b$. Then we use the Chernoff method and set $\alpha/n = t/(bt+\sigma^2) \in [0, 1/b)$. □

Lemma 15. *Let W, Z be mean-zero and sub-Gaussian with parameters σ_W and σ_Z respectively. Then the product WZ satisfies Bernstein's condition with parameter $(8\sigma_W\sigma_Z, 4\sigma_W\sigma_Z)$.*

Proof. In order to use Bernstein's inequality (Proposition 14) we first obtain bounds on

the moments of W and Z. Note that $W^{2k} = \int_0^\infty \mathbb{1}_{\{x<W^{2k}\}} dx$. Thus by Fubini's theorem

$$\begin{aligned}
\mathbb{E}(W^{2k}) &= \int_0^\infty \mathbb{P}(W^{2k} > x) dx \\
&= 2k \int_0^\infty t^{2k-1} \mathbb{P}(|W| > t) dt \qquad \text{substituting } t^{2k} = x \\
&\leq 4k \int_0^\infty t^{2k-1} \exp\{-t^2/(2\sigma_W^2)\} dt \qquad \text{by Proposition 10} \\
&= 4k\sigma_W^2 \int_0^\infty (2\sigma_W^2 x)^{k-1} e^{-x} dx \qquad \text{substituting } t^2/(2\sigma_W^2) = x \\
&= 2^{k+1} \sigma_W^{2k} k!.
\end{aligned}$$

Next note that for any random variable Y,

$$\begin{aligned}
|\mathbb{E}(Y - \mathbb{E}Y)^k| &\leq \mathbb{E}|Y - \mathbb{E}Y|^k \\
&\leq \mathbb{E} \sum_{t=0}^k \binom{k}{t} |Y|^t |\mathbb{E}Y|^{k-t} \\
&\leq \sum_{t=0}^k \binom{k}{t} \mathbb{E}(|Y|^t) \mathbb{E}(|Y|^{k-t}) \qquad \text{by Jensen's inequality } |\mathbb{E}Y|^{k-t} \leq \mathbb{E}|Y|^{k-t}, \\
&\leq \mathbb{E}(|Y|^k) \sum_{t=0}^k \binom{k}{t} \qquad \text{by Jensen's inequality } \mathbb{E}|Y|^{k\frac{t}{k}} \leq (\mathbb{E}|Y|^k)^{t/k} \text{ for } t \leq k, \\
&\leq 2^k \mathbb{E}|Y|^k.
\end{aligned}$$

Therefore

$$\begin{aligned}
\mathbb{E}(|WZ - \mathbb{E}WZ|^k) &\leq 2^k \mathbb{E}|WZ|^k \\
&\leq 2^k (\mathbb{E}W^{2k})^{1/2} (\mathbb{E}Z^{2k})^{1/2} \qquad \text{by Cauchy–Schwarz} \\
&\leq 2^k 2^{k+1} \sigma_W^k \sigma_Z^k k! \\
&= \frac{k!}{2} (8\sigma_W\sigma_Z)^2 (4\sigma_W\sigma_Z)^{k-2}.
\end{aligned}$$

□

2.2.3 Some facts from optimisation theory and convex analysis

In order to study the Lasso in detail, it will be helpful to review some basic facts from optimisation and convex analysis.

Convexity

A set $A \subseteq \mathbb{R}^d$ is *convex* if

$$x, y \in A \Rightarrow (1-t)x + ty \in A \qquad \text{for all } t \in (0,1).$$

In certain settings it will be convenient to consider functions that take, in addition to real values, the value ∞. Denote $\bar{\mathbb{R}} = \mathbb{R} \cup \{\infty\}$. A function $f : \mathbb{R}^d \to \bar{\mathbb{R}}$ is *convex* if

$$f\big((1-t)x + ty\big) \leq (1-t)f(x) + tf(y)$$

for all $x, y \in \mathbb{R}^d$ and $t \in (0,1)$, and $f(x) < \infty$ for at least one x. [This is in fact known in the literature as a *proper convex function*]. It is *strictly convex* if the inequality is strict for all $x, y \in \mathbb{R}^d$, $x \neq y$ and $t \in (0,1)$. Define the *domain* of f, to be $\operatorname{dom} f = \{x : f(x) < \infty\}$. Note that when f is convex, $\operatorname{dom} f$ must be a convex set.

Proposition 16. *(i) Let $f_1, \ldots, f_m : \mathbb{R}^d \to \bar{\mathbb{R}}$ be convex functions with $\operatorname{dom} f_1 \cap \cdots \cap \operatorname{dom} f_m \neq \emptyset$. Then if $c_1, \ldots, c_m \geq 0$, $c_1 f_1 + \cdots c_m f_m$ is a convex function.*

(ii) If $f : \mathbb{R}^d \to \mathbb{R}$ is twice continuously differentiable then

(a) f is convex iff. its Hessian $H(x)$ is positive semi-definite for all x,

(b) f is strictly convex if $H(x)$ is positive definite for all x.

The Lagrangian method

Consider an optimisation problem of the form

$$\text{minimise } f(x), \text{ subject to } g(x) = 0 \tag{2.2.5}$$

where $g : \mathbb{R}^d \to \mathbb{R}^b$. Suppose the optimal value is $c^* \in \mathbb{R}$. The Lagrangian for this problem is defined as

$$L(x, \theta) = f(x) + \theta^T g(x)$$

where $\theta \in \mathbb{R}^b$. Note that

$$\inf_{x \in \mathbb{R}^d} L(x, \theta) \leq \inf_{x \in \mathbb{R}^d : g(x) = 0} L(x, \theta) = c^*$$

for all θ. The Lagrangian method involves finding a θ^* such that the minimising x^* on the LHS satisfies $g(x^*) = 0$. This x^* must then be a minimiser in the original problem (2.2.5).

Subgradients

Definition 5. A vector $v \in \mathbb{R}^d$ is a *subgradient* of a convex function $f : \mathbb{R}^d \to \bar{\mathbb{R}}$ at x if

$$f(y) \geq f(x) + v^T(y - x) \qquad \text{for all } \ y \in \mathbb{R}^d.$$

The set of subgradients of f at x is called the *subdifferential* of f at x and denoted $\partial f(x)$.

In order to make use of subgradients, we will require the following two facts:

Proposition 17. *Let $f : \mathbb{R}^d \to \bar{\mathbb{R}}$ be convex, and suppose f is differentiable at $x \in \operatorname{int}(\operatorname{dom} f)$. Then $\partial f(x) = \{\nabla f(x)\}$.*

Proposition 18. *Let $f, g : \mathbb{R}^d \to \bar{\mathbb{R}}$ be convex with $\operatorname{int}(\operatorname{dom} f) \cap \operatorname{int}(\operatorname{dom} g) \neq \emptyset$ and let $\alpha > 0$. Then*

$$\partial(\alpha f)(x) = \alpha \partial f(x) = \{\alpha v : v \in \partial f(x)\},$$
$$\partial(f + g)(x) = \partial f(x) + \partial g(x) = \{v + w : v \in \partial f(x),\, w \in \partial g(x)\}.$$

The following easy (but key) result is often referred to in the statistical literature as the Karush–Kuhn–Tucker (KKT) conditions, though it is actually a much simplified version of them.

Proposition 19. $x^* \in \operatorname*{arg\,min}_{x \in \mathbb{R}^d} f(x)$ *if and only if* $0 \in \partial f(x^*)$.

Proof.

$$f(y) \geq f(x^*) \quad \text{for all} \quad y \in \mathbb{R}^d \Leftrightarrow f(y) \geq f(x^*) + 0^T(y - x) \quad \text{for all} \quad y \in \mathbb{R}^d$$
$$\Leftrightarrow 0 \in \partial f(x^*).$$

□

Let us now compute the subdifferential of the ℓ_1-norm. First note that $\|\cdot\|_1 : \mathbb{R}^d \to \mathbb{R}$ is convex. Indeed it is a norm so the triangle inequality gives $\|tx + (1-t)y\|_1 \leq t\|x\|_1 + (1-t)\|y\|_1$. We introduce some notation that will be helpful here and throughout the rest of the course.

For $x \in \mathbb{R}^d$ and $A = \{k_1, \ldots, k_m\} \subseteq \{1, \ldots, d\}$ with $k_1 < \cdots < k_m$, by x_A we will mean $(x_{k_1}, \ldots, x_{k_m})^T$. Similarly if X has d columns we will write X_A for the matrix

$$X_A = (X_{k_1} \cdots X_{k_m}).$$

Further in this context, by A^c, we will mean $\{1, \ldots, d\} \setminus A$. Additionally, when in subscripts we will use the shorthand $-j = \{j\}^c$ and $-jk = \{j, k\}^c$. Note these column and component extraction operations will always be considered to have taken place first before any further operations on the matrix, so for example $X_A^T = (X_A)^T$. Finally, define

$$\operatorname{sgn}(x_1) = \begin{cases} -1 & \text{if } x_1 < 0 \\ 0 & \text{if } x_1 = 0 \\ 1 & \text{if } x_1 > 0, \end{cases}$$

and

$$\operatorname{sgn}(x) = (\operatorname{sgn}(x_1), \ldots, \operatorname{sgn}(x_d))^T.$$

Proposition 20. *For $x \in \mathbb{R}^d$ let $A = \{j : x_j \neq 0\}$. Then*

$$\partial\|x\|_1 = \{v \in \mathbb{R}^d : \|v\|_\infty \leq 1 \text{ and } v_A = \operatorname{sgn}(x_A)\}$$

Proof. For $j = 1, \ldots, d$, let

$$g_j : \mathbb{R}^d \to \mathbb{R}$$
$$x \mapsto |x_j|.$$

Then $\|\cdot\| = \sum_j g_j(\cdot)$ so by Proposition 18, $\partial\|x\|_1 = \sum_j \partial g_j(x)$. When x has $x_j \neq 0$, g_j is differentiable at x so by Proposition 17 $\partial g_j(x) = \{\text{sgn}(x_j)e_j\}$ where e_j is the jth unit vector. When $x_j = 0$, if $v \in \partial g_j(x)$ we must have

$$g_j(y) \geq g_j(x) + v^T(y - x) \qquad \text{for all } y \in \mathbb{R}^d,$$

so

$$|y_j| \geq v^T(y - x) \qquad \text{for all } y \in \mathbb{R}^d. \tag{2.2.6}$$

we claim that the above holds iff. $v_j \in [-1, 1]$ and $v_{-j} = 0$. For the 'if' direction, note that $v^T(y - x) = v_j y_j \leq |y_j|$. Conversely, set $y_{-j} = x_{-j} + v_{-j}$ and $y_j = 0$ in (2.2.6) to get $0 \geq \|v_{-j}\|_2^2$, so $v_{-j} = 0$. Then take y with $y_{-j} = x_{-j}$ to get $|y_j| \geq v_j y_j$ for all $y_j \in \mathbb{R}$, so $|v_j| \leq 1$. Forming the set sum of the subdifferentials then gives the result. □

2.2.4 Lasso solutions

Equipped with these tools from convex analysis, we can now fully characterise the solutions to the Lasso. We have that $\hat{\beta}^{\text{L}}_\lambda$ is a Lasso solution if and only if $0 \in \partial Q_\lambda(\hat{\beta}^{\text{L}}_\lambda)$, which is equivalent to

$$\frac{1}{n} X^T(Y - X\hat{\beta}^{\text{L}}_\lambda) = \lambda\hat{\nu},$$

for $\hat{\nu}$ with $\|\hat{\nu}\|_\infty \leq 1$ and writing $\hat{S}_\lambda = \{k : \hat{\beta}^{\text{L}}_{\lambda,k} \neq 0\}$, $\hat{\nu}_{\hat{S}_\lambda} = \text{sgn}(\hat{\beta}^{\text{L}}_{\lambda,\hat{S}_\lambda})$.

