Machine Learning

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Contents

Machine learning in the 1980s have been focused on developing rigorous theory of learning algorithms, and the field has been dominated by statisticians. They strived to develop the theoretical foundation of algorithms that can be implemented and applied to real-world data. These days, machine learning is more of an engineering discipline than a science. With the advent of deep learning, the theory behind these black box algorithms has slowed down, but their applications have exploded. It is now a field of trying out a bunch of things and sticking to what works. These set of notes are for the former theory, while my deep learning notes are for the latter. It is covered in a separate set of notes since a lot of space is needed to talk about recent developments and architectures (e.g. RCNN, YOLO, LSTMs, Transformers, VAEs, GANs, etc.). We will focus more on establishing the theoretical foundations of most learning algorithms and analyze interpretable algorithms.

I've spent a good amount of time trying to create a map of machine learning, but after rewriting these notes multiple times. I've come to the conclusion that it is impossible to create a nice chronological map of machine learning. Like math, you keep on revisiting the same topics over and over again, but at a higher level, and it's not as simple to organize everything into parametric vs nonparametric[1], supervised vs unsupervised[2], or discriminative vs generative models.[3] Therefore, this is what I recommend.

1. If you are new to machine learning, go over my notes on Stanford CS229, which simply covers basic algorithms and their implementation.
2. Now you can learn the deeper theory of machine learning. This is what these notes are for.

You should know measure (probability) theory, a bit of functional analysis, and some statistics. I will reintroduce all the necessary definitions in a way that is as general as possible, as we move along. Some places where I got this information from

1. Larry Wasserman's Statistical Machine Learning course at CMU.
2. Bishop's Pattern Recognition and Machine Learning by Christopher Bishop.
3. Cynthia Rudin's CS671 Machine Learning course at Duke.
4. Olivier Bousquet's Introduction to Statistical Learning Theory notes at MPI.

1 Statistical Learning Theory

Unlike unsupervised learning, which comes in many different shapes and forms (anomaly detection, feature extraction, density estimation, dimensionality reduction, etc.), supervised learning comes in a much cleaner format. In supervised learning, we consider an input space $\mathcal{X}$ and an output space $\mathcal{Y}$. We assume that there exists some unknown measure $\mathbb{P}$ over $\mathcal{X} \times \mathcal{Y}$, making this some probability space. We then assume that some data $\mathcal{D} = \{(x^{(i)}, y^{(i)})\}$ is generated sampled *independently and identically (iid)* from $\mathbb{P}$. Now this assumption is quite strong and is almost always not the case, as different data can be correlated, but we will relax this assumption later. Let's formally construct this from the bottom up.

1. We start off with a general probability space $(\Omega, \mathcal{F}, \mathbb{P})$. This is our model of the world and everything that we are interested in.
2. A measurable function $X : \Omega \to \mathcal{X}$ extracts a set of features, which we call the **covariates** and induces a probability measure on $\mathcal{X}$, say $\mathbb{P}_X$.
3. Another measurable function $Y : \Omega \to \mathcal{Y}$ extracts another set of features called the **labels** and induces another probability measure on $\mathcal{Y}$, the **label set**, say $\mathbb{P}_Y$.
4. At this point the function $X \times Y$ is all we are interested in, and we throw away Ω since we only care about the distribution over $\mathcal{X} \times \mathcal{Y}$.

[1] K nearest neighbors is a nonparameteric model given that the data is not fixed. When the data is fixed, then our function search space is finite.

[2] There are semi-supervised or weakly supervised models, and models like autoencoders use a supervised algorithm without any labels.

[3] Using Bayes rule, we can always reduce generative models into discriminative models.

5. We model the generation of data from Ω by sampling N samples from $\mathbb{P}_{X\times Y}$, which we assume to be iid (this assumption will be relaxed later). This gives us the **dataset**

$$\mathcal{D} = \{(\mathbf{x}^{(i)}, \mathbf{y}^{(i)})\}_{i=1}^{N}$$

Now our goal is to construct a function $f : \mathcal{X} \to \mathcal{Y}$ that predicts Y from X, but we want to define some measure of how good our function is. We can use a loss function L to talk about this.

Definition 1.1 (Risk)

The **risk**, or **expected risk**, of function f is defined as

$$R(f) = \mathbb{E}_{X\times Y}[L(Y, f(X))] = \int_{\mathcal{X}\times\mathcal{Y}} L(y, f(x))\, d\mathbb{P}(x, y) \tag{1}$$

Clearly, we don't know what this risk is since we don't know the true measure $\mathbb{P}$, so we try to approximate it with the *empirical risk*.

Definition 1.2 (Empirical Risk)

The **empirical risk** of function f is defined as

$$\hat{R}_n(f) = \frac{1}{n}\sum_{i=1}^{n} L(y^{(i)}, f(x^{(i)})) \tag{2}$$

Definition 1.3 (Generlize)

A function f is said to **generalize** if

$$\lim_{n\to+\infty} \hat{R}_n(f) = R(f) \tag{3}$$

This gives us a way of computing with the actual data. Now two questions arise from this. First, how do we even choose the loss function L? Second, how do we know that the empirical risk is a good approximation of the true risk? The first question can be quite convoluted, but we introduce it with decision theory. The second has a simple answer with concentration of measure.

1.1 Decision Theory

How can we choose our loss functions? There are two ways of doing this, either through model assumptions or with domain knowledge. When talking about model assumptions, we assume that the residual distribution is of certain form, and the maximum likelihood formulation leads to a certain loss function. For example, assuming that the residuals are normally distributed leads to the squared loss or Laplacian residuals leads to the absolute value loss. These are just modeling assumptions, and if there are no specific assumptions, we are lost. The other way is through domain expertise which allows us to construct our own loss functions. Fortunately, there is a deeper theory behind the choice of loss functions, known as decision theory, which allows us to define loss functions from the get go rather than assume distributions taking particular forms.[4]

[4]Credits to Edric for telling me this.

Definition 1.4 (Misclassification Loss)

The **misclassification loss** is defined as

$$L(y, \hat{y}) = \begin{cases} 0 & \text{if } y = \hat{y} \\ 1 & \text{if } y \neq \hat{y} \end{cases} \tag{4}$$

Example 1.1 (Misclassification Risk)

Substituting the misclassification loss function into the risk gives the **misclassification risk**.

$$R(f) = \mathbb{E}[\mathbb{1}_{\{Y \neq f(X)\}}] = \mathbb{P}(Y \neq f(X)) \tag{5}$$

and therefore our empirical risk is

$$\hat{R}(f) = \frac{1}{n} \sum_{i=1}^{n} \mathbb{1}_{\{y^{(i)} \neq f(x^{(i)})\}} \tag{6}$$

which is just the number of misclassifications over the total number of samples.

However, depending on the context, the loss for misclassification one one label can be quite different from that of another label. Consider the medical example where you're trying to detect cancer. Falsely detecting a non-cancer patient as having cancer is not as bad as falsely detecting a cancer patient as not having cancer.

Definition 1.5 (Weighted Misclassification Loss)

The **loss matrix** K defines the loss that we incur when predicting the ith class on a sample with true label j.

$$L(y, \hat{y}) = \begin{cases} 0 & \text{if } y = \hat{y} \\ K_{ij} & \text{if } y = i \neq j = \hat{y} \end{cases} \tag{7}$$

Definition 1.6 (Squared Loss)

The **squared loss** is defined as

$$L(y, \hat{y}) = (y - \hat{y})^2 \tag{8}$$

Example 1.2 (Mean Squared Risk)

Substituting the squared loss function into the risk gives the **mean squared risk**.

$$R(f) = \mathbb{E}[(Y - f(X))^2] \tag{9}$$

and therefore our empirical risk is

$$\hat{R}(f) = \frac{1}{n} \sum_{i=1}^{n} (y^{(i)} - f(x^{(i)})^2 \tag{10}$$

Definition 1.7 (Absolute Loss)

The **absolute loss** is defined as

$$L(y, \hat{y}) = |y - \hat{y}| \tag{11}$$

1.2 Function Classes

Now that we've defined the risk and empirical risk, the true function that we want to find is the one that minimizes the empirical risk.

$$f^* = \underset{f \in \mathcal{F}}{\operatorname{argmin}} \hat{R}(f) \tag{12}$$

However, this depends on the function space $\mathcal{F}$ that we are minimizing over. If we chose f to be the space of all functions, then we just interpolate (fit perfectly over) the data[5], which is not good since we're **overfitting**. This is a problem especially in nonparametric supervised learning, and there are generally two ways to deal with this. The first is to use *localization*, which deals with local smoothing methods. The second is with **regularization**. The third is to restrict our class of functions to a smaller set. Perhaps we assume that nature is somewhat smooth and so naturally we want to work with smooth functions. There are two ways that we define smoothness, through Holder spaces that focus on local smoothness and Sobolev spaces that focus on global smoothness.

Definition 1.8 (L^p Space)

The $L^p(\mu)$ space is the normed vector space of all functions from $f : \mathcal{X} \to \mathbb{R}$ such that

$$||f||_p = \left(\int |f(x)|^p \, d\mu \right)^{1/p} < \infty \tag{13}$$

Theorem 1.1 (Countable Basis)

You can construct a countable orthonormal basis in $L^2(\mu)$ space.

There are a lot of well known orthonormal bases. For example, the Fourier basis, Legendre polynomials, Hermite polynomials, or wavelets. Therefore, every function can be expressed as a linear combination of this basis, and you can calculate coefficients by taking the inner product with the basis functions.

$$f(x) = \sum_{i=1}^{\infty} \alpha_i \phi_i(x) \text{ and } \alpha_i = \langle f, \phi_i \rangle \tag{14}$$

Now we can define Holder spaces. Holder spaces are used whenever we want to talk about local smoothness. For example, when we want to talk about local smoothing methods for regression and classification, talking about this smoothing is not quite possible if we don't have certain assumptions on the function. To make theory easier, we assume that the function has basic smoothness properties and this property is Holder smoothness. But note that these are ultimately assumptions.

Definition 1.9 (Holder Space)

For some $\beta \in \mathbb{N}$ and $L \in \mathbb{R}^+$, the $H(\beta, L)$ **Holder space** is the set of all functions $f : \mathcal{X} \subset \mathbb{R} \to \mathbb{R}$ such that

$$|f^{(\beta-1)}(y) - f^{(\beta-1)}(x)| \leq L||y - x|| \tag{15}$$

for all x, y. If we want $\mathcal{X}$ to be d-dimensional, then we want to bound the higher order total derivatives, and so $H(\beta, L)$ becomes all functions $f : \mathcal{X} \subset \mathbb{R}^d \to \mathbb{R}$ such that for all $\mathbf{s} = (s_1, \dots, s_d)$ with $|\mathbf{s}| = \beta - 1$,

$$|D^{\mathbf{s}} f(x) - D^{\mathbf{s}} f(x)| \leq L||y - x|| \tag{16}$$

for all $x, y \in \mathcal{X}$, where

$$D^{\mathbf{s}} = \frac{\partial^{|\mathbf{s}|}}{\partial x_1^{s_1} \dots \partial x_d^{s_d}} \tag{17}$$

The higher β is, the more smoothness we're demanding.

[5] unless there were two different values of Y for the same X

If $\beta = 1$, then this reduces to the set of all Lipschitz functions. It is most common to assume that $\beta = 2$, which means that the derivative is Lipschitz. This is not rigorously true, but by dividing both sides by $||y - x||$ and taking the limit to 0, we can say that it implies that there exists some finite second derivative bounded by L.

Definition 1.10 (Sobolev Space)

The **Sobelov space** $W_{m,p}$ is the space of all functions $f \in L_p(\mu)$ such that

$$||D^m f||_p \in L^p(\mu) \tag{18}$$

This is slightly stronger than the usual definition of Sobolev spaces since we requiring the derivative rather than the weak derivative. So m tells us how many derivatives we want well behaved and p tells us under which norm are the derivatives well behaved.

Now there is a related definition of a Sobelov ellipsoid that we'll be working with.

Definition 1.11 (Sobelov Ellipsoid)

Let $\theta = (\theta_1, \theta_2, \dots)$ be a sequence of real numbers. Then the set

$$\Theta_m = \left\{ \theta \mid \sum_{j=1}^{\infty} a_j^2 \theta_j^2 < C^2 \right\} \tag{19}$$

where $a_j^2 = (\pi \cdot j)^{2m}$. Note that since a_j is exploding, to stay finite the θ_j must be decaying.