Lasso solutions need not be unique (e.g. if X has duplicate columns), though for most reasonable design matrices, Lasso solutions will be unique. We will often tacitly assume Lasso solutions are unique in the statement of our theoretical results. It is however straightforward to show that the Lasso fitted values are unique.

Proposition 21. *$X\hat{\beta}^{\text{L}}_\lambda$ is unique.*

Proof. Fix λ and suppose $\hat{\beta}^{(1)}$ and $\hat{\beta}^{(2)}$ are two Lasso solutions giving an optimal objective value of c^*. Now for $t \in (0, 1)$, by strict convexity of $\|\cdot\|_2^2$,

$$\|Y - tX\hat{\beta}^{(1)} - (1-t)X\hat{\beta}^{(2)}\|_2^2 \leq t\|Y - X\hat{\beta}^{(1)}\|_2^2 + (1-t)\|Y - X\hat{\beta}^{(2)}\|_2^2,$$

with equality if and only if $X\hat{\beta}^{(1)} = X\hat{\beta}^{(2)}$. Since $\|\cdot\|_1$ is also convex, we see that

$$\begin{aligned}
c^* &\leq Q_\lambda(t\hat{\beta}^{(1)} + (1-t)\hat{\beta}^{(2)}) \\
&= \|Y - tX\hat{\beta}^{(1)} - (1-t)X\hat{\beta}^{(2)}\|_2^2/(2n) + \lambda\|t\hat{\beta}^{(1)} + (1-t)\hat{\beta}^{(2)}\|_1 \\
&\leq t\|Y - X\hat{\beta}^{(1)}\|_2^2/(2n) + (1-t)\|Y - X\hat{\beta}^{(2)}\|_2^2/(2n) + \lambda\|t\hat{\beta}^{(1)} + (1-t)\hat{\beta}^{(2)}\|_1 \\
&\leq t\{\|Y - X\hat{\beta}^{(1)}\|_2^2/(2n) + \lambda\|\hat{\beta}^{(1)}\|_1\} + (1-t)\{\|Y - X\hat{\beta}^{(2)}\|_2^2/(2n) + \lambda\|\hat{\beta}^{(2)}\|_1\} \\
&= tQ(\hat{\beta}^{(1)}) + (1-t)Q(\hat{\beta}^{(2)}) \leq c^*.
\end{aligned}$$

Equality must prevail throughout this chain of inequalities, so $X\hat{\beta}^{(1)} = X\hat{\beta}^{(2)}$. □

2.2.5 Variable selection

Consider now the "noiseless" version of the high-dimensional linear model (2.2.3), $Y = X\beta^0$. The case with noise can dealt with by similar arguments to those we'll use below when we work on an event that $\|X^T\varepsilon\|_\infty$ is small (see example sheet).

Let $S = \{k : \beta^0_k \neq 0\}$, $N = \{1, \dots, p\} \setminus S$ and assume wlog that $S = \{1, \dots, s\}$, and also that $\operatorname{rank}(X_S) = s$.

Theorem 22. *Let $\lambda > 0$ and define $\Delta = X_N^T X_S (X_S^T X_S)^{-1} \operatorname{sgn}(\beta^0_S)$. If $\|\Delta\|_\infty \leq 1$ and for $k \in S$,*

$$|\beta^0_k| > \lambda |\operatorname{sgn}(\beta^0_S)^T [\{\tfrac{1}{n} X_S^T X_S\}^{-1}]_k|, \tag{2.2.7}$$

then there exists a Lasso solution $\hat\beta^{\mathrm{L}}_\lambda$ with $\operatorname{sgn}(\hat\beta^{\mathrm{L}}_\lambda) = \operatorname{sgn}(\beta^0)$. As a partial converse, if there exists a Lasso solution $\hat\beta^{\mathrm{L}}_\lambda$ with $\operatorname{sgn}(\hat\beta^{\mathrm{L}}_\lambda) = \operatorname{sgn}(\beta^0)$, then $\|\Delta\|_\infty \leq 1$.

Remark 1. We can interpret $\|\Delta\|_\infty$ as the maximum in absolute value over $k \in N$ of the dot product of $\operatorname{sgn}(\beta^0_S)$ and $(X_S^T X_S)^{-1} X_S^T X_k$, the coefficient vector obtained by regressing X_k on X_S. The condition $\|\Delta\|_\infty \leq 1$ is known as the irrepresentable condition.

Proof. Fix $\lambda > 0$ and write $\hat\beta = \hat\beta^{\mathrm{L}}_\lambda$ and $\hat S = \{k : \hat\beta_k \neq 0\}$ for convenience. The KKT conditions for the Lasso give

$$\frac{1}{n} X^T X (\beta^0 - \hat\beta) = \lambda \hat\nu$$

where $\|\hat\nu\|_\infty \leq 1$ and $\hat\nu_{\hat S} = \operatorname{sgn}(\hat\beta_{\hat S})$. We can expand this into

$$\frac{1}{n} \begin{pmatrix} X_S^T X_S & X_S^T X_N \\ X_N^T X_S & X_N^T X_N \end{pmatrix} \begin{pmatrix} \beta^0_S - \hat\beta_S \\ -\hat\beta_N \end{pmatrix} = \lambda \begin{pmatrix} \hat\nu_S \\ \hat\nu_N \end{pmatrix}. \tag{2.2.8}$$

We prove the converse first. If $\operatorname{sgn}(\hat\beta) = \operatorname{sgn}(\beta^0)$ then $\hat\nu_S = \operatorname{sgn}(\beta^0_S)$ and $\hat\beta_N = 0$. The top block of (2.2.8) gives

$$\beta^0_S - \hat\beta_S = \lambda (\tfrac{1}{n} X_S^T X_S)^{-1} \operatorname{sgn}(\beta^0_S).$$

Substituting this into the bottom block, we get

$$\lambda \tfrac{1}{n} X_N^T X_S (\tfrac{1}{n} X_S^T X_S)^{-1} \operatorname{sgn}(\beta^0_S) = \lambda \hat\nu_N.$$

Thus as $\|\hat\nu_N\|_\infty \leq 1$, we have $\|\Delta\|_\infty \leq 1$.

For the positive statement, we need to find a $\hat\beta$ and $\hat\nu$ such that $\operatorname{sgn}(\hat\beta_S) = \operatorname{sgn}(\beta^0_S)$ and $\hat\beta_N = 0$, for which the KKT conditions hold. We claim that taking

$$\begin{aligned} (\hat\beta_S,\, \hat\beta_N) &= (\beta^0_S - \lambda (\tfrac{1}{n} X_S^T X_S)^{-1} \operatorname{sgn}(\beta^0_S),\, 0) \\ (\hat\nu_S,\, \hat\nu_N) &= (\operatorname{sgn}(\beta^0_S),\, \Delta) \end{aligned}$$

satisfies (2.2.8). We only need to check that $\operatorname{sgn}(\beta^0_S) = \operatorname{sgn}(\hat\beta_S)$, but this follows from (2.2.7). □

2.2.6 Prediction and estimation

Consider again the model $Y = X\beta^0 + \varepsilon - \bar{\varepsilon}\mathbf{1}$ where the components of ε are independent mean-zero sub-Gaussian random variables with common parameter σ. Let S, s and N be defined as in the previous section. As we have noted before, in an artificial situation where S is known, we could apply OLS on X_S and have an MSPE of $\sigma^2 s/n$. Under a so-called *compatibility condition* on the design matrix, we can obtain a similar MSPE for the Lasso.

Definition 6. Given a matrix of predictors $X \in \mathbb{R}^{n\times p}$ and support set S, define

$$\phi^2 = \inf_{\beta\in\mathbb{R}^p:\beta_S\neq 0,\, \|\beta_N\|_1\leq 3\|\beta_S\|_1} \frac{\frac{1}{n}\|X\beta\|_2^2}{\frac{1}{s}\|\beta_S\|_1^2},$$

where $s = |S|$ and we take $\phi \geq 0$. The *compatibility condition* is that $\phi^2 > 0$.

Note that if X^TX/n has minimum eigenvalue $c_{\min} > 0$ (so necessarily $p \leq n$), then $\phi^2 > c_{\min}$. Indeed by the Cauchy–Schwarz inequality,

$$\|\beta_S\|_1 = \operatorname{sgn}(\beta_S)^T\beta_S \leq \sqrt{s}\|\beta_S\|_2 \leq \sqrt{s}\|\beta\|_2.$$

Thus

$$\phi^2 \geq \inf_{\beta\neq 0} \frac{\frac{1}{n}\|X\beta\|_2^2}{\|\beta\|_2^2} = c_{\min}.$$

Although in the high-dimensional setting we would have $c_{\min} = 0$, the fact that the infimum in the definition of ϕ^2 is over a restricted set of β can still allow ϕ^2 to be positive even in this case, as we discuss after the presentation of the theorem.

Theorem 23. *Suppose the compatibility condition holds and let $\hat{\beta}$ be the Lasso solution with $\lambda = A\sigma\sqrt{\log(p)/n}$ for $A > 0$. Then with probability at least $1 - 2p^{-(A^2/8-1)}$, we have*

$$\frac{1}{n}\|X(\beta^0 - \hat{\beta})\|_2^2 + \lambda\|\hat{\beta} - \beta^0\|_1 \leq \frac{16\lambda^2 s}{\phi^2} = \frac{16A^2\log(p)}{\phi^2}\frac{\sigma^2 s}{n}.$$

Proof. As in Theorem 9 we start with the "basic inequality":

$$\frac{1}{2n}\|X(\hat{\beta} - \beta^0)\|_2^2 + \lambda\|\hat{\beta}\|_1 \leq \frac{1}{n}\varepsilon^T X(\hat{\beta} - \beta^0) + \lambda\|\beta^0\|_1.$$

We work on the event $\Omega = \{2\|X^T\varepsilon\|_\infty/n \leq \lambda\}$ where after applying Hölder's inequality, we get

$$\frac{1}{n}\|X(\hat{\beta} - \beta^0)\|_2^2 + 2\lambda\|\hat{\beta}\|_1 \leq \lambda\|\hat{\beta} - \beta^0\|_1 + 2\lambda\|\beta^0\|_1. \tag{2.2.9}$$

Lemma 13 shows that $\mathbb{P}(\Omega) \geq 1 - 2p^{-(A^2/8-1)}$.

To motivate the rest of the proof, consider the following idea. We know

$$\frac{1}{n}\|X(\hat{\beta} - \beta^0)\|_2^2 \leq 3\lambda\|\hat{\beta} - \beta^0\|_1.$$

If we could get

$$3\lambda\|\hat{\beta} - \beta^0\|_1 \leq \frac{c\lambda}{\sqrt{n}}\|X(\hat{\beta} - \beta^0)\|_2$$

for some constant $c > 0$, then we would have that $\|X(\hat{\beta} - \beta^0)\|_2^2/n \leq c^2\lambda^2$ and also $3\lambda\|\beta^0 - \hat{\beta}\|_1 \leq c^2\lambda^2$.

Returning to the actual proof, write $a = \|X(\hat{\beta} - \beta^0)\|_2^2/(n\lambda)$. Then from (2.2.9) we can derive the following string of inequalities:

$$\begin{aligned}
a + 2(\|\hat{\beta}_N\|_1 + \|\hat{\beta}_S\|_1) &\leq \|\hat{\beta}_S - \beta_S^0\|_1 + \|\hat{\beta}_N\|_1 + 2\|\beta_S^0\|_1 \\
a + \|\hat{\beta}_N\|_1 &\leq \|\hat{\beta}_S - \beta_S^0\|_1 + 2\|\beta_S^0\|_1 - 2\|\hat{\beta}_S\|_1 \\
a + \|\hat{\beta}_N - \beta_N^0\|_1 &\leq 3\|\beta_S^0 - \hat{\beta}_S\|_1 \\
a + \|\hat{\beta} - \beta^0\|_1 &\leq 4\|\beta_S^0 - \hat{\beta}_S\|_1,
\end{aligned}$$

the final inequality coming from adding $\|\beta_S^0 - \hat{\beta}_S\|_1$ to both sides.

Now using the compatibility condition with $\beta = \hat{\beta} - \beta^0$ we have

$$\begin{aligned}
\frac{1}{n}\|X(\hat{\beta} - \beta^0)\|_2^2 + \lambda\|\beta^0 - \hat{\beta}\|_1 &\leq 4\lambda\|\beta_S^0 - \hat{\beta}_S\|_1 \\
&\leq \frac{4\lambda}{\phi}\sqrt{\frac{s}{n}}\|X(\hat{\beta} - \beta^0)\|_2. \qquad (2.2.10)
\end{aligned}$$

From this we get

$$\frac{1}{\sqrt{n}}\|X(\hat{\beta} - \beta^0)\|_2 \leq \frac{4\lambda\sqrt{s}}{\phi},$$

and substituting this into the RHS of (2.2.10) gives the result. □

The compatibility condition and random design

How strong is the compatibility condition? In order to answer this question, we shall think of X as random and try to understand what conditions on the population covariance matrix $\Sigma^0 := \mathbb{E}(X^T X/n)$ imply that X satisfies a compatibility condition with high probability. To this end let us define

$$\phi_\Sigma^2(S) = \inf_{\beta:\|\beta_S\|_1 \neq 0, \|\beta_N\|_1 \leq 3\|\beta_S\|_1} \frac{\beta^T\Sigma\beta}{\|\beta_S\|_1^2/|S|}$$

where $\Sigma \in \mathbb{R}^{p\times p}$. Note then our $\phi^2 = \phi_{\hat{\Sigma}}^2(S)$ where $\hat{\Sigma} := X^T X/n$ and S is the support set of β^0. The following result shows that if $\hat{\Sigma}$ is close to a matrix $\check{\Sigma}$ for which $\phi_{\check{\Sigma}}^2(S) > 0$, then also $\phi_{\hat{\Sigma}}^2(S) > 0$.

Lemma 24. *Suppose* $\phi_{\check{\Sigma}}^2(S) > 0$ *and* $\max_{jk}|\hat{\Sigma}_{jk} - \check{\Sigma}_{jk}| \leq \phi_{\check{\Sigma}}^2(S)/(32|S|)$. *Then* $\phi_{\hat{\Sigma}}^2(S) \geq \phi_{\check{\Sigma}}^2(S)/2$.

Proof. In the following we suppress dependence on S. Let $s = |S|$ and let $t = \phi^2_{\check{\Sigma}}/(32s)$. We have

$$\begin{aligned} |\beta^T(\check{\Sigma} - \hat{\Sigma})\beta| &\leq \|\beta\|_1 \|(\check{\Sigma} - \hat{\Sigma})\beta\|_\infty \text{ (Hölder)} \\ &\leq t\|\beta\|_1^2 \text{ (Hölder again).} \end{aligned}$$

If $\|\beta_N\|_1 \leq 3\|\beta_S\|_1$ then

$$\|\beta\|_1 = \|\beta_N\|_1 + \|\beta_S\|_1 \leq 4\|\beta_S\|_1 \leq 4\frac{\sqrt{\beta^T\check{\Sigma}\beta}}{\phi_{\check{\Sigma}}/\sqrt{s}}.$$

Thus if $\|\beta_N\|_1 \leq 3\|\beta_S\|_1$,

$$\beta^T\check{\Sigma}\beta - \frac{\phi^2_{\check{\Sigma}}}{32s}\frac{16\beta^T\check{\Sigma}\beta}{\phi^2_{\check{\Sigma}}/s} = \frac{1}{2}\beta^T\check{\Sigma}\beta \leq \beta^T\hat{\Sigma}\beta. \qquad \square$$

We may now apply this with $\check{\Sigma} = \Sigma^0$. To make the result more readily interpretable, we shall state it in an asymptotic framework. Imagine a sequence of design matrices with n and p growing, each with their own compatibility condition. We will however suppress the asymptotic regime in the notation.

Theorem 25. *Suppose the rows of X are i.i.d. and each entry of X is mean-zero sub-Gaussian with parameter v. Suppose $s\sqrt{\log(p)/n} \to 0$ (and $p > 1$) as $n \to \infty$. Let*

$$\begin{aligned} \phi^2_{\hat{\Sigma},s} &= \min_{S:|S|=s} \phi^2_{\hat{\Sigma}}(S) \\ \phi^2_{\Sigma^0,s} &= \min_{S:|S|=s} \phi^2_{\Sigma^0}(S), \end{aligned}$$

and suppose the latter is bounded away from 0. Then $\mathbb{P}(\phi^2_{\hat{\Sigma},s} \geq \phi^2_{\Sigma^0,s}/2) \to 1$ as $n \to \infty$.

Proof. In view of Lemma 24, we need only show that

$$\mathbb{P}(\max_{jk} |\hat{\Sigma}_{jk} - \Sigma^0_{jk}| \geq \phi^2_{\Sigma^0,s}/(32s)) \to 0.$$

Let $t = \phi^2_{\Sigma^0,s}/(32s)$. By a union bound and then Lemma 15 we have

$$\begin{aligned} \mathbb{P}(\max_{jk} |\hat{\Sigma}_{jk} - \Sigma^0_{jk}| \geq \phi^2_{\Sigma^0,s}/(32s)) &< p^2 \max_{jk} \mathbb{P}\Big(\Big|\sum_{i=1}^n X_{ij}X_{ik}/n - \Sigma^0_{jk}\Big| \geq t\Big) \\ &\leq 2\exp\left(-\frac{nt^2}{2(64v^4 + 4v^2t))} + 2\log(p)\right) \\ &\leq c_1\exp(-c_2 n/s^2 + c_3\log(p)) \to 0. \qquad \square \end{aligned}$$

Corollary 26. *Suppose the rows of X are independent with distribution $N_p(0, \Sigma^0)$. Suppose the diagonal entries of Σ^0 are bounded above and the minimum eigenvalue of Σ^0, $c_{\min}$ is bounded away from 0. Then $\mathbb{P}(\phi^2_{\hat{\Sigma},s} \geq c_{\min}/2) \to 1$ provided $s\sqrt{\log(p)/n} \to 0$.*

2.2.7 Computation

One of the most efficient ways of computing Lasso solutions is to use a optimisation technique called *coordinate descent*. This is a quite general way of minimising a function $f : \mathbb{R}^d \to \mathbb{R}$ and works particularly well for functions of the form

$$f(x) = g(x) + \sum_{j=1}^{d} h_j(x_j)$$

where g is convex and differentiable and each $h_j : \mathbb{R} \to \mathbb{R}$ is convex (and so continuous). We start with an initial guess of the minimiser $x^{(0)}$ (e.g. $x^{(0)} = 0$) and repeat for $m = 1, 2, \ldots$

$$\begin{aligned}
x_1^{(m)} &= \arg\min_{x_1 \in \mathbb{R}} f(x_1, x_2^{(m-1)}, \ldots, x_d^{(m-1)}) \\
x_2^{(m)} &= \arg\min_{x_2 \in \mathbb{R}} f(x_1^{(m)}, x_2, x_3^{(m-1)}, \ldots, x_d^{(m-1)}) \\
&\vdots \\
x_d^{(m)} &= \arg\min_{x_d \in \mathbb{R}} f(x_1^{(m)}, x_2^{(m)}, \ldots, x_{d-1}^{(m)}, x_d).
\end{aligned}$$

Tseng [2001] proves that provided $A_0 = \{x : f(x) \leq f(x^{(0)})\}$ is compact, then every converging subsequence of $x^{(m)}$ will converge to a minimiser of f.

Corollary 27. *Suppose A^0 is compact. Then*

(i) There exists a minimiser of f, x^* and $f(x^{(m)}) \to f(x^*)$.

(ii) If x^* is the unique minimiser of f then $x^{(m)} \to x^*$.

Proof. f is a continuous function so it attains its infimum on the compact set A_0. Suppose $f(x^{(m)}) \nrightarrow f(x^*)$. Then there exists $\epsilon > 0$ and a subsequence $(x^{(m_j)})_{j=0}^{\infty}$ such that $f(x^{(m_j)}) \geq f(x^*) + \epsilon$ for all j. Note that since $f(x^{(m)}) \leq f(x^{(m-1)})$, we know that $x^{(m)} \in A_0$ for all m. Thus if A_0 is compact then any subsequence of $(x^{(m)})_{m=0}^{\infty}$ has a further subsequence that converges by the Bolzano–Weierstrass theorem. Let $\tilde{x}$ be the limit of the converging subsequence of $(x^{(m_j)})_{j=0}^{\infty}$. Then $f(\tilde{x}) \geq f(x^*) + \epsilon$, contradicting the result of Tseng [2001]. Thus (i) holds. The proof of (ii) is similar. □

We can replace individual coordinates by blocks of coordinates and the same result holds. That is if $x = (x_1, \ldots, x_B)$ where now $x_b \in \mathbb{R}^{d_b}$ and

$$f(x) = g(x) + \sum_{b=1}^{B} h_b(x_b)$$

with g convex and differentiable and each $h_b : \mathbb{R}^{d_b} \to \mathbb{R}$ convex, then block coordinate descent can be used.

We often want to solve the Lasso on a grid of λ values $\lambda_0 > \cdots > \lambda_L$ (for the purposes of cross-validation for example). To do this, we can first solve for λ_0, and then solve at subsequent grid points by using the solution at the previous grid points as an initial guess (known as a *warm start*). An active set strategy can further speed up computation. This works as follows: For $l = 1, \ldots, L$

1. Initialise $A_l = \{k : \hat{\beta}^{\mathrm{L}}_{\lambda_{l-1},k} \neq 0\}$.

2. Perform coordinate descent only on coordinates in A_l obtaining a solution $\hat{\beta}$ (all components $\hat{\beta}_k$ with $k \notin A_l$ are set to zero).

3. Let $V = \{k : |X_k^T(Y - X\hat{\beta})|/n > \lambda_l\}$, the set of coordinates which violate the KKT conditions when $\hat{\beta}$ is taken as a candidate solution.

4. If V is empty, we set $\hat{\beta}^{\mathrm{L}}_{\lambda_l} = \hat{\beta}$. Else we update $A_l = A_l \cup V$ and return to 2.

2.3 Extensions of the Lasso

We can add an ℓ_1 penalty to many other log-likelihoods, or more generally other loss functions besides the squared-error loss that arises from the normal linear model. For Lasso-penalised generalised linear models, such as logistic regression, similar theoretical results to those we have obtained are available and computations can proceed in a similar fashion to above.

2.3.1 Structural penalties

The Lasso penalty encourages the estimated coefficients to be shrunk towards 0 and sometimes exactly to 0. Other penalty functions can be constructed to encourage different types of sparsity.

Group Lasso

Suppose we have a partition $G_1, \ldots, G_q$ of $\{1, \ldots, p\}$ (so $\cup_{k=1}^q G_k = \{1, \ldots, p\}$, $G_j \cap G_k = \emptyset$ for $j \neq k$). The *group Lasso* penalty [Yuan and Lin, 2006] is given by

$$\lambda \sum_{j=1}^{q} m_j \|\beta_{G_j}\|_2.$$

The multipliers $m_j > 0$ serve to balance cases where the groups are of very different sizes; typically we choose $m_j = \sqrt{|G_j|}$. This penalty encourages either an entire group G to have $\hat{\beta}_G = 0$ or $\hat{\beta}_k \neq 0$ for all $k \in G$. Such a property is useful when groups occur through coding for categorical predictors or when expanding predictors using basis functions.