This is useful because of the following theorem.

Theorem 1.2 (Conditions for Function being in Sobelov Space)

Given a function $f \in L^2(\mu)$ expanded in some orthonormal basis ϕ_j, then $f \in W_{m,2}$ if and only if the coefficients α_j die off fast enough in the sense that it is in the Sobelov ellipsoid.

Now let's talk about RKHS. Let's take the $L^2(\mu)$ space of functions $f : [0, 1] \to \mathbb{R}$ with $||f|| = \int f^2 \, d\mu < \infty$ and inner product $\langle f, g \rangle = \int f(x) g(x) \, d\mu$. It is known that if f_n converges to f in L^2, then it is not necessarily true that f converges pointwise since it can diverge on a sequence of sets that converge to measure 0. You probably don't want to work with functions that look like this, and that's what a RKHS is for. It gives you a nice class of functions that have good statistical properties but also are easy to compute with.

Definition 1.12 (Mercer Kernels)

A **Mercer kernel** is a function $K : \mathbb{R} \times \mathbb{R} \to \mathbb{R}$ that is symmetric and positive definite in the sense that for any collection $x_1, \dots, x_n$ of arbitrary size n,

$$\sum_i \sum_j c_i c_j K(x_i, x_j) \geq 0 \tag{20}$$

which is equivalent to saying that the matrix formed by evaluating these kernels at the pairs of points is positive semi-definite.

Example 1.3 (Gaussian Kernel)

The Gaussian kernel is defined

$$K(x,y) = \exp\left(-\frac{||x-y||^2}{\sigma^2}\right) \tag{21}$$

Now this kernel should tell us roughly how similar two points x and y are. Using this kernel, we want to build a function space. For this, we need Mercer's theorem.

Theorem 1.3 (Mercer's Theorem)

If we have a kernel K that is bounded

$$\sup_{x,y} K(x,y) < \infty \tag{22}$$

we can define a new operator T_K that maps functions to functions

$$T_K f(x) = \int K(x,y)f(y)\,dy = \iint K(x,y)f(x)f(y)\,dx\,dy \tag{23}$$

This operator is linear, meaning that it has an eigendecomposition and therefore there exists eigenfunctions ϕ_i s.t.

$$T_K\phi_i(x) = \int K(x,y)\phi_i(y)\,dy = \lambda_i\phi_i(x) \tag{24}$$

Then these eigenvalues are bounded and we can write the kernel as a sum of the eigenfunctions.

$$\sum_i \lambda_i < \infty, \quad K(x,y) = \sum_{i=1}^{\infty} \lambda_i\phi_i(x)\phi_i(y) \tag{25}$$

These ϕ_i's are the implicit high-dimensional features.

What do these eigenfunctions ϕ_i look like? Well, they tend to look like functions that tend to get wigglier and wigglier as i increases, indicating that λ_i must decrease in such a way that it still keeps the function smooth.

Now, we can fix the first term in the kernel and it will be function of the second term $K_x(\cdot) = K(x,\cdot)$. We do this for all $x \in \mathbb{R}$, which form the basis of our RKHS, and it consists of all functions that are linear combinations of these K_x's. For example, the functions

$$f = \sum_i \alpha_i K_{x_i} \text{ and } g = \sum_j \beta_j K_{x_j} \tag{26}$$

can consist of a finite number of perhaps different basis functions. Now this is clearly a vector space, and to upgrade this to a Hilbert space, we must define an inner product. This inner product (with respect to some kernel K) is defined as

$$\langle f,g\rangle_K = \sum_{i,j} \alpha_i\beta_j K(x_i,x_j) \tag{27}$$

Exercise 1.1 (Inner Product of RKHS)

Show that the inner product of the RKHS is indeed an inner product.

The inner product induces a norm, and so by taking the completion of all linear combinations of the kernel basis functions we get our RKHS. Now since K_x is itself in the RKHS, we can take the inner product of f and K_x, which just gives us back the evaluation of f at x.

Definition 1.13 (Reproducing Kernel Hilbert Space)

Given a kernel K, the **reprducing kernel Hilbert space** $\mathcal{H}$ is the Hilbert space of all functions $f : \mathcal{X} \to \mathcal{Y}$ that can be expressed as a linear combination of the functions $\{K_x = K(x, \cdot)\}$. It has the inner product

$$\langle f, g \rangle_{\mathcal{H}} = \sum_{i,j} \alpha_i \beta_j K(x_i, x_j) \tag{28}$$

and also includes all of its limit points under this norm, making it a complete space.

Theorem 1.4 (Reproducing Property of RKHS)

An RKHS satisfies the **reproducing property**, which means that taking the inner product of a function f and a kernel K_x gives you the evaluation of f at x.

$$\langle f, K_x \rangle_{\mathcal{H}} = f(x) \tag{29}$$

and therefore it also means that $\langle K_x, K_x \rangle_{\mathcal{H}} = K(x, x)$. This also means that K_x is the evaluation functional in the dual space of $\mathcal{H}$ and this evaluation functional δ_x is continuous, which is not always true in functional analysis.

Proof.

We can evaluate from the inner product

$$f = \sum_i \alpha_i K_{x_i} \implies \langle f, K_x \rangle_K = \sum_i \alpha_i \langle K_{x_i}, K_x \rangle_K = \sum_i \alpha_i K(x_i, x) = f(x) \tag{30}$$

This reproducing property tends to be very useful, especially in the corollary below.

Corollary 1.1 (Convergence in RKHS)

Convergence in norm implies pointwise convergence in RKHS.

Proof.

Given that $f_n \to f$ in norm, we have that $||f_n - f|| \to 0$. Then for all points $x \in \mathcal{X}$,

$$|f_n(x) - f(x)| = |\langle f_n - f, K_x \rangle_{\mathcal{H}}| \leq ||f_n - f|| \cdot ||K_x|| \to 0 \tag{31}$$

Theorem 1.5 (Moore-Aronszajn)

Any positive definite function K is a reproducing kernel for some RKHS.

Proof.

We won't be too rigorous about this since this is not a functional analysis course. Assume that we have a positive definite kernel $K : X \times X \to \mathbb{R}$, where X is some measurable set, and we will show how to make a RKHS $\mathcal{H}_k$ such that K is the reproducing kernel on $\mathcal{H}$. It turns out that $\mathcal{H}_k$ is unique up to isomorphism. Since X exists, let us first define the set $S = \{k_x \mid x \in X\}$ such that $k_x(y) \coloneqq K(x, y)$. Now let us define the vector space V to be the span of S. Therefore, each element

$v \in V$ can be written as

$$v = \sum_i \alpha_i k_{x_i}$$

Now we want to define an inner product on V. By expanding out the vectors w.r.t. the basis and the properties of bilinearity, we have

$$\langle k_x, k_y \rangle_V = \left\langle \sum_i \alpha_i k_{x_i}, \sum_i \beta_i k_{y_i} \right\rangle = \sum_{i,j} \alpha_i \beta_j K(x_i, y_j)$$

At this point, V is not necessarily complete, but we can force it to be complete by taking the limits of all Cauchy sequences and adding them to V. In order to complete the construction, we need to ensure that K is continuous and doesn't diverge, i.e.

$$\iint K^2(x,y)\,dx\,dy < +\infty$$

which is a property known as finite trace.[a]

Now at first glance, this abstract construction makes it hard to determine what kind of functions there are in a RKHS generated by some kernel. Conversely, given some RKHS, it's not always easy to know which kernel it came from.

Example 1.4 (Fourier Basis)

Let us take the vector space of all real functions f for which its Fourier transform is supported on some finite interval $[-a, a]$. This is a RKHS with the kernel function

$$K(x,y) = \frac{\sin(a(y-x))}{a(y-x)} \tag{32}$$

with the inner product $\langle f, g \rangle = \int f(x)g(x)\,dx$.

Example 1.5 (Some Sobelov Spaces are RKHS)

Let us take the Sobelov space $W_{1,2}$ of all functions $f : [0,1] \to \mathbb{R}$ satisfying

$$\int (f'(x))^2\,dx < \infty \tag{33}$$

This is a RKHS with the kernel function

$$K(x,y) = \begin{cases} 1 + xy + \frac{xy^2}{2} - \frac{y^3}{6} & \text{if } 0 \le y \le x \le 1 \\ 1 + xy + \frac{x^2 y}{2} - \frac{x^3}{6} & \text{if } 0 \le x \le y \le 1 \end{cases} \tag{34}$$

Finally, remembering Mercer's theorem, we can decompose the Kernel into its eigenfunctions

$$K(x,y) = \sum_{j=1}^{\infty} \lambda_j \phi_j(x) \phi_j(y) \tag{35}$$

When you talk about feature maps (e.g. in support vector machines), you're really just creating the map from $x \in \mathcal{X}$ into the infinite dimensional vector space

$$x \mapsto \Phi(x) = \left(\sqrt{\lambda_1}\phi_1(x), \sqrt{\lambda_2}\phi_2(x), \dots\right) \tag{36}$$

[a] Too much to write down here at this point, but for further information look at *thearticlehere*.

and the inner product between two functions is actually the inner product between their feature maps. Therefore, you can either just work with x in the RKHS or work with the features Φ in a higher dimensional Euclidean space. Therefore, we can either work with f as a combination of kerenels or a linear combination of the eigenfunctions. The eigenfunctions are easier conceptually, but when we actually do computations, the kernel expansion is much easier.

$$f(x) = \sum_i \alpha_i K(x_i, x) = \sum_j \beta_j \phi_j(x) \tag{37}$$

When you're expanding with the eigenfunctions, you can just compute the inner product as

$$\langle f, g \rangle = \sum_i \frac{\alpha_i \beta_i}{\lambda_i} \tag{38}$$

and because f, g must satisfy some smoothness constraints, the α_i and β_i must die off quickly, making the sum finite. But we're never going to be actually computing this way since it's much easier to compute with the kernel expansion. This means that the ϕ_i's, which get wigglier (think of sine and cosine eigenbases) as i increases, must have decreasing coefficients.

When working with function classes, we tend to divide them into two broad categories.

Definition 1.14 (Parametric Models)

A **parametric model** is a set of functions $\mathcal{M}_{\boldsymbol{\theta}}$ that can be parameterized by a finite-dimensional vector. The elements of this model are hypotheses functions $h_{\boldsymbol{\theta}}$, with the subscript used to emphasize that its parameters are $\boldsymbol{\theta}$. We have the flexibility to choose any form of h that we want, and that is ultimately a model assumption that we are making.

Example 1.6 (Examples of Parametric Models)

1. If we assume $h : \mathbb{R}^D \to \mathbb{R}$ to be linear, then h lives in the dual of $\mathbb{R}^D$, which we know to be D-dimensional.
2. If we assume h to be affine, then this just adds one more dimension.
3. If we assume $h : \mathbb{R} \to \mathbb{R}$ to be a kth degree polynomial, then g can be parameterized by a $k+1$ dimensional θ.

However, parametric models may be limited in the way that we are assuming some form about the data. For certain forms of data, where we may have domain knowledge, it is reasonable to use parametric models, but there are cases when we will have absolutely no idea what the underlying distribution is. For example, think of classifying a $3 \times N \times N$ image as a cat or a dog. There is some underlying distribution in the space $[255]^{3N^2} \times \{\text{cat}, \text{dog}\}$, but we have absolutely no idea how to parameterize this. Should it be a linear model or something else? This is when nonparametric models come in. They are not restricted by the assumptions concerning the nature of the population from which the sample is drawn.

Definition 1.15 (Nonparametric Models)

Nonparametric models are ones that cannot be expressed in a finite set of parameters. They may be countably or uncountably infinite.

1.3 Concentration of Measure

Concentration of measure is a tool used to prove a lot of theorems in statistical machine learning. I have another series of notes on this, but we'll stick to the key points.