Fused Lasso

If there is a sense in which the coefficients are ordered, so β_j^0 is expected to be close to β_{j+1}^0, a *fused Lasso* penalty [Tibshirani et al., 2005] may be appropriate. This takes the form

$$\lambda_1 \sum_{j=1}^{p-1} |\beta_j - \beta_{j+1}| + \lambda_2 \|\beta\|_1,$$

where the second term may be omitted depending on whether shrinkage towards 0 is desired. As an example, consider the simple setting where $Y_i = \mu_i^0 + \varepsilon_i$, and it is thought that the $(\mu_i^0)_{i=1}^n$ form a piecewise constant sequence. Then one option is to minimise over $\mu \in \mathbb{R}^n$, the following objective

$$\frac{1}{n}\|Y - \mu\|_2^2 + \lambda \sum_{i=1}^{n-1} |\mu_i - \mu_{i+1}|.$$

2.3.2 Reducing the bias of the Lasso

One potential drawback of the Lasso is that the same shrinkage effect that sets many estimated coefficients exactly to zero also shrinks all non-zero estimated coefficients towards zero. One possible solution is to take $\hat{S}_\lambda = \{k : \hat{\beta}^{\mathrm{L}}_{\lambda,k} \neq 0\}$ and then re-estimate $\beta^0_{\hat{S}_\lambda}$ by OLS regression on $X_{\hat{S}_\lambda}$.

Another option is to re-estimate using the Lasso on $X_{\hat{S}_\lambda}$; this procedure is known as the *relaxed Lasso* [Meinshausen, 2007]. The *adaptive Lasso* [Zou, 2006] takes an initial estimate of β^0, $\hat{\beta}^{\mathrm{init}}$ (e.g. from the Lasso) and then performs weighted Lasso regression:

$$\hat{\beta}^{\mathrm{adapt}}_\lambda = \underset{\beta \in \mathbb{R}^p : \beta_{\hat{S}^c_{\mathrm{init}}} = 0}{\arg\min} \left\{ \frac{1}{2n}\|Y - X\beta\|_2^2 + \lambda \sum_{k \in \hat{S}_{\mathrm{init}}} \frac{|\beta_k|}{|\hat{\beta}^{\mathrm{init}}_k|} \right\},$$

where $\hat{S}_{\mathrm{init}} = \{k : \hat{\beta}^{\mathrm{init}}_k \neq 0\}$.

Yet another approach involves using a family of non-convex penalty functions $p_{\lambda,\gamma} : [0,\infty) \to [0,\infty)$ and attempting to minimise

$$\frac{1}{2n}\|Y - X\beta\|_2^2 + \sum_{k=1}^{p} p_{\lambda,\gamma}(|\beta_k|).$$

A prominent example is the *minimax concave penalty* (MCP) [Zhang, 2010] which takes

$$p'_\lambda(u) = \left(\lambda - \frac{u}{\gamma}\right)_+.$$

One disadvantage of using a non-convex penalty is that there may be multiple local minima which can make optimisation problematic. However, typically if the non-convexity is not too severe, coordinate descent can produce reasonable results.

Chapter 3

High-dimensional covariance estimation and PCA

We shall denote the ℓ_2 norm $\|\cdot\|$, and its unit sphere, $S^{d-1} = \{v \in \mathbb{R}^d; \|v\| = 1\}$. The operator norm of a matrix $M \in \mathbb{R}^{d\times d}$ is defined by

$$\|M\|_{op} = \max_{v\in S^{d-1}} \|Mv\|$$

which is equal to the largest singular value of M. Recall that any symmetric matrix $M \in \mathbb{R}^{d\times d}$ is diagonalisable and denote its eigenvalues $\gamma_1(M) \geq \gamma_2(M) \geq \cdots \geq \gamma_d(M)$. We shall exploit the variational characterisation of eigenvalues

$$\gamma_1(M) = \max_{v\in S^{d-1}} v^T M v; \qquad \gamma_d(M) = \min_{v\in S^{d-1}} v^T M v.$$

Furthermore $\|M\|_{op} = \max\{\gamma_1(M), |\gamma_d(M)|\}$, so we also have the variational representation $\|M\|_{op} = \max_{v\in S^{d-1}} |v^T M v|$. The Frobenius norm will be denoted $\|M\|_F = \sqrt{\mathrm{Tr}(M^T M)}$.

3.1 Covariance estimation

3.1.1 Maximum-likelihood

Let $x_1, \ldots, x_n$ be an i.i.d. sample from $N_d(\mu, \Sigma)$, and suppose we wish to estimate the covariance matrix Σ. Recall that the density of $N_d(\mu, \Sigma)$ is

$$f(z) = \frac{1}{(2\pi)^{d/2}\det(\Sigma)^{1/2}} \exp\bigg(-\frac{1}{2}(z-\mu)^T\Sigma^{-1}(z-\mu)\bigg).$$

The log-likelihood of (μ, Σ) is then

$$\ell(\mu, \Omega) = \frac{n}{2}\log\det(\Omega) - \frac{1}{2}\sum_{i=1}^{n}(x_i-\mu)^T\Omega(x_i-\mu).$$

Write

$$\bar{X} = \frac{1}{n}\sum_{i=1}^{n} x_i, \qquad \hat{\Sigma} = \frac{1}{n}\sum_{i=1}^{n}(x_i - \bar{X})(x_i - \bar{X})^T,$$

where $\hat{\Sigma}$ is often called the empirical or sample covariance. Then

$$\begin{aligned}\sum_{i=1}^{n}(x_i - \mu)^T\Omega(x_i - \mu) &= \sum_{i=1}^{n}(x_i - \bar{X} + \bar{X} - \mu)^T\Omega(x_i - \bar{X} + \bar{X} - \mu) \\ &= \sum_{i=1}^{n}(x_i - \bar{X})^T\Omega(x_i - \bar{X}) + n(\bar{X} - \mu)^T\Omega(\bar{X} - \mu) \\ &\quad + 2\sum_{i=1}^{n}(x_i - \bar{X})^T\Omega(\bar{X} - \mu).\end{aligned}$$

Also,

$$\begin{aligned}\sum_{i=1}^{n}(x_i - \bar{X})^T\Omega(x_i - \bar{X}) &= \sum_{i=1}^{n}\mathrm{tr}\{(x_i - \bar{X})^T\Omega(x_i - \bar{X})\} \\ &= \sum_{i=1}^{n}\mathrm{tr}\{(x_i - \bar{X})(x_i - \bar{X})^T\Omega\} \\ &= n\mathrm{tr}(\hat{\Sigma}\Omega).\end{aligned}$$

Thus

$$\ell(\mu, \Omega) = -\frac{n}{2}\{\mathrm{tr}(\hat{\Sigma}\Omega) - \log\det(\Omega) + (\bar{X} - \mu)^T\Omega(\bar{X} - \mu)\}$$

and

$$\max_{\mu\in\mathbb{R}^p}\ell(\mu, \Omega) = -\frac{n}{2}\{\mathrm{tr}(\hat{\Sigma}\Omega) - \log\det(\Omega)\}.$$

Hence the maximum likelihood estimate of Ω, $\hat{\Omega}^{ML}$ can be obtained by solving

$$\min_{\Omega:\Omega\succ 0}\{-\log\det(\Omega) + \mathrm{tr}(\hat{\Sigma}\Omega)\},$$

where $\Omega \succ 0$ means Ω is positive definite. One can show that the objective is convex and we are minimising over a convex set. As

$$\begin{aligned}\frac{\partial}{\partial\Omega_{jk}}\log\det(\Omega) &= (\Omega^{-1})_{kj} = (\Omega^{-1})_{jk}, \\ \frac{\partial}{\partial\Omega_{jk}}\mathrm{tr}(\hat{\Sigma}\Omega) &= \hat{\Sigma}_{kj} = \hat{\Sigma}_{jk},\end{aligned}$$

if X has full column rank so $\hat{\Sigma}$ is positive definite, $\hat{\Omega}^{ML} = \hat{\Sigma}^{-1}$. As matrix inversion is a bijection on the set of positive definite matrices, we deduce that $\hat{\Sigma}$ is also the maximum likelihood estimator of the covariance Σ.

3.1.2 Non-asymptotic error bounds

In the rest of this section, we will assume for simplicity that $\mu = 0$ and $\hat{\Sigma} = n^{-1}X^TX$, as the mean estimator $\bar{X}$ converges to μ quickly (see example sheet). We start by proving a generic error bound in the operator norm, which is non-asymptotic, in that it holds for any finite problem dimensions (n, d).

Theorem 28. *Let X be an $n \times d$ random matrix with i.i.d. rows $x_1, \dots, x_n$, each of mean 0 and covariance Σ, satisfying the sub-Gaussian condition*

$$\mathbb{E}(e^{\lambda\langle x_1, v\rangle}) \le e^{\frac{\lambda^2\sigma^2}{2}} \quad \text{for all } v \in S^{d-1}.$$

Then, there are universal constants c, C such that $\hat{\Sigma} = n^{-1}X^TX$ satisfies

$$\mathbb{E}(e^{\lambda\|\hat{\Sigma}-\Sigma\|_{op}}) \le e^{c_0\left[\frac{\lambda^2\sigma^4}{n}+d\right]} \qquad \text{for all } |\lambda| < \frac{n}{16\sigma^2} \tag{3.1.1}$$

and with probability at least $1 - e^{-\delta}$,

$$\frac{\|\hat{\Sigma}-\Sigma\|_{op}}{\sigma^2} \le C\left(\frac{d+\delta}{n} \vee \sqrt{\frac{d+\delta}{n}}\right) \qquad \text{for all } \delta > 0. \tag{3.1.2}$$

The theorem guarantees that the sample covariance matrix $\hat{\Sigma}$ is consistent in an asymptotic regime where the number of samples grows more quickly than the dimension of the samples, or $d/n \to 0$.

Proof. The deviation bound (3.1.2) follows from the first inequality (3.1.1) through the Chernoff technique: apply Markov's inequality and minimise the upper bound over $\{\lambda; |\lambda| \le n/(16\sigma^2)\}$. The details will be left as an exercise. It remains to prove the exponential moment bound (3.1.1).

Writing $Q = \hat{\Sigma} - \Sigma$, the operator norm is $\|Q\|_{op} = \max_{v\in S^{d-1}} |v^TQv|$. To bound this, we will use a discretisation argument, covering the sphere S^{d-1} with balls of radius $1/8$ centred at points $v_1, \dots, v_N$. It is possible to find such a covering with $N = e^{4d}/2$. Then, for an arbitrary $v \in S^{d-1}$, there is an i such that $\|v_i - v\| \le 1/8$ and

$$\begin{aligned}|v^TQv| &\le |v_i^TQv_i| + 2|v_i^TQ(v-v_i)| + |(v-v_i)^TQ(v-v_i)| \\ &\le |v_i^TQv_i| + \frac{2}{8}\|Q\|_{op} + \frac{1}{64}\|Q\|_{op} \le v_i^TQv_i + \frac{1}{2}\|Q\|_{op}.\end{aligned}$$

Maximising the right hand side over $v \in S^{d-1}$, we obtain

$$\|Q\|_{op} \le 2\max_{i=1,\dots,N} |v_i^TQv_i|.$$

This implies

$$\mathbb{E}[e^{\lambda\|Q\|_{op}}] \le \mathbb{E}[e^{2\lambda\max_i |v_i^TQv_i|}] \le \sum_{i=1}^N \mathbb{E}[e^{2\lambda v_i^TQv_i}] + \mathbb{E}[e^{-2\lambda v_i^TQv_i}].$$

We claim that for a fixed $u \in S^{d-1}$,

$$\mathbb{E}[e^{tu^TQu}] \leq e^{64\frac{t^2\sigma^4}{n}} \quad \text{for } |t| \leq \frac{n}{8\sigma^2}. \tag{3.1.3}$$

Applying this bound with $t = 2\lambda$ and $t = -2\lambda$ in the previous inequality yields the desired exponential moment bound (3.1.1):

$$\mathbb{E}[e^{\lambda\|Q\|_{op}}] \leq 2Ne^{256\frac{\lambda^2\sigma^4}{n}} = e^{256\frac{\lambda^2\sigma^4}{n}+4d}$$

which holds for $|\lambda| < n/16\sigma^2$.