Definition 1.16 (Hoeffding's Inequality)

Given $X_1, \dots, X_n$ are iid random variables with $a \leq X_i \leq b$, then for any $\epsilon > 0$,

$$\mathbb{P}\left(\left| \frac{1}{n} \sum_{i=1}^{n} X_i - \mathbb{E}[X] \right| \geq \epsilon \right) \leq 2 \exp\left(- \frac{2n\epsilon^2}{(b-a)^2} \right) \tag{39}$$

Therefore, if we apply it to some binary classifier $f : \mathcal{X} \to \{0, 1\}$, then we can say that the probability that the empirical risk deviates from the true risk is exponentially small.

$$\mathbb{P}(|\hat{R}(f) - R(f)| \geq \epsilon) \leq 2e^{-2n\epsilon^2} \tag{40}$$

But when we do empirical risk minimization (ERM), we not given a classifier, but we must *choose* it. So given our space of classifiers f, we can plot the true risk and the noisy empirical risk. The equation above states that at any given point the probability of it deviating by more than ϵ is exponentially small. But we want something stronger: we want to bound the probability of the supremum of the difference over the whole class $\mathcal{F}$.

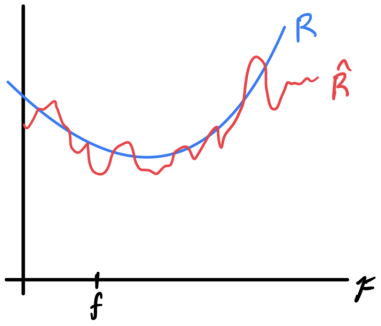


Figure 1: True risk of functions over $\mathcal{F}$ and its noisy empirical risk. We want to bound the maximum deviation of these two over the whole class.

$$\mathbb{P}\big(\sup_{f \in \mathcal{F}} |\hat{R}(f) - R(f)| \geq \epsilon \big) \tag{41}$$

This bound will depend on how *complex* the function class $\mathcal{F}$ is, and to measure this complexity, we introduce some definitions.

Definition 1.17 (Rademacher Complexity)

Given **Rademacher random variables** $\sigma_1, \dots, \sigma_n$ with $\mathbb{P}(\sigma_i = 1) = \mathbb{P}(\sigma_i = -1) = \frac{1}{2}$, the **Rademacher complexity** of a function class $\mathcal{F}$ is defined

$$\text{Rad}_n(\mathcal{F}) = \mathbb{E}\left[\sup_{f \in \mathcal{F}} \left| \frac{1}{n} \sum_{i=1}^{n} \sigma_i f(Z_i) \right| \right] \tag{42}$$

where the expectation is across the random σ_i's and the Z_i's, which are independent.

To get some intuition of what this is, let's consider a function class of a single function f. Then, the sup disappears and the term inside the absolute value sign becomes a 0-mean random variable. Now if we have a very complex function class $\mathcal{F}$ with a lot of "wiggly" functions, then this value should be large. In this case, imagine a game where you pick generate some random variables σ_i and the Z_i. Then, I pick a function that maximizes this value. How can I do that? If I can find a function f that matches the sign of the σ_i's (+1 or

-1) at each of the values of Z_i, then this would be maximized. Therefore, if I have a sufficiently complex class, then I can pick a function that tracks your σ_i's. Another way of looking at it is given noise variables σ and Z, we're looking at the correlation between σ and $f(Z)$. If we can maximize this correlation, then this is a complex class.

Now this is the most natural way of defining the complexity of the class, and in some cases it can be explicitly computed. However, in most cases it cannot be, but it can be bounded be something that is computable, like the VC dimension.

Lemma 1.1 (Bigger Class, Bigger Complexity)

If $\mathcal{F} \subset \mathcal{G}$, then $\text{Rad}_n(\mathcal{F}) \leq \text{Rad}_n(\mathcal{G})$.

Lemma 1.2 (Convex Hull)

If $\mathcal{F}$ is a convex set, then $\text{Rad}_n(\mathcal{F}) = \text{Rad}_n(\text{conv}(\mathcal{F}))$, where $\text{conv}(\mathcal{F})$ is the convex hull of $\mathcal{F}$.

This lemma is quite useful since if we have a certain finite set of functions, then their convex hull can encompass quite a bit, and we can also easily compute that convex hull's Rademacher complexity. Since the extremes haven't changed, the complexity doesn't change, and this might suggest that the Rademacher complexity is a good measure.

Lemma 1.3 (Change of Complexity with Lipschitz Functions)

Consider a L-Lipschitz function g with $g(0) = 0$ and consider the class $\mathcal{F}$, then we can bound the class of functions $g \circ \mathcal{F} = \{g \circ f \mid f \in \mathcal{F}\}$.

$$\text{Rad}_n(g \circ \mathcal{F}) \leq 2L\text{Rad}_n(\mathcal{F}) \tag{43}$$

This constant multiplicative bound is also useful.

Definition 1.18 (Projection of Function Class onto Points)

Given a binary function class $\mathcal{F}$ with functions $f : \mathcal{X} \to \{0, 1\}$, let us denote the projection of $\mathcal{F}$ onto a set of points $z_1, \dots, z_n \in \mathcal{X}$ to be

$$\mathcal{F}_z = \mathcal{F}_{z_1,\dots,z_n} = \{(f(z_1), \dots, f(z_n)) \mid f \in \mathcal{F}\} \tag{44}$$

This projection determines the set of all possible binary labels that can be perfectly classified by some function f.

Definition 1.19 (Shattering Number)

The **shattering number** of $\mathcal{F}$ is defined

$$s_n(\mathcal{F}) = s(\mathcal{F}, n) = \sup_{z_1,\dots,z_n} |\mathcal{F}_{z_1,\dots,z_n}| \tag{45}$$

The highest number that this can be is 2^n, since this is the number of possible binary vectors of length n. Given a set of n points $z_1, \dots, z_n$, we say that the function class $\mathcal{F}$ **shatters** this set if $\mathcal{F}_{z_1,\dots,z_n} = |2^n|$. That is, for every one of the 2^n labels on the points, there exists a function that can perfectly classify them.

Example 1.7 (Binary Functions)

Consider the function class $\mathcal{F}$ of all binary functions of the form

$$f(x) = \begin{cases} 1 & \text{if } x > t \\ 0 & \text{if } x \leq t \end{cases} \tag{46}$$

Then, the projection of $\mathcal{F}$ onto some $n = 3$ points is the set

$$\{(0,0,0), (0,0,1), (0,1,1), (1,1,1)\} \tag{47}$$

and this is true no matter how I pick the z_1, z_2, z_3, and so the Shattering number is $s_n(\mathcal{F}) = 4$.

Definition 1.20 (VC Dimension)

We know that the shattering number is bounded above by 2^n. For $n = 1$, it is reasonable that it achieves this bound, but as n grows, the Shattering number may die off. The point at which it dies off is the VC dimension.

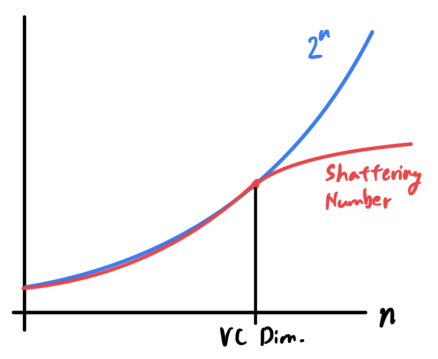


Figure 2: The Shattering number of $\mathcal{F}$ will grow exponentially until it reaches the VC dimension, at which point it will grow polynomially.

That is, it is the largest n number of points that can be shattered by the function class without misclassification.

$$n^{\text{VC}} := \sup_n \{s_n(\mathcal{F}) = 2^n\} \tag{48}$$

It turns out that there are very interesting properties about the VC dimension. One such fact is Sawyer's lemma, which states that if the VC dimension is finite, then the rate of growth of the shattering number suddenly changes from exponential 2^n to polynomial n^{VC}, and this is what makes a lot of machine learning work.

Definition 1.21 (Subgaussian Random Variables)

A random variable X is **subgasussian** if

$$\mathbb{E}[e^{\lambda X}] \leq e^{\frac{\lambda^2 \sigma^2}{2}} \tag{49}$$

Gaussians and bounded random variables are subgaussian.

Lemma 1.4 (Bound on Subgaussian Random Variables)

Given a set of iid subgaussian random variables $X_1, \dots, X_n$

$$\mathbb{E}\big[\max_{1\le i\le d} X_i\big] \le \sigma\sqrt{2\log d} \tag{50}$$

Theorem 1.6 (Bound of Rademacher Complexity with Shattering Number)

The Rademacher complexity of a binary function class $\mathcal{F}$ is bounded by

$$\text{Rad}_n(\mathcal{F}) \le \sqrt{\frac{2\log s_n(\mathcal{F})}{n}} \tag{51}$$

Proof.

Given the projection $\mathcal{F}_{z_1,\dots,z_n}$, we can use the law of iterated expectations on the Rademacher complexity.

$$\text{Rad}_n(\mathcal{F}) = \mathbb{E}\left[\sup_{f\in\mathcal{F}}\left|\frac{1}{n}\sum_{i=1}^n \sigma_i f(Z_i)\right|\right] \tag{52}$$

$$= \mathbb{E}_Z\left[\mathbb{E}_\sigma\left[\sup_{f\in\mathcal{F}}\left|\frac{1}{n}\sum_{i=1}^n \sigma_i f(Z_i)\right| \;\middle|\; Z_1, \dots Z_n\right]\right] \tag{53}$$

Note that in the inner expectation, since $f(Z_i)$ is now fixed, then are bounding a linear combination of a bunch of σ_i's, which are subgaussian. Using the bound above, we can reduce it to

$$\mathbb{E}_Z\left[\sqrt{\frac{2\log|F_{z_1,\dots,z_n}|}{n}}\right] \le \sqrt{\frac{2\log s_n(\mathcal{F})}{n}} \le \sqrt{\frac{2d\log n}{n}} \tag{54}$$

However, this is not the best possible bound, and in cases such as K means clustering in high dimensions, this VC bound is terrible. Now we move onto the big VC theorem which now bounds the supremum of the difference between the empirical risk and the true risk. To prove this, we need a few tricks, the first being the symmetrization trick using ghost samples.

Lemma 1.5 (Symmetrization Lemma)

Given a set of random variables $Z_1, \dots, Z_n$ and a function class $\mathcal{F}$, we can define ghost samples $Z_1', \dots, Z_n'$ that are iid copies of $Z_1, \dots, Z_n$. Then, we can bound the Rademacher complexity of the function class $\mathcal{F}$ by

$$\mathbb{P}\left(\sup_{f\in\mathcal{F}}|\hat{R}(f) - R(f)| \ge \epsilon\right) \le 2\mathbb{P}\left(\sup_{f\in\mathcal{F}}|\hat{R}(f) - \hat{R}'(f)| \ge \epsilon/2\right) \tag{55}$$

where $\hat{R}, \hat{R}'$ is the empirical risk over the original and ghost samples, respectively.

Proof.

Assume that we have a function f that achieves this minimum. By the triangle inequality,

$$|\hat{R}(f) - R(f)| > t \text{ and } |\hat{R}'(f) - R(f)| < \frac{t}{2} \implies |\hat{R}(f) - \hat{R}'(f)| > \frac{t}{2} \tag{56}$$

We write this again as an indicator function.

$$\mathbb{1}(|\hat{R}(f) - R(f)| > t, |\hat{R}'(f) - R(f)| < \frac{t}{2}) \implies \mathbb{1}(|\hat{R}(f) - \hat{R}'(f)| > \frac{t}{2}) \tag{57}$$

and since the samples and the ghost samples are independent, we can take the probability over the ghost samples to get

$$\mathbb{1}(|\hat{R}(f) - R(f)| > t)\, \mathbb{P}_{Z'}(|\hat{R}'(f) - R(f)| < \frac{t}{2}) \implies \mathbb{P}_{Z'}(|\hat{R}(f) - \hat{R}'(f)| > \frac{t}{2}) \tag{58}$$

and the rest of the proof can be found online.

The reason we want this is that it removes the $R(f)$, which is some unknown true mean that can be hard to deal with since it takes infinite values. It's easier to work with two empirical risks than deal with the true risk.

Theorem 1.7 (VC Theorem/Inequality)

Given a binary function class $\mathcal{F}$, we have

$$\mathbb{P}\left(\sup_{f \in \mathcal{F}} |\hat{R}(f) - R(f)| \geq \epsilon \right) \leq 2S(\mathcal{F}, n) e^{-n\epsilon^2/8} \approx n^d e^{-n\epsilon^2/8} \tag{59}$$

You can see that the exponential term is from Hoeffding but there is an extra cost of taking the supremum over the whole function class, which is the shattering number.

Proof.

Given $Z_1, \dots, Z_n \sim \mathbb{P}$, we take a new set of random variables $Z_1', \dots, Z_n'$ that are iid copies of $Z_1, \dots, Z_n$, called *ghost samples*.

Therefore, for some classes of sets with finite VC dimension, the shattering term will grow polynomially in n but the exponential term decays faster, which is what makes this work. That's why as n grows, we can get a good bound on the supremum of this difference.

Theorem 1.8 ()

With probability $\geq 1 - \delta$, we have

$$\sup_{f \in \mathcal{F}} |\hat{R}(f) - R(f)| \leq 2\text{Rad}_n(\mathcal{F}) + \sqrt{\frac{\log(2/\delta)}{2n}} \tag{60}$$

1.4 Bias Variance Noise Decomposition

Let's do some further analysis on this. When you take a supremum over a function class, it decomposes into 3 terms.

1. One of which quantifies how big the function class is (more variance).
2. One of which quantifies the distance between the truth and the function class (bias).
3. One is the noise term, which is the irreducible error.

Example 1.8 (Bias and Variance Tradeoff in Polynomial Regression)

Let's motivate this by trying to fit a polynomial on some data.

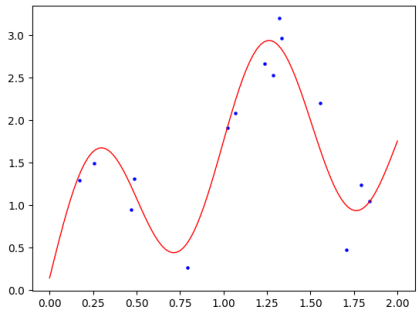
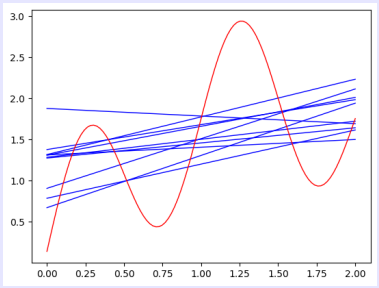
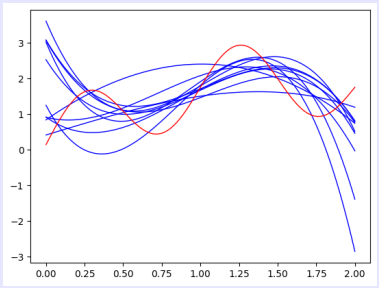


Figure 3: A sample of $|\mathcal{D}| = 15$ data points are generated from the function $f(x) = \sin(2\pi x) + 2\cos(x - 1.5)$ with Gaussian noise $N(0, 0.3)$ on the interval $[0, 1]$.

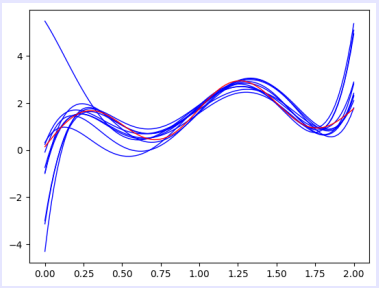
If we try to fit a polynomial function, how do we know which degree is best? Well the most simple thing is to just try all of them. To demonstrate this even further, I generated 10 different datasets $\mathcal{D}$ of size 15 taken from the same true distribution. The best fitted polynomials for each dataset is shown below.



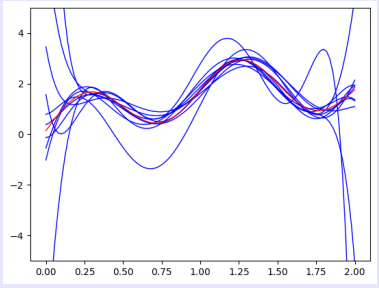
(a) 1st Degree



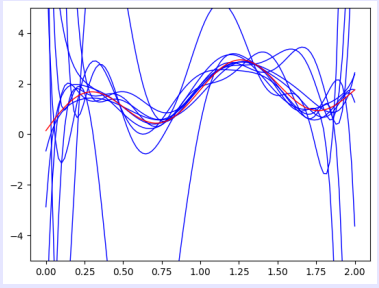
(b) 3rd Degree



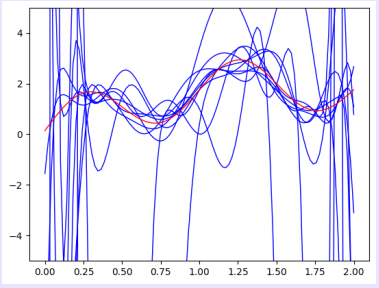
(c) 5th Degree



(d) 7th Degree



(e) 9th Degree



(f) 11th Degree

Figure 4: Different model complexities (i.e. different polynomial degrees) lead to different fits of the data generated from the true distribution. The lower degree best fit polynomials don't have much variability in their best fits but have high bias, while the higher degree best fit polynomials have very high variability in their best fits but have low bias. The code used to generate this data is here

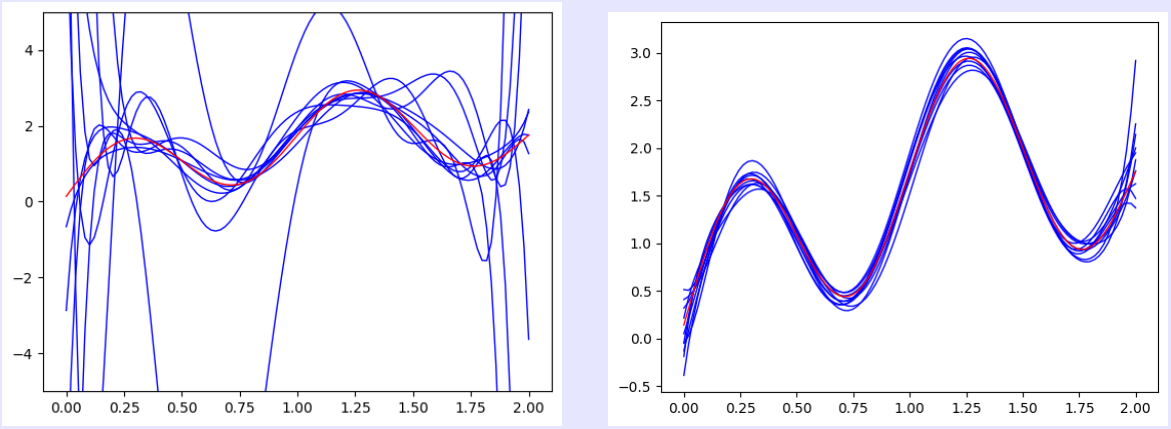
.

We already know that the 5th degree approximation is most optimal, and the lower degree ones are **underfitting** the data, while the higher degree ones are **overfitting**. As mentioned before, we can describe the underfitting and overfitting phenomena through the bias variance decomposition.

1. If we underfit the data, this means that our model is not robust and does not capture the patterns inherent in the data. It has a high bias since the set of function it encapsulates is not large enough to model $\mathbb{E}[Y \mid X]$. However, it has a low variance since if we were to take different samples of the dataset $\mathcal{D}$, the optimal parameters would not fluctuate.
2. What overfitting essentially means is that our model is too complex to the point where it starts to fit to the *noise* of the data. This means that the variance is high, since different samples of the dataset $\mathcal{D}$ would cause huge fluctuations in the optimal trained parameters $\boldsymbol{\theta}$. However, the function set would be large, and thus it would be close to $\mathbb{E}[Y \mid X]$, leading to a low bias.

Example 1.9 (Polynomial Regression Continued)

Another way to reduce the overfitting problem is if we have more training data to work with. That is, if we were to fit a 9th degree polynomial on a training set of not $N = 15$, but $N = 100$ data points, then we can see that this gives a much better fit. This makes sense because now the random variable $\mathcal{D}$, as a function of more random variables, has lower variance. Therefore, the lower variance in the dataset translates to lower variance in the optimal parameter.



(a) $M = 9, N = 15$ (b) $M = 9, N = 100$

Figure 5: Increasing the number of data points helps the overfitting problem. Now, we can afford to fit a 9th degree polynomial with reasonable accuracy.

1.5 Minimax Theory

2 Low Dimensional Linear Regression

In introductory courses, we start with linear predictors since it is easy to understand. We still start with linear predictors because in high-dimensional machine learning, even linear prediction can be hard as we will see. Low dimensional linear regression is what statisticians worked in back in the early days, where data was generally low dimensional.[6] Generally, we had $d < n$, but these days, we are in the regime where $d > n$. For example, in genetic data, you could have a sample of $n = 100$ people but each of them have genetic sequences at $d = 10^6$. When the dimensions become high, the original methods of linear regression tend to break down, which is why I separate low and high dimensional linear regression. The line tends to be fuzzy between these two regimes, but we will not worry about strictly defining that now.

In here, we start with **multiple linear regression**, which assumes that we have several covariates and one response. If we extend this to multiple responses (i.e. a response vector), this is called **multivariate linear**

[6] Quoting Larry Wasserman, even 5 dimensions was considered high and 10 was considered massive.

regression. The simple case for one response is called **simple linear regression**, and we will mention some nice formulas and intuition that come out from working with this.

Definition 2.1 (Linear Regression Model)

Given a dataset $\mathcal{D} = \{(x^{(i)}, y^{(i)})\}_{i=1}^n$, where $x^{(i)} \in \mathbb{R}^d$ with $x_1 = 1$ (which is what we do in practice to include an intercept term) and $y^{(i)} \in \mathbb{R}$, the multiple linear regression model is

$$y = \beta^T x + \epsilon \tag{61}$$

with the following assumptions:

1. *Weak exogeneity*: the covariates are observed without error.
2. *Linearity*: the mean of the variate is a linear combination of the parameters and the covariates.
3. *Gaussian errors*: the errors are Gaussian.[a]
4. *Homoscedasticity*: the errors (the observations of Y) have constant variance.
5. *Independence of errors*: The errors are uncorrelated.
6. *No multicollinearity*: more properly, the lack of perfect multicollinearity. Assume that the covariates aren't perfectly correlated.[b]

In order to check multicollinearity, we compute the correlation matrix.

Definition 2.2 (Correlation Matrix)

The correlation matrix of random variables $X_1, \dots, X_d$ is

$$\mathbf{C}_{ij} = \text{Corr}(X_i, X_j) = \frac{\text{Cov}(X_i, X_j)}{\sigma_{X_i}\sigma_{X_j}}$$

given that $\sigma_{X_i}\sigma_{X_j} > 0$. Clearly, the diagonal entries are 1, but if there are entries that are very close to 1, then we have multicollinearity.

Assume that two variables are perfectly correlated. Then, there would be pairs of parameters that are indistinguishable if moved in a certain linear combination. This means that the variance of $\hat{\boldsymbol{\beta}}$ will be very ill conditioned, and you would get a huge standard error in some direction of the β_i's. We can fix this by making sure that the data is not redundant and manually removing them, standardizing the variables, making a change of basis to remove the correlation, or just leaving the model as it is.

If these assumptions don't hold,

1. *Weak exogeneity*: the sensitivity of the model can be tested to the assumption of weak exogeneity by doing bootstrap sampling for the covariates and seeing how the sampling affects the parameter estimates. Covariates measured with error used to be a difficult problem to solve, as they required errors-in-variables models, which have very complicated likelihoods. In addition, there is no universal fitting library to deal with these. But nowadays, with the availability of Markov Chain Monte Carlo (MCMC) estimation through probabilistic programming languages, it is a lot easier to deal with these using Bayesian hierarchical models (or multilevel models, or Bayesian graphical models—these have many names).
2. *Linearity*: the linear regression model only assumes linearity in the parameters, not the covariates. Therefore you could build a regression using non-linear transformations of the covariates, for instance,

$$Y = X_1\beta_1 + X_1^2\beta_2 + \log(X_1)\beta_3 \tag{62}$$

   If you need to further relax the assumption, you are better off using non-linear modelling.

[a] We can relax this assumption when we get into generalized linear models, and in most cases we assume some closed form of the error for computational convenience, like when computing the maximum likelihood.

[b] This is the assumption that breaks down in high dimensional linear regression.