It only remains to prove the inequality (3.1.3). Observe that

$$u^TQu = \frac{1}{n}u^TX^TXu - u^T\Sigma u = \frac{1}{n}\sum_{i=1}^{n}(u^Tx_i)^2 - u^T\Sigma u,$$

and, as the rows $x_1, \ldots, x_n$ of X are i.i.d.,

$$\mathbb{E}(e^{tu^TQu}) = \prod_{i=1}^{n}\mathbb{E}(e^{\frac{t}{n}[(u^Tx_i)^2 - u^T\Sigma u]}) = \mathbb{E}(e^{\frac{t}{n}[(u^Tx_1)^2 - u^T\Sigma u]})^n \tag{3.1.4}$$

Writing $Z^2 = t(u^Tx_1)^2/n$, the above can be expressed $\mathbb{E}(e^{u^TQu}) \leq \mathbb{E}(e^{Z^2-\mathbb{E}(Z^2)})^n$. By assumption, Z is sub-Gaussian with parameter $\sqrt{|t|\sigma^2/n}$, so Z^2 satisfies the Berstein condition with parameters $(8|t|\sigma^2/n, 4|t|\sigma^2/n)$.Thus,

$$\begin{aligned}
\mathbb{E}(e^{Z^2-\mathbb{E}(Z^2)}) &= 1 + \sum_{k=2}^{\infty}\frac{\mathbb{E}((Z^2-\mathbb{E}(Z^2))^k)}{(k)!} \\
&\leq 1 + \sum_{k=2}^{\infty} 2^{2k+1}\sigma^{2k}\left(\frac{|t|}{n}\right)^k && \text{(by Bernstein condition)} \\
&\leq 1 + \frac{2^5\sigma^4t^2}{n}\frac{1}{1-4\sigma^2|t|/n} && (\text{as } |t| < \frac{n}{4\sigma^2}) \\
&\leq 1 + \frac{64\sigma^4t^2}{n} && (\text{as } |t| < \frac{n}{8\sigma^2}) \\
&\leq e^{64\sigma^4t^2/n^2}.
\end{aligned}$$

Exponentiating by n yields desired upper bound in (3.1.3) when $|t| < n/(8\sigma^2)$. □

Theorem 28 applies to a generic random matrix with sub-Gaussian rows, and because of this generality the proof relies on weak techniques that do not afford fine control over the constants c_0, C. When we assume that the rows of the matrix are Gaussian, $x_i \sim N(0, \Sigma)$ i.i.d. for $i = 1, \ldots, n$, it is possible to obtain tighter constants. More importantly, while the error bound in (3.1.2) is sharp when $\Sigma = I_d$, it can be improved when the true covariance Σ is constrained.

Definition 7. The *effective rank* $r(\Sigma)$ of a covariance matrix is the ratio

$$r(\Sigma) = \frac{\mathrm{Tr}(\Sigma)}{\|\Sigma\|_{op}} = \frac{\sum_{i=1}^{d} \gamma_i(\Sigma)}{\gamma_1(\Sigma)}.$$

The effective rank is in fact a lower bound for the rank, $r(\Sigma) \leq \mathrm{rank}(\Sigma)$, with equality when the non-zero singular values of Σ are equal. The following theorem gives a tighter bound when Σ has low effective rank.

Theorem 29. *Suppose X is a matrix with i.i.d. $N(0, \Sigma)$ rows, with $r(\Sigma) \leq cn$. Then, there exists a constant C such that with probability at least $1 - e^{-\delta}$,*

$$\frac{\|\hat{\Sigma} - \Sigma\|_{op}}{\|\Sigma\|_{op}} \leq C \left(\frac{r(\Sigma) + \delta}{n} \vee \sqrt{\frac{r(\Sigma) + \delta}{n}} \right) \text{ for all } \delta > 0. \tag{3.1.5}$$

Comparing this deviation bound with that in Theorem 28, the main difference is that the dimension of the samples d is replaced by the effective rank $r(\Sigma)$. So the sample covariance is a consistent estimator in the operator norm as long as $r(\Sigma)/n \to 0$, a much weaker assumption.

The bound is in fact dimension free and holds in an infinite-dimensional setting where the samples are realisations of a Gaussian process in a Banach space. A proof in this nonparametric setting may be found in [Koltchinskii and Lounici, 2014]. The proof uses the generic chaining method of Talagrand to bound the supremum of the stochastic process $(v^T Q v)_{v \in S^{d-1}}$ in expectation and its fluctuations.

A slightly weaker result is shown more succinctly in Theorem 6.1 of [Wainwright, 2019], using Gaussian process comparison techniques. Section 6.4 of [Wainwright, 2019] includes non-asymptotic error bounds which relax the sub-Gaussian assumption and apply to more general distributions.

3.1.3 The Graphical Lasso

We have seen that the sample covariance matrix $\hat{\Sigma}$ can be an efficient estimator of Σ when the effective rank, $r(\Sigma)$, is low relative to the number of samples, n. However, in very high-dimensional applications, it may become necessary to make further structural assumptions on Σ and to use regularised estimators. The graphical Lasso [Yuan and Lin, 2007] is one example.

For a normal variable $Z \sim N(\mu, \Sigma)$, it can be reasonable to assume that the precision matrix $\Omega = \Sigma^{-1}$ is sparse. This is because zeros of the precision matrix encode conditional independence relationships between pairs of variables, as shown in the following proposition. The assumption that two entries, Z_j and Z_k, are conditionally independent given all the other entries Z_{-jk}, is often a natural one, implying that one variable only influences the other *through* the remaining variables.

Proposition 30. *Let $Z \sim N(\mu, \Omega^{-1})$ and assume that Ω is of full rank, then $Z_k \perp\!\!\!\perp Z_j \mid Z_{-jk}$ if and only if $\Omega_{jk} = 0$.*

Proof. The conditional density of $Z_j, Z_k \mid Z_{-jk}$ is

$$\begin{aligned} f(z_j, z_k \mid z_{-jk}) &\propto \exp\left(-\frac{1}{2}(z-\mu)^T\Omega(z-\mu)\right) \\ &= \exp\left(-\frac{1}{2}\sum_{i,\ell}(z-\mu)_i\Omega_{i,\ell}(z-\mu)_\ell\right) \\ &= g(z_j)h(z_k)\exp\left(-z_jz_k\Omega_{jk}\right) \end{aligned}$$

where $g(z_j)$ collects factors depending only on z_j and $h(z_k)$ factors depending only on z_k. Clearly, the density factorises over z_j and z_k if and only if $\Omega_{jk} = 0$. □

The *graphical Lasso* penalises the log-likelihood for Ω and solves

$$\min_{\Omega:\Omega\succ 0}\{-\log\det(\Omega) + \operatorname{tr}(\hat{\Sigma}\Omega) + \lambda\|\Omega\|_1\},$$

where $\|\Omega\|_1 = \sum_{j,k}|\Omega_{jk}|$; this results in a sparse estimate of the precision matrix. Often the $\|\Omega\|_1$ is modified such that the diagonal elements are not penalised.

3.2 Principal Components Analysis

Principal Components Analysis (PCA) is a classical technique invented by Karl Pearson in 1901. The procedure is based on estimating the eigenvectors of the covariance matrix using the sample covariance matrix. We assume the rows of $X \in \mathbb{R}^{n\times d}$ are i.i.d. with covariance Σ, and let $\lambda_1 \geq \lambda_2 \geq \ldots \lambda_d \geq 0$ be eigenvalues of Σ with eigenvectors $u_i \in S^{d-1}$ with $\Sigma u_i = \lambda_i u_i$ for each $i = 1, \ldots, d$. For any $s \leq d$, the span of $u_1, \ldots, u_s$ can be interpreted as the linear subspace with maximum variance:

$$\operatorname{span}(u_1, \ldots, u_s) = \underset{S\subseteq\mathbb{R}^d, \dim(S)=s}{\arg\max} \mathbb{E}(\|\Pi_S x_1\|^2) \tag{3.2.1}$$

where Π_S is the orthogonal projection onto S. Alternatively, it may be seen as the subspace which lies closest to the data in the Euclidean distance

$$\operatorname{span}(u_1, \ldots, u_s) = \underset{S\subseteq\mathbb{R}^d, \dim(S)=s}{\arg\min} \mathbb{E}(\|x_1 - \Pi_S x_1\|^2). \tag{3.2.2}$$

The residual variance is $\lambda_{s+1} + \cdots + \lambda_d$. If this is small, projecting the samples onto the span of $u_1, \ldots, u_s$ can yield a powerful representation of data with many variables, allowing us to visualise the samples in a low-dimensional plot.

PCA approximates the eigenfunctions $u_1, \ldots, u_d$ with the *principal directions*, which are the eigenvectors $\hat{u}_1, \ldots, \hat{u}_d$ of the sample covariance $\hat{\Sigma}$. The principal directions have similar variational characterisations as (3.2.1) and (3.2.2) where the expectations are replaced by their empirical counterparts. Finally a dual eigendecomposition of the Gram matrix

$$(X - \mathbf{1}\bar{X}^T)(X - \mathbf{1}\bar{X}^T)^T$$

yields a useful low-dimensional representation of the variables, or columns of X.

Understanding the accuracy of PCA thus amounts to understanding the error of eigenvectors estimated from a noisy matrix $\hat{\Sigma} = \Sigma + E$. We will see that PCA is not consistent when d is comparable or larger than n. This will motivate the development of regularised estimators, and we will discuss sparse PCA as one example.

3.2.1 Perturbation of eigenvalues and eigenvectors

In this section, we assume the error matrix E is deterministic and symmetric. Eigenvalues are in general robust to small perturbations. For the top eigenvalue, this is a straightforward consequence of the variational characterisation

$$\begin{aligned}\hat{\lambda}_1 &= \max_{v \in S^{d-1}} v^T(\Sigma + E)v \\ &\leq \max_{v \in S^{d-1}} v^T \Sigma v + \max_{v \in S^{d-1}} v^T E v \\ &\leq \lambda_1 + \|E\|_{op}\end{aligned}$$

Writing $\Sigma = \hat{\Sigma} - E$ and applying the same argument yields $|\hat{\lambda}_1 - \lambda_1| \leq \|E\|_{op}$. The following theorem due to Hermann Weyl generalises this to other eigenvalues.

Theorem 31 (Weyl's theorem)**.** $\max_{i=1,\dots,d} |\hat{\lambda}_i - \lambda_i| \leq \|E\|_{op}$.

The eigenvectors of the sample covariance are not in general robust to noise (see example sheet). This is because a slight perturbation in the matrix can change the order of the eigenvalues. To avoid this, we must assume there is a gap in the spectrum separating the eigenvectors of interest from the rest.

We will characterise the error in eigenvectors using the $\sin\Theta$ distance between linear subspaces of $\mathbb{R}^d$. Let S and U be two matrices with orthonormal columns and equal rank; the $\sin\Theta$ distance between the column space of S and U is

$$\sin\Theta(S, U) = \|\Pi_S(I - \Pi_U)\|_F = \|\Pi_U(I - \Pi_S)\|_F.$$

The $\sin\Theta$ distance satisfies the following inequality (see example sheet),

$$\min_{O \in \mathbb{R}^{d\times d} \text{ orthogonal}} \|S - UO\|_F \leq \sqrt{2}\sin\Theta(S, U). \tag{3.2.3}$$

Theorem 32 (Davis–Kahan)**.** *For a covariance matrix Σ, suppose $\Sigma u_i = \lambda_i u_i$ for $i = 1, \dots, d$ with $\lambda_1 \geq \cdots \geq \lambda_d$. Write $\Sigma = U_0\Lambda_0 U_0^T + U_1\Lambda_1 U_1^T$ where $U_0 = [u_1, \dots, u_r]$, $U_1 = [u_{r+1}, \dots, u_d]$. For a perturbed matrix $\hat{\Sigma} = \Sigma + E$ with E symmetric, we define the decomposition $\hat{\Sigma} = \hat{U}_0\hat{\Lambda}_0\hat{U}_0^T + \hat{U}_1\hat{\Lambda}_1\hat{U}_1^T$ in the same way. If $\lambda_r - \hat{\lambda}_{r+1} > 0$, then*

$$\sin\Theta(U_0, \hat{U}_0) = \|\Pi_{U_0}(I - \Pi_{\hat{U}_0})\|_F \leq \frac{\|E\|_F}{\lambda_r - \hat{\lambda}_{r+1}}.$$

Proof. Rewrite the left hand side

$$\|\Pi_{U_0}(I - \Pi_{\hat{U}_0})\|_F = \|U_0 U_0^T(\hat{U}_1\hat{U}_1^T)\|_F = \|U_0^T\hat{U}_1\|_F.$$

Now, as $\Sigma U_0 = U_0\Lambda_0 U_0^T U_0 + U_1\Lambda_1 U_1^T U_0 = U_0\Lambda_0$, we have

$$EU_0 = EU_0 + \Sigma U_0 - \Sigma U_0 = \hat{\Sigma}U_0 - U_0\Lambda_0.$$

By the same reasoning $\hat{\Sigma}\hat{U}_1 = \hat{U}_1\hat{\Lambda}_1$, and multiplying the equation above by $\hat{U}_1^T$,

$$\hat{U}_1^T EU_0 = \hat{U}_1^T\hat{\Sigma}U_0 - \hat{U}_1^T U_0\Lambda_0 = \hat{\Lambda}_1\hat{U}_1^T U_0 - \hat{U}_1^T U_0\Lambda_0.$$

Now, letting $a = (\lambda_1 + \lambda_r)/2$ and $b = (\lambda_1 - \lambda_r)/2$,

$$\begin{aligned}\|\hat{U}_1^T EU_0\|_F &= \|(\hat{\Lambda}_1 - aI)\hat{U}_1^T U_0 - \hat{U}_1^T U_0(\Lambda_0 - aI)\|_F \\ &\geq \|(\hat{\Lambda}_1 - aI)\hat{U}_1^T U_0||_F - \|\hat{U}_1^T U_0(\Lambda_0 - aI)\|_F, \end{aligned} \tag{3.2.4}$$

by the triangle inequality. Now, the entries of $\Lambda_0 - aI$ are by construction in $[-b, b]$ and those of $\hat{\Lambda}_1 - bI$ are outside $[-b - |\lambda_r - \hat{\lambda}_{r+1}|, b + |\lambda_r - \hat{\lambda}_{r+1}|]$, hence

$$\begin{aligned}\|(\Lambda_0 - aI)\hat{U}_1^T U_0||_F &\leq b\|\hat{U}_1^T U_0||_F \\ \|\hat{U}_1^T U_0(\hat{\Lambda}_1 - aI)||_F &\geq (b + |\lambda_r - \hat{\lambda}_{r+1}|)\|\hat{U}_1^T U_0||_F.\end{aligned}$$

Plugging these bounds into (3.2.4),

$$\|\hat{U}_1^T EU_0\|_F \geq (\lambda_r - \hat{\lambda}_{r+1})\|\hat{U}_1^T U_0\|_F.$$

Noting that $\|\hat{U}_1^T EU_0\|_F \leq \|E\|_F$ yields the desired inequality. □

The following variant of the Davis–Kahan theorem due to Yu et al. [2014] makes the spectral gap in the denominator depend only on the eigenvalues of the population covariance Σ.

Theorem 33. *Under the assumptions of the previous theorem,*

$$\sin\Theta(U_0, \hat{U}_0) \leq \frac{2\min\{\sqrt{r}\|E\|_{op}, \|E\|_F\}}{|\lambda_r - \lambda_{r+1}|}.$$

This theorem will allow us to control the error in the dominant eigenspace of the sample covariance using bounds on $\|\hat{\Sigma} - \Sigma\|_{op}$, like those derived in the previous section.

3.2.2 The spiked covariance model

A useful model for a covariance matrix with a spectral gap is a mixture of a rank-1 matrix and the identity:

$$\Sigma = \theta v v^T + I_d,$$

for some $v \in S^{d-1}$. A random vector with covariance Σ can be thought of as a sum $\eta\sqrt{\theta}v + \varepsilon$, where $\eta, \varepsilon_1, \ldots, \varepsilon_d$ are independent, variance 1 random variables. In words, the samples are a random "spike" with scale $\sqrt{\theta}$ in a fixed direction v, with independent noise added to each entry.

The eigenvalues of Σ are $1+\theta, 1, \ldots, 1$, where the eigenvector with eigenvalue $1+\theta$ is v. We're interested estimating v using the top eigenvector $\hat{v}$ of the sample covariance matrix $\hat{\Sigma}$. Theorem 33 and inequality (3.2.3) imply that, with probability 1,

$$\min_{\epsilon \in \{-1,1\}} \|v - \epsilon\hat{v}\| \leq 2^{3/2} \frac{\|\hat{\Sigma} - \Sigma\|_{op}}{\theta}.$$

If we assume that the rows of X are sub-Gaussian, as in Theorem 28, we can bound $\|\hat{\Sigma} - \Sigma\|_{op}$ in probability, leading to

$$\mathbb{P}\left(\min_{\epsilon \in \{-1,1\}} \|v - \epsilon\hat{v}\| \geq C\frac{1+\theta}{\theta}\left(\frac{d+\delta}{n} \vee \sqrt{\frac{d+\delta}{n}}\right)\right) \leq e^{-\delta}$$

for some constant C and any $\delta > 0$. Therefore, if the signal strength θ is fixed, PCA will be consistent if $d/n \to 0$.

3.2.3 High-dimensional asymptotics

How good is PCA in the spiked covariance model when d/n stays bounded away from 0? Much work at the intersection of Probability and Statistical Physics has been devoted to this question in the regime $d/n \to \gamma > 0$. A celebrated result of Marčenko and Pastur is a formula for the limiting CDF of sample eigenvalues, $F(\cdot) = \lim_{n\to\infty} d^{-1}\sum_{i=1}^{d} \mathbb{1}(\hat{\lambda}_i \leq \cdot)$. When $\Sigma = I$, F is a semi-circle law, supported on the interval $[1-\sqrt{\gamma})^2, (1+\sqrt{\gamma})^2]$. Whereas the eigenvalues of $\Sigma = I$ are all 1, the empirical eigenvalues are spread out.

In the spiked covariance model $\Sigma = \theta v v^T + I$, a phase transition occurs at $\theta = \sqrt{\gamma}$. Below the critical value, $\theta < \sqrt{\gamma}$, the sample eigenvalue $\hat{\lambda}_1$ is buried in the Marčenko–Pastur distribution. It is located around $(1+\sqrt{\gamma})^2$, with fluctuations of order $d^{-2/3}$ following the Tracy–Widom distribution. The eigenvector estimator $\hat{v}$ is asymptotically orthogonal to v, i.e. PCA is no better than estimating a random principal direction.

On the other hand, above the critical value $\theta > \sqrt{\gamma}$, the top eigenvalue $\hat{\lambda}_1$ emerges from the "bulk" of the Marčenko–Pastur distribution, with an upward bias of known magnitude. Its fluctuations around the expected value are asymptotically Gaussian with scale $n^{-1/2}$. In this case, the overlap $|\hat{v}^T v|$ is bounded away from zero asymptotically. These facts are summarised in Fig. 3.1 from Johnstone and Paul [2018], where you may find a friendly introduction to this vast literature.

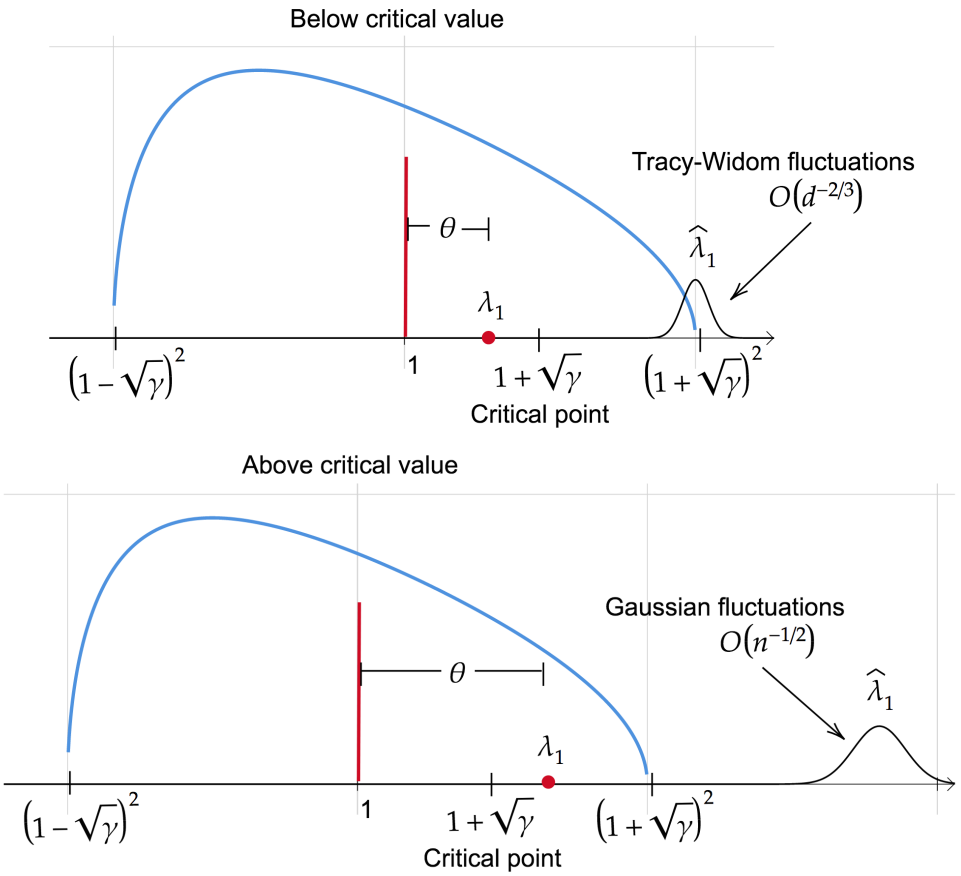

Figure 3.1: [Johnstone and Paul, 2018]. Asymptotic behaviour of sample eigenvalues in the spiked covariance model when $d/n \to \gamma = 1/4$. The true eigenvalues are shown in red. The Marčenko–Pastur distribution of sample eigenvalues is shown in blue. The top panel illustrates the subcritical case $\lambda_1 < 1+\sqrt{\gamma}$, where the sample eigenvector $\hat{v}$ is asymptotically orthogonal to v. The bottom panel shows the supercritical case $\lambda_1 < 1 + \sqrt{\gamma}$.

3.3 Sparse PCA

We have seen that in the spiked covariance model, PCA is consistent when $d/n \to 0$, but when d/n is bounded away from zero it can fail dramatically. This begs the question of whether a more sophisticated estimator could be consistent for general θ when, for example, $d/n \to \gamma > 0$. The answer is negative, as minimax lower bounds show that the dependence of the risk on d/n cannot be improved without making further assumptions about the eigenvector v.