3. *Constant variance*: the simplest fix is to do a variance-stabilising transformation on the data. Assuming a constant coefficient of variation rather than a constant mean could also work. Some estimation libraries (such as the `glm` package in R) allow specifying the variance as a function of the mean.
4. *Independence of errors*: this is dangerous because in the financial world things are usually highly correlated in times of crisis. The most important thing is to understand how risky this assumption is for your setting. If necessary, add a correlation structure to your model, or do a multivariate regression. Both of these require significant resources to estimate parameters, not only in terms of computational power but also in the amount of data required.
5. *No multicollinearity*: If the covariates are correlated, they can still be used in the regression, but numerical problems might occur depending on how the fitting algorithms invert the matrices involved. The t-tests that the regression produces can no longer be trusted. All the covariates must be included regardless of what their significance tests say. A big problem with multicollinearity, however, is overfitting. Depending on how bad the situation is, the parameter values might have huge uncertainties around them, and if you fit the model using new data their values might change significantly.[7] Multicollinearity is a favourite topic of discussion for quant interviewers, and they usually have strong opinions about how it should be handled. The model's intended use will determine how sensitive it is to ignoring the error distribution. In many cases, fitting a line using least-squares estimation is equivalent to assuming errors have a normal distribution. If the real distribution has heavier tails, like the t-distribution, how risky will it make decisions based on your outputs? One way to address this is to use a technique like robust-regression. Another way is to think about the dynamics behind the problem and which distribution would be best suited to model them—as opposed to just fitting a curve through a set of points.

2.1 Ordinary Least Squares

If we use a squared loss function, this is called **ordinary least squares**. It is a well known fact that the true regressor that minimizes this loss is

$$f^*(x) = \mathbb{E}[Y \mid X = x] \tag{63}$$

which is the conditional expectation of Y given X. This is the true regressor function, which is the best approximation of Y over the σ-algebra generated by X. This may or may not be linear.

Theorem 2.1 (Least Squares Solution For Linear Regression)

Given the design matrix $\mathbf{X}$, we can present the linear model in vectorized form:

$$\mathbf{Y} = \mathbf{X}\boldsymbol{\beta} + \boldsymbol{\epsilon},\ \boldsymbol{\epsilon} \sim N(\mathbf{0}, \sigma^2\mathbf{I}) \tag{64}$$

The solution that minimizes the squared loss is

$$\boldsymbol{\beta} = (\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{Y} \in \mathbb{R}^d$$
$$\text{Var}(\hat{\boldsymbol{\beta}}) = \hat{\sigma}^2(\mathbf{X}^T\mathbf{X})^{-1} \in \mathbb{R}^{d\times d}$$

Proof.

The errors can be written as $\boldsymbol{\epsilon} = \mathbf{Y} - \mathbf{X}\boldsymbol{\beta}$, and you have the following total sum of squared errors:

$$S(\boldsymbol{\beta}) = \boldsymbol{\epsilon}^T\boldsymbol{\epsilon} = (\mathbf{Y} - \mathbf{X}\boldsymbol{\beta})^T(\mathbf{Y} - \mathbf{X}\boldsymbol{\beta})$$

We want to find the value of $\boldsymbol{\beta}$ that minimizes the sum of squared errors. In order to do this, remember the following matrix derivative rules when differentiating with respect to vector $\mathbf{x}$.

[7] I suggest reading this Wikipedia article on multicollinearity, as it contains useful information: `https://en.wikipedia.org/wiki/Multicollinearity`

1. $\mathbf{x}^T\mathbf{A} \mapsto \mathbf{A}$
2. $\mathbf{x}^T\mathbf{A}\mathbf{x} \mapsto 2\mathbf{A}\mathbf{x}$

Now this should be easy.

$$\begin{aligned} S(\boldsymbol{\beta}) &= \mathbf{Y}^T\mathbf{Y} - \boldsymbol{\beta}^T\mathbf{X}^T\mathbf{Y} - \mathbf{Y}^T\mathbf{X}\boldsymbol{\beta} + \boldsymbol{\beta}^T\mathbf{X}^T\mathbf{X}\boldsymbol{\beta} \\ &= \mathbf{Y}^T\mathbf{Y} - 2\mathbf{Y}^T\mathbf{X}\boldsymbol{\beta} + \boldsymbol{\beta}^T\mathbf{X}^T\mathbf{X}\boldsymbol{\beta} \\ \frac{\partial}{\partial \boldsymbol{\beta}} S(\boldsymbol{\beta}) &= -2\mathbf{X}^T\mathbf{Y} + 2\mathbf{X}^{\mathbf{X}}\boldsymbol{\beta} \end{aligned}$$

and setting it to $\mathbf{0}$ gives

$$2\mathbf{X}^T\mathbf{X}\boldsymbol{\beta} - 2\mathbf{X}^T\mathbf{Y} = 0 \implies \mathbf{X}^T\mathbf{X}\boldsymbol{\beta} = \mathbf{X}^T\mathbf{Y}$$

and the variance of $\boldsymbol{\beta}$, by using the fact that $\text{Var}[\mathbf{A}\mathbf{X}] = \mathbf{A}\,\text{Var}[X]\mathbf{A}^T$, is

$$\text{Var}(\hat{\boldsymbol{\beta}}) = (\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\,\sigma^2\mathbf{I}\,\mathbf{X}(\mathbf{X}'\mathbf{X})^{-1} = \sigma^2(\mathbf{X}'\mathbf{X})^{-1}(\mathbf{X}'\mathbf{X})(\mathbf{X}'\mathbf{X})^{-1} = \sigma^2(\mathbf{X}'\mathbf{X})^{-1}$$

But we don't know the true σ^2, so we estimate it with $\hat{\sigma}^2$ by taking the variance of the residuals. Therefore, we have

$$\begin{aligned} \boldsymbol{\beta} &= (\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{Y} \in \mathbb{R}^d \\ \text{Var}(\hat{\boldsymbol{\beta}}) &= \hat{\sigma}^2(\mathbf{X}^T\mathbf{X})^{-1} \in \mathbb{R}^{d\times d} \end{aligned}$$

Example 2.1 (Copying Data)

What happens if you copy your data in OLS? In this case, our MLE estimate becomes

$$\begin{aligned} &\left(\begin{pmatrix} X \\ X \end{pmatrix}^T \begin{pmatrix} X \\ X \end{pmatrix}\right)^{-1} \begin{pmatrix} X \\ X \end{pmatrix}^T \begin{pmatrix} Y \\ Y \end{pmatrix} = \\ &\qquad = (X^TX + X^TX)^{-1}(X^TY + X^TY) = (2X^TX)^{-1}2X^TY = \hat{\beta} \end{aligned}$$

and our estimate is unaffected. However, the variance shrinks by a factor of 2 to

$$\frac{\sigma^2}{2}(\mathbf{X}^T\mathbf{X})^{-1} \tag{65}$$

A consequence of that is that confidence intervals will shrink with a factor of $1/\sqrt{2}$. The reason is that we have calculated as if we still had iid data, which is untrue. The pair of doubled values are obviously dependent and have a correlation of 1.

Another way to solve the solution is through likelihood estimation.

Theorem 2.2 (Maximum Likelihood Estimation of Linear Regression)

Given a dataset $\mathcal{D} = \{(x^{(i)}, y^{(i)})\}_{i=1}^N$, our likelihood is

$$L(\theta; \mathcal{D}) = \prod_{i=1}^N p(y^{(i)} \mid x^{(i)}; \theta) = \prod_{i=1}^N \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{(y^{(i)} - \theta^T x^{(i)})^2}{2\sigma^2}\right)$$

We can take its negative log, remove additive constants, and scale accordingly to get

$$\begin{aligned}\ell(\theta) &= -\frac{N}{2}\ln\sigma^2 - \frac{N}{2}\ln(2\pi) + \frac{1}{2\sigma^2}\sum_{i=1}^{N}\left(y^{(i)} - \boldsymbol{\theta}^T\mathbf{x}^{(i)}\right)^2 \\ &= \frac{1}{2}\sum_{i=1}^{N}\left(y^{(i)} - \boldsymbol{\theta}^T\mathbf{x}^{(i)}\right)^2\end{aligned}$$

which then corresponds to minimizing the sum of squares error function.

Theorem 2.3 (Gradient Descent for Linear Regression)

Taking the gradient of this log likelihood w.r.t. θ gives

$$\nabla_\theta \ell(\theta) = \sum_{i=1}^{N}(y^{(i)} - \theta^T x^{(i)})x^{(i)}$$

and running gradient descent over a minibatch $M \subset \mathcal{D}$ gives

$$\begin{aligned}\theta &= \theta - \eta\nabla_\theta\ell(\theta) \\ &= \theta - \eta\sum_{(x,y)\in M}(y - \theta^T x)x\end{aligned}$$

This is guaranteed to converge since $\ell(\theta)$, as the sum of convex functions, is also convex.
Note that since we can solve this in closed form, by setting the gradient to 0, we have

$$0 = \sum_{n=1}^{N} y^{(n)}\boldsymbol{\phi}(\mathbf{x}^{(n)})^T - \mathbf{w}^T\left(\sum_{n=1}^{N}\boldsymbol{\phi}(\mathbf{x}^{(n)})\boldsymbol{\phi}(\mathbf{x}^{(n)})^T\right)$$

which is equivalent to solving the least squares equation

$$\mathbf{w}_{ML} = (\boldsymbol{\Phi}^T\boldsymbol{\Phi})^{-1}\boldsymbol{\Phi}^T\mathbf{Y}$$

Note that if we write out the bias term out explicitly, we can see that it just accounts for the translation (difference) between the average of the outputs $\bar{y} = \frac{1}{N}\sum_{n=1}^{N} y_n$ and the average of the basis functions $\bar{\phi_j} = \frac{1}{N}\sum_{n=1}^{N}\phi_j(\mathbf{x}^{(n)})$.

$$w_0 = \bar{y} - \sum_{j=1}^{M-1} w_j\bar{\phi_j}$$

We can also maximize the log likelihood w.r.t. σ^2, which gives the MLE

$$\sigma^2_{ML} = \frac{1}{N}\sum_{n=1}^{N}\left(y^{(n)} - \mathbf{w}_{ML}^T\boldsymbol{\phi}(\mathbf{x}^{(n)})\right)^2$$

2.1.1 Bias Variance Decomposition

We can use what we have learned to prove a very useful result for the mean squared loss.

Theorem 2.4 (Pythagorean's Theorem)

The expected square loss over the joint measure $\mathbb{P}_{X\times Y}$ can be decomposed as

$$\mathbb{E}_{X\times Y}[(Y-h(X))^2] = \mathbb{E}_{X\times Y}[\big(Y-\mathbb{E}[Y\mid X]\big)^2] + \mathbb{E}_X[\big(\mathbb{E}[Y\mid X]-h(X)\big)^2] \tag{66}$$

That is, the squared loss decomposes into the squared loss of $\mathbb{E}[Y\mid X]$ and $g(X)$, which is the intrinsic misspecification of the model, plus the squared difference of Y with its best approximation $\mathbb{E}[Y\mid X]$, which is the intrinsic noise inherent in Y beyond the σ-algebra of X.

Proof.

We can write

$$\begin{aligned}
\mathbb{E}_{X\times Y}[L] &= \mathbb{E}_{X\times Y}\big[\big(Y-g(X)\big)^2\big] \\
&= \mathbb{E}_{X\times Y}\big[\big((Y-\mathbb{E}[Y\mid X])+(\mathbb{E}[Y\mid X]-g(X))\big)^2\big] \\
&= \mathbb{E}_{X\times Y}[\big(Y-\mathbb{E}[Y\mid X]\big)^2] + \mathbb{E}_{X\times Y}[\{Y-\mathbb{E}[Y\mid X]\}\{\mathbb{E}[Y\mid X]-g(X)\}] \\
&\qquad + \mathbb{E}_X[\big(\mathbb{E}[Y\mid X]-g(X)\big)^2] \\
&= \mathbb{E}_{X\times Y}[\big(Y-\mathbb{E}[Y\mid X]\big)^2] + \mathbb{E}_X[\big(\mathbb{E}[Y\mid X]-g(X)\big)^2]
\end{aligned}$$

where the middle term cancels out due to the tower property.