In many applications, it is reasonable to assume that the leading eigenvectors of Σ are sparse. For example, in a gene expression study where gene expressions are recorded for a large number of genes (variables) across a range of conditions (samples), it is plausible that the principal directions involve only a small number of genes. This motivates the

development of sparse PCA.

Suppose $\Sigma = \theta vv^T + I_d$ with $\|v\|_0 \leq k$. Our first estimator is the solution to the following optimisation, which is similar in spirit to best subset selection,

$$\hat{v}^{(0,k')} = \underset{v \in S^{d-1}, \|v\|_0 \leq k'}{\arg\max} v^T \hat{\Sigma} v$$

The following proposition will be proven in the examples class, using the tools developed thus far.

Proposition 34. *Let $\hat{\Sigma}$ be the sample covariance of i.i.d. $N(0, \Sigma)$ random variables. Suppose $k \leq d/2$ and $k \leq k'$, then*

$$\mathbb{P}\left(\min_{\epsilon \in \{-1,1\}} \|v - \epsilon \hat{v}^{(0,k')}\| \geq C \frac{1+\theta}{\theta} \left[\sqrt{\eta_n} \vee \eta_n \right] \right) \leq e^{-\delta} \text{ for all } \delta > 0,$$

with

$$\eta_n = \frac{(k+k') \log(de^2/(k+k')) + \delta}{n}.$$

The dependence of the error on d is now logarithmic. While this estimator has good properties, computing it naïvely would require searching over all subsets of $\{1, \ldots, d\}$ with k' elements. The SCoTLASS estimator proposed by Jolliffe et al. [2003] produces sparse estimators by constraining an ℓ_1 norm:

$$\hat{v}^{(1,\lambda)} = \underset{v \in S^{d-1}, \|v\|_1 \leq \lambda}{\arg\max} v^T \hat{\Sigma} v. \tag{3.3.1}$$

The SCoTLASS estimator $\hat{v}^{(1,\lambda)}$ for well-chosen λ enjoys similar convergence rates as the estimator $\hat{v}^{(0,k')}$, with the error scaling as $\sqrt{k \log d / n}$ [Wainwright, 2019, Corollary 8.12].

Unlike the Lasso, (3.3.1) is not a convex optimisation problem, as we are maximising a convex function. To remedy this, we can define a semidefinite relaxation of the problem which can be solved quickly (see example sheet). Nonetheless, sparse PCA seems to be inherently difficult computationally, and Wang et al. [2016] have shown that there are no estimators computable in polynomial time which achieve the minimax rate for certain distribution classes.

Chapter 4

Multiple testing and high-dimensional inference

In many modern applications, we may be interested in testing many hypotheses simultaneously. Suppose we are interested in testing null hypotheses $H_1, \dots, H_m$ of which m_0 are true and $m - m_0$ are not (we do not mention the alternative hypotheses explicitly). Consider the following contingency table:

	Claimed non-significant	Claimed significant (reject)	Total
True null hypotheses	N_{00}	N_{01}	m_0
False null hypotheses	N_{10}	N_{11}	$m - m_0$
Total	$m - R$	R	m

The N_{jj} are unobserved random variables; R is observed.

Suppose we have p-values $p_1, \dots, p_m$ associated with $H_1, \dots, H_m$ and H_i, $i \in I_0$ are the true null hypotheses, so

$$\mathbb{P}(p_i \leq \alpha) \leq \alpha$$

for all $\alpha \in [0, 1]$, $i \in I_0$. Traditional approaches to multiple testing have sought to control the familywise error rate (FWER) defined by

$$\text{FWER} = \mathbb{P}(N_{01} \geq 1)$$

at a prescribed level α; i.e. find procedures for which FWER $\leq \alpha$. The simplest such procedure is the *Bonferroni correction*, which rejects H_i if $p_i \leq \alpha/m$.

Theorem 35. *Using Bonferroni correction,*

$$\mathbb{P}(N_{01} \geq 1) \leq \mathbb{E}(N_{01}) \leq \frac{m_0 \alpha}{m} \leq \alpha.$$

Proof. The first inequality comes from Markov's inequality. Next

$$\begin{aligned}\mathbb{E}(N_{01}) &= \mathbb{E}\left(\sum_{i\in I_0} \mathbb{1}_{\{p_i \leq \alpha/m\}}\right) \\ &= \sum_{i\in I_0} \mathbb{P}(p_i \leq \alpha/m) \\ &\leq \frac{m_0\alpha}{m}.\end{aligned}$$

□

A more sophisticated approach is the closed testing procedure.

4.1 The closed testing procedure

Given our family of hypotheses $\{H_i\}_{i=1}^m$, define the *closure* of this family to be

$$\{H_I : I \subseteq \{1,\ldots,m\},\ I \neq \emptyset\}$$

where $H_I = \cap_{i\in I} H_i$ is known as an *intersection hypothesis* (H_I is the hypothesis that all H_i $i \in I$ are true).

Suppose that for each I, we have an α-level test ϕ_I taking values in $\{0,1\}$ for testing H_I (we reject if $\phi_I = 1$), so under H_I,

$$\mathbb{P}_{H_I}(\phi_I = 1) \leq \alpha.$$

The ϕ_I are known as *local tests*.

The *closed testing procedure* [Marcus et al., 1976] is defined as follows:

Reject H_I if and only if for all $J \supseteq I$,
H_J is rejected by the local test ϕ_J.

Typically we only make use of the individual hypotheses that are rejected by the procedure i.e. those rejected H_I where I is a singleton.

We consider the case of 4 hypotheses as an example. Suppose the underlined hypotheses are rejected by the local tests.

$$\begin{array}{cccccc} & & & \underline{H_{1234}} & & \\ & & \underline{H_{123}} & \underline{H_{124}} & \underline{H_{134}} & \underline{H_{234}} \\ \underline{H_{12}} & \underline{H_{13}} & \underline{H_{14}} & \underline{H_{23}} & H_{24} & H_{34} \\ & & \underline{H_1} & \underline{H_2} & H_3 & H_4 \end{array}$$

- Here H_1 is rejected be the closed testing procedure.
- H_2 is not rejected by the closed testing procedure as H_{24} is not rejected by the local test.

- H_{23} is rejected by the closed testing procedure.

Theorem 36. *The closed testing procedure makes no false rejections with probability* $1-\alpha$. *In particular it controls the FWER at level* α.

Proof. Assume I_0 is not empty (as otherwise no rejection can be false anyway). Define the events

$$A = \{\text{at least one false rejection}\} \supseteq \{N_{01} \geq 1\},$$
$$B = \{\text{reject } H_{I_0} \text{ with the local test}\} = \{\phi_{I_0} = 1\}.$$

In order for there to be a false rejection, we must have rejected H_{I_0} with the local test. Thus $B \supseteq A$, so

$$\text{FWER} \leq \mathbb{P}(A) \leq \mathbb{P}(\phi_{I_0} = 1) \leq \alpha. \qquad \square$$

Different choices for the local tests give rise to different testing procedures. *Holm's procedure* takes ϕ_I to be the Bonferroni test i.e.

$$\phi_I = \begin{cases} 1 & \text{if } \min_{i \in I} p_i \leq \frac{\alpha}{|I|} \\ 0 & \text{otherwise.} \end{cases}$$

It can be shown (see example sheet) that Holm's procedure amounts to ordering the p-values $p_1, \ldots, p_m$ as $p_{(1)} \leq \cdots \leq p_{(m)}$ with corresponding hypothesis tests $H_{(1)}, \ldots, H_{(m)}$, so (i) is the index of the ith smallest p-value, and then performing the following.

Step 1. If $p_{(1)} \leq \alpha/m$ reject $H_{(1)}$, and go to step 2. Otherwise accept $H_{(1)}, \ldots, H_{(m)}$ and stop.

Step i. If $p_{(i)} \leq \alpha/(m-i+1)$, reject $H_{(i)}$ and go to step $i+1$. Otherwise accept $H_{(i)}, \ldots, H_{(m)}$.

Step m. If $p_{(m)} \leq \alpha$, reject $H_{(m)}$. Otherwise accept $H_{(m)}$.

The p-values are visited in ascending order and rejected until the first time a p-value exceeds a given critical value. This sort of approach is known (slightly confusingly) as a *step-down* procedure.

4.2 The False Discovery Rate

A different approach to multiple testing does not try to control the FWER, but instead attempts to control the *false discovery rate* (FDR) defined by

$$\text{FDR} = \mathbb{E}(\text{FDP})$$
$$\text{FDP} = \frac{N_{01}}{\max(R, 1)},$$

where FDP is the *false discovery proportion*. Note the maximum in the denominator is to ensure division by zero does not occur. The FDR was introduced in Benjamini and Hochberg [1995], and it is now widely used across science, particularly biostatistics.

The *Benjamini–Hochberg procedure* attempts to control the FDR at level α and works as follows. Let

$$\hat{k} = \max\left\{ i : p_{(i)} \leq \frac{i\alpha}{m} \right\}.$$

Reject $H_{(1)}, \ldots, H_{(\hat{k})}$ (or perform no rejections if $\hat{k}$ is not defined).

Theorem 37. *Suppose that the p_i, $i \in I_0$ are independent, and independent of $\{p_i : i \notin I_0\}$. Then the Benjamini–Hochberg procedure controls the FDR at level α; in fact $FDR \leq \alpha m_0/m$.*

Proof. For each $i \in I_0$, let R_i denote the number of rejections we get by applying a modified Benjamini–Hochberg procedure to

$$p^{\setminus i} := \{p_1, p_2, \ldots, p_{i-1}, p_{i+1}, \ldots, p_m\}$$

with cutoff

$$\hat{k}_i = \max\left\{ j : p^{\setminus i}_{(j)} \leq \frac{\alpha(j+1)}{m} \right\},$$

where $p^{\setminus i}_{(j)}$ is the jth smallest p-value in the set $p^{\setminus i}$.

For $r = 1, \ldots, m$ and $i \in I_0$, note that

$$\begin{aligned}
\left\{ p_i \leq \frac{\alpha r}{m},\, R = r \right\} &= \left\{ p_i \leq \frac{\alpha r}{m},\, p_{(r)} \leq \frac{\alpha r}{m},\, p_{(s)} > \frac{\alpha s}{m} \text{ for all } s > r \right\} \\
&= \left\{ p_i \leq \frac{\alpha r}{m},\, p^{\setminus i}_{(r-1)} \leq \frac{\alpha r}{m},\, p^{\setminus i}_{(s-1)} > \frac{\alpha s}{m} \text{ for all } s > r \right\} \\
&= \left\{ p_i \leq \frac{\alpha r}{m},\, R_i = r - 1 \right\}.
\end{aligned}$$

Thus

$$\begin{aligned}
\mathrm{FDR} &= \mathbb{E}\left(\frac{N_{01}}{\max(R,1)}\right) \\
&= \sum_{r=1}^{m} \mathbb{E}\left(\frac{N_{01}}{r}\mathbb{1}_{\{R=r\}}\right) \\
&= \sum_{r=1}^{m} \frac{1}{r}\mathbb{E}\left(\sum_{i\in I_0} \mathbb{1}_{\{p_i \le \alpha r/m\}}\mathbb{1}_{\{R=r\}}\right) \\
&= \sum_{r=1}^{m} \frac{1}{r}\sum_{i\in I_0} \mathbb{P}(p_i \le \alpha r/m,\, R=r) \\
&= \sum_{r=1}^{m} \frac{1}{r}\sum_{i\in I_0} \mathbb{P}(p_i \le \alpha r/m)\mathbb{P}(R_i = r-1) \\
&\le \frac{\alpha}{m}\sum_{i\in I_0}\sum_{r=1}^{m} \mathbb{P}(R_i = r-1) \\
&= \frac{\alpha m_0}{m}.
\end{aligned}$$

□

4.3 Inference in high-dimensional regression

Consider the normal linear model $Y = X\beta^0 + \varepsilon$ where $\varepsilon \sim N_n(0, \sigma^2 I)$. In the low-dimensional setting, the fact that $\hat{\beta}^{\mathrm{OLS}} - \beta^0 \sim N_p(0, \sigma^2(X^TX)^{-1})$ allows us to form confidence intervals for components of β_j^0 and perform hypothesis tests with $H_0 : \beta_j^0 = 0$, for example.