We also proved a second fact: Since $\mathbb{E}[\big(\mathbb{E}[Y\mid X]-g(X)\big)^2]$ is the misspecification of the model, we cannot change this (positive) constant, so $\mathbb{E}\big[\big(Y-g(X)\big)^2\big] \geq \mathbb{E}[(Y-\mathbb{E}[Y\mid X])^2]$, with equality achieved when we perfectly fit g as $\mathbb{E}[Y\mid X]$ (i.e. the model is well-specified). Therefore, denoting $\mathcal{F}$ as the set of all $\sigma(X)$-measurable functions, then the minimum of the loss is attained when

$$\operatorname*{argmin}_{g\in\mathcal{F}} \mathbb{E}[L] = \operatorname*{argmin}_{g\in\mathcal{F}} \mathbb{E}\big[\big(Y-g(X)\big)^2\big] = \mathbb{E}[Y\mid X] \tag{67}$$

Even though this example is specific for the mean squared loss, this same decomposition, along with the bias variance decomposition, exists for other losses. It just happens so that the derivations are simple for the MSE, which is why this is introduced first. However, the derivations for other losses are much more messy, and sometimes may not hold rigorously. However, the general intuition that more complex models tend to overfit still hold true.

Now if we approximate $\mathbb{E}[Y\mid X]$ with our parameterized hypothesis $h_{\boldsymbol{\theta}}$, then from a Bayesian perspective the uncertainty in our model is expressed through a poseterior distribution over $\boldsymbol{\theta}$. A frequentist treatment, however, involves making a point estimate of $\boldsymbol{\theta}$ based on the dataset $\mathcal{D}$ and tries instead to interpret the uncertainty of this estimate through the following thought experiment: Suppose we had a large number of datasets each of size N and each drawn independently from the joint distribution $X\times Y$. For any given dataset $\mathcal{D}$, we can run our learning algorithm and obtain our best fit function $h^*_{\boldsymbol{\theta};\mathcal{D}}(\mathbf{x})$. Different datasets from the ensemble will give different functions and consequently different values of the squared loss. The performance of a particular learning algorithm is then assessed by taking the average over this ensemble of datasets, which we define $\mathbb{E}_{\mathcal{D}}[h_{\boldsymbol{\theta};\mathcal{D}}(\mathbf{x})] = \mathbb{E}_{(X\times Y)^N}[h_{\boldsymbol{\theta};\mathcal{D}}(\mathbf{x})]$. We are really taking an expectation over all datasets, meaning that the N points in each $\mathcal{D}$ must be sampled from $(X\times Y)^N$.

Consider the term $\big(\mathbb{E}[Y\mid X]-h_{\boldsymbol{\theta}}(X)\big)^2$ above, which models the discrepancy in our optimized hypothesis and the best approximation. Now, over all datasets $\mathcal{D}$, there will be a function $h_{\boldsymbol{\theta};\mathcal{D}}$, and averaged over all datasets $\mathcal{D}$ is $\mathbb{E}_{\mathcal{D}}[h_{\boldsymbol{\theta};\mathcal{D}}]$. So, the random variable below (of $\mathcal{D}$ and X) representing the stochastic difference between our optimized function $h_{\boldsymbol{\theta};\mathcal{D}}(X)$ and our best approximation $\mathbb{E}[Y\mid X]$ can be decomposed into

$$\begin{aligned}\big(\mathbb{E}[Y \mid X] - h_{\boldsymbol{\theta};\mathcal{D}}(X)\big)^2 &= \big[\big(\mathbb{E}[Y \mid X] - \mathbb{E}_{\mathcal{D}}[h_{\boldsymbol{\theta};\mathcal{D}}(X)]\big) + \big(\mathbb{E}_{\mathcal{D}}[h_{\boldsymbol{\theta};\mathcal{D}}(X)] - h_{\boldsymbol{\theta};\mathcal{D}}(X)\big)\big]^2 \\ &= \big(\mathbb{E}[Y \mid X] - \mathbb{E}_{\mathcal{D}}[h_{\boldsymbol{\theta};\mathcal{D}}(X)]\big)^2 + \big(\mathbb{E}_{\mathcal{D}}[h_{\boldsymbol{\theta};\mathcal{D}}(X)] - h_{\boldsymbol{\theta};\mathcal{D}}(X)\big)^2 \\ &\quad + 2\big(\mathbb{E}[Y \mid X] - \mathbb{E}_{\mathcal{D}}[h_{\boldsymbol{\theta};\mathcal{D}}(X)]\big)\big(\mathbb{E}_{\mathcal{D}}[h_{\boldsymbol{\theta};\mathcal{D}}(X)] - h_{\boldsymbol{\theta};\mathcal{D}}(X)\big) \\ &= \big(\mathbb{E}[Y \mid X] - \mathbb{E}_{\mathcal{D}}[h_{\boldsymbol{\theta};\mathcal{D}}(X)]\big)^2 + \big(\mathbb{E}_{\mathcal{D}}[h_{\boldsymbol{\theta};\mathcal{D}}(X)] - h_{\boldsymbol{\theta};\mathcal{D}}(X)\big)^2\end{aligned}$$

Averaging over all datasets $\mathcal{D}$ causes the middle term to vanish and gives us the expected squared difference between the two random variables, now of X.

Theorem 2.5 (Bias Variance Decomposition)

Therefore, we can write out the expected square difference between $h_{\boldsymbol{\theta}}$ and $\mathbb{E}[Y \mid X]$ as the sum of two terms.

$$\mathbb{E}_{\mathcal{D}}\big[\big(\mathbb{E}[Y \mid X] - h_{\boldsymbol{\theta}}(X)\big)^2\big] = \underbrace{\big(\mathbb{E}[Y \mid X] - \mathbb{E}_{\mathcal{D}}[h_{\boldsymbol{\theta};\mathcal{D}}(X)]\big)^2}_{(\text{bias})^2} + \underbrace{\mathbb{E}_{\mathcal{D}}\big[\big(\mathbb{E}_{\mathcal{D}}[h_{\boldsymbol{\theta};\mathcal{D}}(X)] - h_{\boldsymbol{\theta};\mathcal{D}}(X)\big)^2\big]}_{\text{variance}} \tag{68}$$

Let us observe what these terms mean:

1. The **bias** $\mathbb{E}[Y \mid X] - \mathbb{E}_{\mathcal{D}}[h_{\boldsymbol{\theta};\mathcal{D}}(X)]$ is a random variable of X that measures the difference in how the average prediction of our hypothesis function $\mathbb{E}_{\mathcal{D}}[h_{\boldsymbol{\theta};\mathcal{D}}(X)]$ differs from the actual prediction $\mathbb{E}[Y \mid X]$.
2. The **variance** $\mathbb{E}_{\mathcal{D}}\big[\big(\mathbb{E}_{\mathcal{D}}[h_{\boldsymbol{\theta};\mathcal{D}}(X)] - h_{\boldsymbol{\theta};\mathcal{D}}(X)\big)^2\big]$ is a random variable of X that measures the variability of each hypothesis function $h_{\boldsymbol{\theta}}(X)$ about its mean over the ensemble $\mathbb{E}_{\mathcal{D}}[h_{\boldsymbol{\theta};\mathcal{D}}(X)]$.

Therefore, we can substitute this back into our Pythagoras decomposition, where we must now take the expected bias and the expected variance. Therefore, we get

$$\text{Expected Loss} = (\text{Expected Bias})^2 + \text{Expected Variance} + \text{Noise} \tag{69}$$

where

$$\begin{aligned}(\text{Bias})^2 &= \mathbb{E}_X\big[\big(\mathbb{E}[Y \mid X] - \mathbb{E}_{\mathcal{D}}[h_{\boldsymbol{\theta};\mathcal{D}}(X)]\big)^2\big] \\ \text{Variance} &= \mathbb{E}_X\big[\mathbb{E}_{\mathcal{D}}\big[\big(\mathbb{E}_{\mathcal{D}}[h_{\boldsymbol{\theta};\mathcal{D}}(X)] - h_{\boldsymbol{\theta};\mathcal{D}}(X)\big)^2\big]\big] \\ \text{Noise} &= \mathbb{E}_{X\times Y}[\big(Y - \mathbb{E}[Y \mid X]\big)^2]\end{aligned}$$

2.1.2 Convergence Bounds

Let's get a deeper understanding on linear regression by examining the convergence of the empirical risk minimizer to the true risk minimizer. We can develop a naive bound using basic concentration of measure.

Theorem 2.6 (Exponential Bound)

Let $\mathcal{P}$ be the set of all distributions for $X \times Y$ supported on a compact set. There exists constants c_1, c_2 s.t. that the following is true. For any $\epsilon > 0$,

$$\sup_{\mathbb{P}\in\mathcal{P}} \mathbb{P}^n\big(r(\hat{\beta}_n) > r(\beta_*(\mathbb{P}) + 2\epsilon)\big) \leq c_1 e^{-nc_2\epsilon^2} \tag{70}$$

Hence

$$r(\hat{\beta}_n) - r(\beta_*) = O_{\mathbb{P}}\left(\sqrt{\frac{1}{n}}\right) \tag{71}$$

Proof.

However, this is not a very tight bound, and we can do better. Though the proof is very long and will be omitted.

Theorem 2.7 (Gyorfi, Kohler, Krzyzak, Walk, 2002 [1])

Let $\sigma^2 = \sup_x \text{Var}[Y \mid X = x] < \infty$. Assume that all random variables are bounded by $L < \infty$. Then

$$\mathbb{E} \int |\hat{\beta}^T x - m(x)|^2 \, d\mathbb{P}(x) \leq 8 \inf_{\beta} \int |\beta^T x - m(x)|^2 \, d\mathbb{P}(x) + \frac{Cd(\log(n) + 1)}{n} \tag{72}$$

You can see that the bound contains a term of the form

$$\frac{d \log(n)}{n} \tag{73}$$

and under the low dimensional case, d is small and bound is good. However, as d becomes large, then we don't have as good of theoretical guarantees.

Theorem 2.8 (Central Limit Theorem of OLS)

We have

$$\sqrt{n}(\hat{\beta} - \beta) \xrightarrow{d} N(0, \Gamma) \tag{74}$$

where

$$\Gamma = \Sigma^{-1} \mathbb{E}\big[(Y - X^T\beta)^2 X X^T\big] \Sigma^{-1} \tag{75}$$

The covariance matrix Γ can be consistently estimated by

$$\hat{\Gamma} = \hat{\Sigma}^{-1} \hat{M} \hat{\Sigma}^{-1} \tag{76}$$

where

$$\hat{M}(j,k) = \frac{1}{n} \sum_{i=1}^{n} X_i(j) X_i(k) \hat{\epsilon}_i^2 \tag{77}$$

and $\hat{\epsilon}_i = Y_i - \hat{\beta}^T X_i$.

2.2 Simple Linear Regression

The simple linear regression is the special case of the linear regression with only one covariate.[8]

$$y = \alpha + x\beta \tag{78}$$

which is just a straight line fit. Interviewers like this model for its aesthetically pleasing theoretical properties. A few of them are described here, beginning with parameter estimation. For n pairs of (x_i, y_i),

$$y_i = \alpha + \beta x_i + \epsilon_i \tag{79}$$

To minimize the sum of squared errors

$$\sum_i \epsilon_i^2 = \sum_i (y_i - \alpha - \beta x_i)^2 \tag{80}$$

[8] I've included a separate section on this since this was especially important for quant interviews.

Taking the partial derivatives w.r.t. α and β and setting them equal to 0 gives

$$\sum_i (y_i - \hat{\alpha} - \hat{\beta} x_i) = 0$$
$$\sum_i (y_i - \hat{\alpha} - \hat{\beta} x_i) x_i = 0$$

From just the first equation, we can write

$$n\bar{y} = n\hat{\alpha} + n\hat{\beta}\bar{x} \implies y = \hat{\alpha} + \hat{\beta}\bar{x} \implies \hat{\alpha} = \bar{y} - \hat{\beta}\bar{x} \tag{81}$$

The second equation gives

$$\sum_i x_i y_i = \hat{\alpha} n \bar{x} + \hat{\beta} \sum_i x_i^2 \tag{82}$$

and substituting what we derived gives

$$\begin{aligned} \sum_i x_i y_i &= (\bar{y} - \hat{\beta}\bar{x}) n\bar{x} + \hat{\beta} \sum_i x_i^2 \\ &= n\bar{x}\bar{y} + \hat{\beta}\left(\left(\sum_i x_i^2 \right) - n\bar{x}^2 \right) \end{aligned}$$

and so we have

$$\hat{\beta} = \frac{\left(\sum_i x_i y_i\right) - n\bar{x}\bar{y}}{\left(\sum x_i^2\right) - n\bar{x}^2} = \frac{\sum_i x_i y_i - \bar{x} y_i}{\sum x_i^2 - \bar{x} x_i} = \frac{\sum_i (x_i - \bar{x}) y_i}{\sum_i (x_i - \bar{x}) x_i} \tag{83}$$

Now we can use the identity

$$\sum_i (x_i - \bar{x})(y_i - \bar{y}) = \sum_i y_i (x_i - \bar{x}) = \sum_i x_i (y_i - \bar{y})$$

to substitute both the numerator and denominator of the equation to

$$\hat{\beta} = \frac{\sum_i (x_i - \bar{x})(y_i - \bar{y})}{\sum_i (x_i - \bar{x})^2} = \frac{\text{cov}(x, y)}{\text{var}(x)} = \rho_{xy} \frac{s_y}{s_x}$$

where ρ_{xy} is the correlation between x and y, and the variance and covariance represent the sample variance and covariance (indicated in lower case letters). Therefore, the correlation coefficient ρ_{xy} is precisely equal to the slope of the best fit line when x and y have been standardized first, i.e. $s_x = s_y = 1$.