One might hope that studying the distribution of $\hat{\beta}_\lambda^{\mathrm{L}} - \beta^0$ would enable us to perform these tasks in the high-dimensional setting when $p \gg n$. However, the distribution of $\hat{\beta}_\lambda^{\mathrm{L}} - \beta^0$ is intractable and depends delicately on the unknown β^0, making it unsuitable as a basis for establishing confidence intervals.

Whilst several methods have been proposed over the years, typically they have involved placing conditions on the unknown β^0, other than the usual assumption of sparsity. Given that the task is to perform inference for β^0, such conditions are undesirable. In the last couple of years, there has been a breakthrough on this front [Zhang and Zhang, 2014, Van de Geer et al., 2014], and here we will aim to cover the main ideas in this exciting development. Our treatment follows Van de Geer et al. [2014].

We begin our investigation by considering the KKT conditions of the Lasso. Fix $\lambda > 0$ and let $\hat{\beta}$ be the Lasso estimator with tuning parameter λ. Recall that the KKT conditions give

$$\frac{1}{n}X^T(Y - X\hat{\beta}) = \lambda\hat{\nu}$$

where $\|\hat{\nu}\|_\infty \le 1$ and writing $\hat{S} = \{k : \hat{\beta}_k \neq 0\}$, $\hat{\nu}_{\hat{S}} = \mathrm{sgn}(\hat{\beta}_{\hat{S}})$. Setting $\hat{\Sigma} = X^TX/n$ and

rearranging we have

$$\hat{\Sigma}(\hat{\beta} - \beta^0) + \lambda\hat{\nu} = \frac{1}{n}X^T\varepsilon.$$

The key idea is now to form an approximate inverse $\hat{\Theta}$ of $\hat{\Sigma}$. Then we have

$$\hat{\beta} + \lambda\hat{\Theta}\hat{\nu} - \beta^0 = \frac{1}{n}\hat{\Theta}X^T\varepsilon + \frac{1}{\sqrt{n}}\Delta$$

where $\Delta = \sqrt{n}(\hat{\Theta}\hat{\Sigma} - I)(\beta^0 - \hat{\beta})$. Define

$$\hat{b} = \hat{\beta} + \lambda\hat{\Theta}\hat{\nu} = \hat{\beta} + \hat{\Theta}X^T(Y - X\hat{\beta})/n,$$

which we shall refer to as the *debiased Lasso*. If we choose $\hat{\Theta}$ such that Δ is small, we will have $\hat{b} - \beta^0 \approx \hat{\Theta}X^T\varepsilon/n$, which can be used as a basis for performing inference.

We already know that under a compatibility condition on the design matrix X, $\|\hat{\beta}-\beta^0\|_1$ is small (Theorem 23) with high probability. If we can also show that the ℓ_∞-norms of rows of $\hat{\Theta}\hat{\Sigma} - I$ are small, we can leverage this fact using Hölder's inequality to show that $\|\Delta\|_\infty$ is small. Let $\hat{\theta}_j$ be the jth row of $\hat{\Theta}$. Then $\|(\hat{\Sigma}\hat{\Theta}^T - I)_j\|_\infty \leq \eta$ is equivalent to

$$\frac{1}{n}\|X_{-j}^T X\hat{\theta}_j\|_\infty \leq \eta \text{ and } |X_j^T X\hat{\theta}_j/n - 1| \leq \eta.$$

The first of these inequalities is somewhat reminiscent of the KKT conditions for the Lasso. Let

$$\hat{\gamma}^{(j)} = \underset{\gamma\in\mathbb{R}^{p-1}}{\arg\min}\left\{\frac{1}{2n}\|X_j - X_{-j}\gamma\|_2^2 + \lambda_j\|\gamma\|_1\right\}. \tag{4.3.1}$$

Further let

$$\hat{\tau}_j^2 = X_j^T(X_j - X_{-j}\hat{\gamma}^{(j)})/n = \frac{1}{n}\|X_j - X_{-j}\hat{\gamma}^{(j)}\|_2^2 + \lambda_j\|\hat{\gamma}^{(j)}\|_1;$$

see the example sheet for the final equality. Then set

$$\hat{\theta}_j = -\frac{1}{\hat{\tau}_j^2}(\hat{\gamma}_1^{(j)}, \ldots, \hat{\gamma}_{j-1}^{(j)}, -1, \hat{\gamma}_j^{(j)}, \ldots, \hat{\gamma}_{p-1}^{(j)})^T.$$

$$\uparrow$$

$$j\text{th position}$$

Note that by construction,

$$X\hat{\theta}_j = \frac{X_j - X_{-j}\hat{\gamma}^{(j)}}{X_j^T(X - X_{-j}\hat{\gamma}^{(j)})/n}.$$

Thus $X_j^T X\hat{\theta}_j/n = 1$ and by the KKT conditions of the Lasso optimisation (4.3.1), we have $\hat{\tau}_j^2\|X_{-j}^T X\hat{\theta}_j\|_\infty/n \leq \lambda_j$.

Thus with the choice of $\hat{\Theta}$ defined as above, we have

$$\|\Delta\|_\infty \leq \sqrt{n}\|\hat{\beta} - \beta^0\|_1 \max_j \frac{\lambda_j}{\hat{\tau}_j^2}$$

When can we expect $\lambda_j/\hat{\tau}_j^2$ to be small? One way of answering this is to consider a random design setting. Let us assume that each row of X is independent and distributed as $N_p(0, \Sigma)$ where Σ is positive definite. Write $\Omega = \Sigma^{-1}$. As a consequence of normality, we can write for each j,

$$X_j = X_{-j}\gamma^{(j)} + \varepsilon^{(j)}, \tag{4.3.2}$$

where $\varepsilon_i^{(j)}|X_{-j} \overset{\text{i.i.d.}}{\sim} N(0, \Omega_{jj}^{-1})$ and $\gamma^{(j)} = -\Omega_{jj}^{-1}\Omega_{-j,j}$. Theorem 23 can therefore be used to understand properties of $\hat{\gamma}^{(j)}$ and hence the $\hat{\tau}_j^2$. In order to apply this result however, we need $\gamma^{(j)}$ to be sparse. Let us therefore define

$$s_j = \sum_{k \neq j} \mathbb{1}_{\{\Omega_{kj} \neq 0\}}$$

and $s_{\max} = \max(\max_j s_j, s)$. In order to make the following result more easily interpretable, we will consider an asymptotic regime where $X, s, s_{\max}$ etc. are all allowed to change as $n \to \infty$, though we suppress this in the notation. We will consider σ as constant.

Theorem 38. *Suppose the minimum eigenvalue of Σ is always at least $c_{\min} > 0$ and $\max_j \Sigma_{jj} \leq 1$. Suppose further that $s_{\max}\sqrt{\log(p)/n} \to 0$. Then there exists constants A_1, A_2 such that setting $\lambda = \lambda_j = A_1\sqrt{\log(p)/n}$, we have*

$$\begin{aligned}\sqrt{n}(\hat{b} - \beta^0) &= W + \Delta \\ W|X &\sim N_p(0, \sigma^2\hat{\Theta}\hat{\Sigma}\hat{\Theta}^T),\end{aligned}$$

and as $n, p \to \infty$,

$$\mathbb{P}(\|\Delta\|_\infty > A_2 s\log(p)/\sqrt{n}) \to 0.$$

Proof. Consider the sequence of events Λ_n described by the following properties:

- $\phi^2_{\hat{\Sigma},s} \geq c_{\min}/2$ and $\phi^2_{\hat{\Sigma}_{-j,-j},s_j} \geq c_{\min}/2$ for all j,
- $2\|X^T\varepsilon\|_\infty/n \leq \lambda$ and $2\|X_{-j}^T\varepsilon^{(j)}\|_\infty/n \leq \lambda$ for all j,
- $\|\varepsilon^{(j)}\|_2^2/n \geq \Omega_{jj}^{-1}(1 - 4\sqrt{\log(p)/n})$ for all j.

You will show on the example sheet that then $\mathbb{P}(\Lambda_n) \to 1$ for A_1 sufficiently large. In the following we work on Λ_n, and $c_1, c_2, \ldots$ will be constants.

By Theorem 23, we have

$$\|\hat{\beta} - \beta^0\|_1 \leq c_1 s\sqrt{\log(p)/n}.$$

We now seek a lower bound for the $\hat{\tau}_j^2$. Consider the linear models in (4.3.2). Note that the maximum eigenvalue of Ω is at most $c_{\min}^{-1}$ so $\Omega_{jj} \leq c_{\min}^{-1}$. Also, $\Omega_{jj}^{-1} = \mathrm{Var}(X_{ij}|X_{i,-j}) \leq \mathrm{Var}(X_{ij}) = \Sigma_{jj} \leq 1$. Thus applying Theorem 23 to the linear models (4.3.2), we know that

$$\|\gamma^{(j)} - \hat{\gamma}^{(j)}\|_1 \leq c_2 s_j \sqrt{\log(p)/n}.$$

Then

$$\begin{aligned}
\hat{\tau}_j^2 \geq \frac{1}{n}\|X_j - X_{-j}\hat{\gamma}^{(j)}\|_2^2 &\geq \frac{1}{n}\|\varepsilon^{(j)}\|_2^2 - \frac{2}{n}\|X_{-j}^T\varepsilon^{(j)}\|_\infty \|\gamma^{(j)} - \hat{\gamma}^{(j)}\|_1 \\
&\geq \Omega_{jj}^{-1}(1 - 4\sqrt{\log(p)/n}) - \frac{c_4 s_{\max}\log(p)}{n} \\
&\geq c_{\min}/2
\end{aligned}$$

for all j when n is sufficiently large. Putting things together we see that on Λ_n,

$$\begin{aligned}
\|\Delta\|_\infty &\leq \lambda\sqrt{n}\|\hat{\beta} - \beta^0\|_1 \max_j \hat{\tau}_j^{-2} \\
&\leq 2A_1\sqrt{\log(p)}(c_1 s\sqrt{\log(p)/n})/c_{\min} \leq A_2 s\log(p)/\sqrt{n}
\end{aligned}$$

where $A_2 = 2c_1A_1/c_{\min}$. Thus

$$\mathbb{P}(\|\Delta\|_\infty > A_2 s\log(p)/\sqrt{n}) \leq \mathbb{P}(\Lambda_n^c) \to 0. \qquad \square$$

4.3.1 Using the debiased Lasso in practice

Theorem 38 shows in particular that

$$\sqrt{n}(\hat{b}_j - \beta_j^0) \approx W_j$$

where $W_j \sim N(0, \sigma^2(\hat{\Theta}\hat{\Sigma}\hat{\Theta}^T)_{jj})$. Let $(\hat{\Theta}\hat{\Sigma}\hat{\Theta}^T)_{jj} = d_j$. The approximate equality above suggests constructing (1-α)-level confidence intervals of the form

$$\Big[\hat{b}_j - z_{\alpha/2}\sigma\sqrt{d_j}/\sqrt{n},\ \hat{b}_j + z_{\alpha/2}\sigma\sqrt{d_j}/\sqrt{n}\Big],$$

where z_α is the upper α point of a standard normal. The only unknown quantity in the confidence interval above is σ: this can be estimated [Sun and Zhang, 2012].

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