Example 2.2 (Switching Variables)

Say that we are fitting Y onto X in a simple regression setting with MLE β_1, and now we wish to fit X onto Y. How will the MLE slope change? We can see that

$$\beta_1 = \rho \frac{s_y}{s_x}, \quad \beta_2 = \rho \frac{s_x}{s_y}$$

and so

$$\beta_2 = \rho^2 \frac{1}{\rho} \frac{s_x}{s_y} = \rho^2 \frac{1}{\beta_1} = \beta_1 \frac{\text{var}(x)}{\text{var}(y)}$$

The reason for this is because regression lines don't necessarily correspond to one-to-one to a casual relationship. Rather, they relate more directly to a conditional probability or best prediction.

The **coefficient of determination** R^2 is a measure tells you how well your line fits the data. When you have your y_i's, their deviation around its mean is captured by the sample variance $s_y^2 = \sum_i (y_i - \bar{y})^2$. When

we fit our line, we want the deviation of y_i around our predicted values $\hat{y}_i$, i.e. our sum of squared loss $\sum_i (y_i - \hat{y}_i)^2$, to be lower. Therefore, we can define

$$R^2 = 1 - \frac{\text{MSELoss}}{\text{var}(y)} = 1 - \frac{\sum_i (y_i - \hat{y}_i)^2}{\sum_i (y_i - \bar{y})^2}$$

In simple linear regression, we have

$$R^2 = \rho_{yx}^2$$

An R^2 of 0 means that the model does not improve prediction over the mean model and 1 indicates perfect prediction. However, a drawback of R^2 is that it can increase if we add predictors to the regression model, leading to a possible overfitting.

Theorem 2.9 ()

The residual sum of squares (RSS) is equal to the a proportion of the variance of the y_i's.

$$\text{RSS} = \sum (y_i - \hat{y}_i)^2 = (1 - \rho^2) \sum (y_i - \bar{y})^2 \tag{84}$$

2.3 Weighted Least Squares

2.4 Mean Absolute Error

2.5 Significance Tests

This is not as emphasized in the machine learning literature, but it is useful to know from a statistical point of view.[9]

2.5.1 T Test

Given some multilinear regression problem where we must estimate $\boldsymbol{\beta} \in \mathbb{R}^{D+1}$ (D coefficients and 1 bias), we must determine whether there is actually a linear relationship between the x and y variables in our dataset $\mathcal{D}$. Say that we have a sample of N points $\mathcal{D} = \{(x_n, y_n)\}_{n=1}^N$. Then, for each ensemble of datasets $\mathcal{D}$ that we sample from the distribution $(X \times Y)^N$, we will have some estimator $\boldsymbol{\beta}$ for each of them. This will create a sampling distribution of $\boldsymbol{\beta}$'s where we can construct our significance test on.

So what should our sampling distribution of $\hat{\boldsymbol{\beta}}$ be? It is clearly normal since it is just a transformation of the normally distributed Y: $\hat{\boldsymbol{\beta}} \sim N(\boldsymbol{\beta}, \sigma^2 (X^T X)^{-1})$. Therefore, only considering one element β_i here,

$$\frac{\hat{\beta}_i - \beta_i}{\sigma \sqrt{(X^T X)_{ii}^{-1}}} \sim N(0, 1)$$

But the problem is that we don't know the true σ^2, and we are estimating it with $\hat{\sigma}^2$. If we knew the true σ^2 then this would be a normal, but because of this estimate, our normalizing factor is also random. It turns out that the residual sum of squares (RSS) for a multiple linear regression

$$\sum_i (y_i - x_i^T \beta)^2$$

follows a χ^2_{n-d} distribution. Additionally from the χ^2 distribution of RSS we have

$$\frac{(n-d)\hat{\sigma}^2}{\sigma^2} \sim \chi^2_{n-d}$$

[9] This is also asked in quant interviews.

where we define $\hat{\sigma}^2 = \frac{\text{RSS}}{n-d}$ which is an unbiased estimator for σ^2. Now there is a theorem that says that if you divide a $N(0,1)$ distribution by a χ_k^2/k distribution (with k degrees of freedom), then it gives you a t-distribution with the same degrees of freedom. Therefore, we divide

$$\frac{\frac{\hat{\beta}_i - \beta_i}{\sqrt{(X^TX)^{-1}_{ii}}}}{\hat{\sigma}} = \frac{\sigma \sim N(0,1)}{\sigma\chi^2_{n-d}/(n-d)} = \frac{\sim N(0,1)}{\chi^2_{n-d}/(n-d)} = t_{n-d}$$

where the standard error of the distribution is

$$\text{SE}(\hat{\beta}_i) = \sigma_{\hat{\beta}_i} = \sigma\sqrt{(X^TX)^{-1}_{ii}}$$

In ordinary linear regression, we have the null hypothesis $h_0 : \beta_i = 0$ and the alternative $h_a : \beta_i \neq 0$ for a two sided test or $h_a : \beta_i > 0$ for a one sided test. Given a certain significance level, we compute the critical values of the t-distribution at that level and compare it with the test statistic

$$t = \frac{\hat{\beta} - 0}{\text{SE}(\hat{\beta})}$$

Now given our β, how do we find the standard error of it? Well this is just the variance of our estimator $\boldsymbol{\beta}$, which is $\hat{\sigma}^2(\mathbf{X}^T\mathbf{X})^{-1}$, where $\hat{\sigma}^2$ is estimated by taking the variance of the residuals ϵ_i. When there is a single variable, the model reduces to

$$y = \beta_0 + \beta_1 x + \epsilon$$

and

$$\mathbf{X} = \begin{pmatrix} 1 & x_1 \\ 1 & x_2 \\ \vdots & \vdots \\ 1 & x_n \end{pmatrix}, \qquad \boldsymbol{\beta} = \begin{pmatrix} \beta_0 \\ \beta_1 \end{pmatrix}$$

and so

$$(\mathbf{X}'\mathbf{X})^{-1} = \frac{1}{n\sum x_i^2 - (\sum x_i)^2}\begin{pmatrix} \sum x_i^2 & -\sum x_i \\ -\sum x_i & n \end{pmatrix}$$

and substituting this in gives

$$\sqrt{\widehat{\text{Var}}(\hat{\beta}_1)} = \sqrt{[\hat{\sigma}^2(\mathbf{X}'\mathbf{X})^{-1}]_{22}} = \sqrt{\frac{\hat{\sigma}^2}{\sum x_i^2 - (\sum x_i)^2}} = \sqrt{\frac{\hat{\sigma}^2}{\sum (x_i - \bar{x}_i)^2}}$$

Example 2.3 ()

Given a dataset

```
Hours Studied for Exam 20 16 20 18 17 16 15 17 15 16 15 17 16 17 14
Grade on Exam 89 72 93 84 81 75 70 82 69 83 80 83 81 84 76
```

The hypotheses are $h_0 : \beta = 0$ and $h_a : \beta \neq 0$, and the degrees of freedom for the t-test is $df = N - (D+1) = 13$, where $N = 15$ is the number of datapoints and $D = 1$ is the number of coefficients (plus the 1 bias term). The critical values is ± 2.160, which can be found by taking the inverse CDF of the t-distribution evaluated at 0.975.

Now we calculate the t score. We have our estimate $\beta_1 = 3.216, \beta_0 = 26.742$, and so we calculate

$$\hat{\sigma}^2 = \frac{1}{15}\sum_{i=1}^{15}\big(y_i - (3.216x_i + 26.742)\big) = 13.426$$
$$\sum_i (x_i - \hat{x}_i)^2 = 41.6$$

and therefore, we can compute

$$t = \frac{\beta_1}{\sqrt{\hat{\sigma}^2 / \sum_i (x_i - \hat{x}_i)^2}} = \frac{3.216}{\sqrt{13.426/41.6}} = 5.661$$

and therefore, this is way further than our critical value of 2.16, meaning that we reject the null hypothesis.

Note that when multicolinearity is present, then $\sum_i (x_i - \hat{x}_i)^2$ will be very small causing the denominator to blow up, and therefore you cannot place too much emphasis on the interpretation of these statistics. While it is hard to see for the single linear regression case, we know that some eigenvalue of $(\mathbf{X}^T\mathbf{X})^{-1}$ will blow up, causing the diagonal entries $(\mathbf{X}^T\mathbf{X})^{-1}_{ii}$ to be very small. When we calculate the standard error by dividing by this small value, the error blows up.

Theorem 2.10 ()

We can compute this t-statistic w.r.t. just the sample size n and the correlation coefficient ρ as such.

$$t = \frac{\hat{\beta} - 0}{\text{SE}(\hat{\beta})}$$

and the denominator is simply

$$\text{SE}(\hat{\beta}) = \sqrt{\frac{\frac{1}{n-1}\sum(y_i - \hat{y})^2}{\sum(x_i - \bar{x})^2}} \implies t = \frac{\hat{\beta}\sqrt{\sum(x_i - \bar{x})^2}\sqrt{n-1}}{\sqrt{\sum(y_i - \hat{y})^2}} = \frac{\hat{\beta}\sqrt{\sum(x_i - \bar{x})^2}\sqrt{n-1}}{\sqrt{(1-\rho^2)}\sqrt{\sum(y_i - \bar{y})^2}}$$
$$= \frac{\rho}{\sqrt{1-\rho^2}}\sqrt{n-1}$$

where the residual sum of squares on the top can be substituted according to our theorem. Therefore

$$t = \frac{\rho}{\sqrt{1-\rho^2}}\sqrt{n-1} \tag{85}$$

2.5.2 F Test

Given that you have n data points that have been fit on a linear model, the F-statistic is based on the ratio of two variances.

2.6 Bayesian Linear Regression

3 High Dimensional Linear Regression

Now supposed that $d > n$, then the first problem is that we can no longer use least squares since X^TX is no longer invertible and the same problem happens with maximum likelihood. This is known as the **high dimensional** or **large p, small n** problem. The most straightforward way is simply to reduce the covariates to a dimension smaller than n. This can be done with three ways.

1. We perform PCA on the X and use the first k principal components where $k < n$.
2. We cluster the covariates based on their correlation. We can use one feature from each cluster or take the average of the covariates within each cluster.
3. We can screen the variables by choosing the k features that have the largest correlation with Y.

Once this is done, we are back in the low dimensional regime and can use least squares. Essentially, this is a way to find a good subset of the covariates, which can be formalized by the following. Let S be a subset of $[d]$ and let $X_S = (X_j : j \in S)$. If the size of S is not too large, we can regress Y on X_S instead of X.

Definition 3.1 (Best Subset Regression)

Fix $k < d$ and let $\mathcal{S}_k$ denote all subsets of size k. For a given $S \in \mathcal{S}_k$, let β_S be the best linear predictor for the subset S. We want to find the best subset S that minimizes the loss

$$\mathbb{E}[(Y - \beta_S^T X_S)^2] \tag{86}$$

which is equivalent to finding

$$\underset{\beta}{\text{argmin}}\, \mathbb{E}[(Y - \beta^T X)^2] \text{ subject to } ||\beta||_0 \leq k \tag{87}$$

where $||\beta||_0$ is the number of non-zero entries in β.

There will be a bias variance tradeoff. As k increases, the bias decreases but the variance increases. We can approximate the risk with the training error, but the minimization is over all subset of size k, and so this is NP-hard. Therefore, best subset regression is infeasible, but we can approximate best subset regression in two different ways.

1. A greedy approximation leads to *forward stepwise regression*.
2. A convex relaxation of the problem leads to the *LASSO* regression.

It turns out that the theoretical guarantees and computational time for both are the same, but the Lasso is much more popular. It may be due to a cleaner form or that it's easier to study, but who knows.

A completely separate way is to use all the covariates, but instead of least squares, we shrink the coefficients towards 0. This is called *ridge regression* and is an example of a *shrinkage model*.

3.1 Ridge Regression

Ridge regression is used both in the high dimensional case or when our function space is too large/complex, which leads to overfitting. In the overfitting case, we have seen that either decreasing our function space or getting more training data helps. Another popular way is to add a **regularizing term** to the error function in order to discourage the coefficients from reaching large values, effectively limiting the variance over $\mathcal{D}$.

Definition 3.2 (Ridge Regression)

In **ridge regression**, we minimize

$$E(\boldsymbol{\theta}) := \frac{1}{2}\sum_{n=1}^{N}\left(h_{\boldsymbol{\theta}}(x^{(n)}) - y^{(n)}\right)^2 + \frac{\lambda}{2}||\boldsymbol{\theta}||_2^2 \tag{88}$$

where we penalize according to the L2 norm of the coefficients.

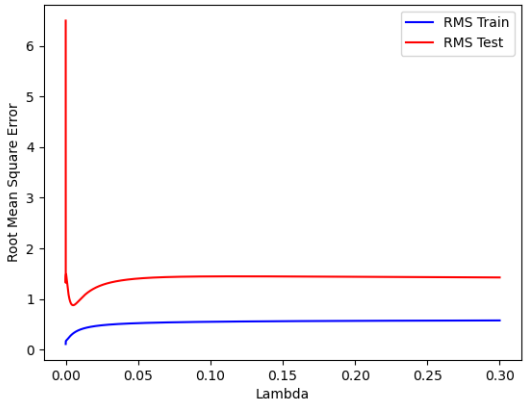


Figure 6: Even with a slight increase in the regularization term λ, the RMS error on the testing set heavily decreases.

Theorem 3.1 (Least Squares Solution for Ridge Regression)

The minimizer of the ridge loss is

$$\hat{\beta} = (X^T X + \lambda I)^{-1} \mathbf{X}^T \mathbf{Y} \tag{89}$$

Proof.

TBD

Theorem 3.2 (Bias Variance Decomposition of Ridge Regression)

TBD

From a computational point of view, we can see that by adding the λI term, it *dampens* the matrix so that it does become invertible (or well conditioned), allowing us to find a solution. The higher the λ term, the higher the damping effect. The next theorem compares the performance of the best ridge regression estimator to the best linear predictor.

Theorem 3.3 (Hsu, Kakade, Zhang, 2014 [2])

Suppose that $||X_i|| \leq r$ and let $\beta^T x$ be the best linear approximation to $m(x)$. Then, with probability at least $1 - 4e^{-t}$, we have

$$r(\hat{\beta}) - r(\beta) \leq \left(1 + O\left(\frac{1 + r^2/\lambda}{n}\right)\right) \frac{\lambda ||\beta||^2}{2} + \frac{\sigma^2}{n} \frac{\text{Tr}(\Sigma)}{2\lambda} \tag{90}$$

We can see that the λ term exists in the numerator on $\frac{\lambda ||\beta||^2}{2}$ and in the denominator on $\frac{\text{Tr}(\Sigma)}{2\lambda}$. This is the bias variance tradeoff. The first term is the bias term, which is the penalty for not being able to fit the data as well. The second term is the variance term, which is the penalty for having a more complex model. So our optimal λ in the theoretical sense would be the one that minimizes the sum of these two terms. In practice, it's not this clean since we have unknown quantities in the formula, but just like how we did cross validation over the model complexity, we can also do cross validation over the λ. The decomposition above just gives you a theoretical feeling of how these things trade off.

Question 3.1 (To Do)

Bayesian interpretation of ridge regression.

3.2 Forward Stepwise Regression

Forward stepwise regression is a greedy algorithm that starts with an empty set of covariates and adds the covariate that most improves the fit.

Definition 3.3 (Greedy Forward Stepwise Regression)

Given your data $\mathcal{D}$, let's first standardize it to have mean 0 and variance 1.[a] With each covariate $X = (X_1, \dots, X_n)$, we compute the correlation between it and the Y, which reduces to the inner product (since we standardized).

$$\rho_j = \langle Y, X_j \rangle = \frac{1}{n} \sum_{i=1}^{n} Y_i X_{ij} \tag{91}$$

3.3 Lasso Regression

The Lasso approximates the best subset regression by using a convex relaxation. In particular, the norm $||\beta||_0$ is not convex, but the L1 norm $||\beta||_1$ is. Therefore, we want relax our constraint equation as such:

$$\underset{||\beta||_0 \leq L}{\operatorname{argmin}} r(\beta) \mapsto \underset{||\beta||_1 \leq L}{\operatorname{argmin}} r(\beta) \tag{92}$$

This gives us a convex problem, which we can then solve. In fact, it turns out that optimizing the risk given the L1 restriction on the norm is equivalent to minimizing the risk plus a L1 penalty. Therefore, there exists a pair (L, λ) for which the two problems are equivalent

$$\underset{||\beta||_1 \leq L}{\operatorname{argmin}} r(\beta) = \underset{\beta}{\operatorname{argmin}} r(\beta) + \lambda ||\beta||_1 \tag{93}$$

Definition 3.4 (LASSO Regression)

In **lasso regression**, we minimize the loss defined

$$\hat{R}(\beta) = \frac{1}{n} \sum_{i=1}^{n} (y^{(i)} - \beta^T x^{(i)})^2 + \lambda ||\beta||_1 \tag{94}$$

where we penalize according to the L1 norm of the coefficients.

Unfortunately, there is no closed form solution for this estimator, but in convex optimization, we can prove that this estimator is sparse. That is, for large enough λ, many of the components of $\hat{\beta}$ are 0. The classical intuition for this is the figure below.

[a] This may or may not be a good idea, since the variance of each covariate can tell you a lot about the importance of the covariate.

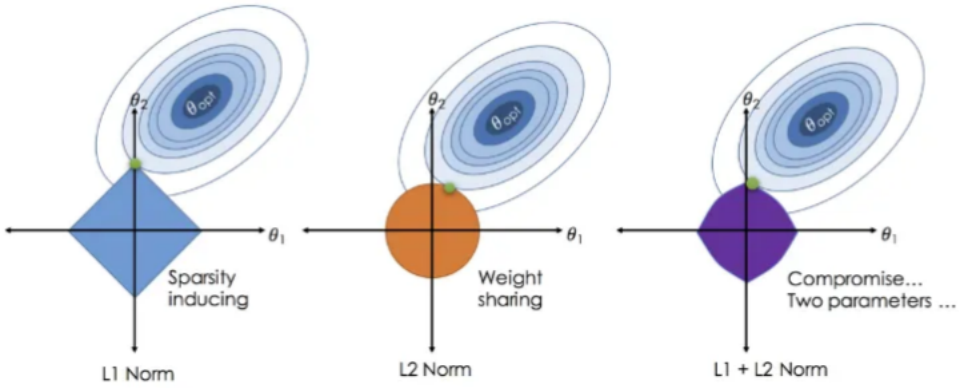


Figure 7: The ridge regularizer draws equipotential circles in our parameter space. The lasso draws a diamond, which tends to give a sparser solution since the loss is most likely to "touch" the corners of the contour plots of the regularizer. The elastic net is a linear combination of the ridge and lasso regularizers.

This now raises the question of how to determine a suitable regularization parameter λ. The next theorem shows a nice concentration property of the Lasso for bounded covariates.

Theorem 3.4 (Concentration of Lasso)

Given (X, Y), assume that $|Y| \leq B$ and $\max_j |X_j| \leq B$. Let

$$\beta^* = \underset{||\beta||_1 \leq L}{\operatorname{argmin}}\, r(\beta) \tag{95}$$

be the best sparse linear predictor in the L1 sense, where $r(\beta) = \mathbb{E}[(Y - \beta^T X)^2]$. Let our lasso estimator be

$$\hat{\beta} = \underset{||\beta||_1 \leq L}{\operatorname{argmin}}\, \hat{r}(\beta) = \underset{||\beta||_1 \leq L}{\operatorname{argmin}}\, \frac{1}{n} \sum_{i=1}^{n} (Y_i - \beta^T X_i)^2 \tag{96}$$

which minimizes the empirical risk. Then, with probability at least $1 - \delta$,

$$r(\hat{\beta}) \leq r(\beta^*) + \sqrt{\frac{16(L+1)^4 B^2}{n} \log\left(\frac{\sqrt{2}d}{\sqrt{\delta}}\right)} \tag{97}$$

Proof.

4 Nonparametric Regression

4.1 Kernel Regression

This is a local linear smoother.

Linear smoothers, Kernel regression, Gaussian smoothing, Kernel smoothers, but has the desgin bias and boundary bias problem. Good fix is local linear regression.

4.2 Local Polynomial Regression

Local linear regression, and polynomial regression. This is a local linear smoother.

4.3 Regularized: Spline Smoothing

This is not local, but it's a linear smoother.

4.4 Regularized: RKHS Regression

This is not local, but it's a linear smoother.

4.5 Additive Models

We've learned about linear smoothers to create nonparametric models in 1 dimension. We can then extend this to multiple input dimensions with additive models, which aren't as flexible since they can't capture dependencies, but we can create dependency functions.

4.6 Nonlinear Smoothers, Trend Filtering

Tough example of the Dobbler function (like topologists sine curve). It's a pretty good fit but it's not too good since it's using a linear smoother (homogeneous). So we might need to fit it with nonlinear smoothers.

4.7 High Dimensional Nonparametric Regression

4.8 Regression Trees

5 Cross Validation

We have understood the theoretical foundations of overfitting and underfitting with the bias variance decomposition. But in practice, we don't have an ensemble of datasets; we just have one. Therefore, we don't actually know what the bias, the variance, or the noise is at all. Therefore, how do we actually *know* in practice when we are underfitting or overfitting? Easy. We just split our dataset into 2 different parts: the training set and testing sets.

$$\mathcal{D} = \mathcal{D}_{train} \sqcup \mathcal{D}_{test} \tag{98}$$

What we usually have is a **training set** that allows us to train the model, and then to check its performance we have a **test set**. We would train the model on the training set, where we will always minimize the loss, and then we would look at the loss on the test set. Though we haven't made a testing set, since we know the true model let us just generate more data and use that as our testing set. For each model, we can calculate the optimal $\boldsymbol{\theta}$, which we will denote $\boldsymbol{\theta}^*$, according to the **root mean squared loss**

$$h_{\boldsymbol{\theta}^*} = \underset{h_{\boldsymbol{\theta}}}{\text{argmin}} \sqrt{\frac{1}{N} \sum_{i=1}^{N} \left(y^{(i)} - h_{\boldsymbol{\theta}}(\mathbf{x}^{(i)}) \right)^2} \tag{99}$$

where division of N allows us to compare different sizes of datasets on equal footing, and the square root ensures that this is scaled correctly. Let us see how well these different order models perform on a separate set of data generated by the same function with Gaussian noise.

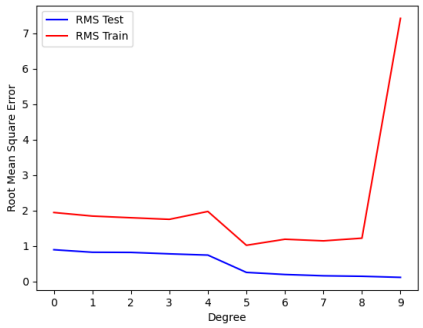


Figure 8: We can see that the RMS decreases monotonically on the training error as more complex functions become more fine-tuned to the data. However, when we have a 9th degree polynomial the RMS for the testing set dramatically increases, meaning that this model does not predict the testing set well, and performance drops.

Now we know that a more complex model (i.e. that captures a greater set of functions) is not necessarily the best due to overfitting. Therefore, researchers perform **cross-validation** by taking the training set $(\mathcal{X}, \mathcal{Y})$. We divide it into S equal pieces

$$\bigcup_{s=1}^{S} D_s = (\mathcal{X}, \mathcal{Y}) \tag{100}$$

Then, we train the model $\mathcal{M}$ on $S-1$ pieces of the data and then test it across the final piece, and do this S times for every test piece, averaging its perforance across all S test runs. Therefore, for every model $\mathcal{M}_k$, we must train it S times, for all K models, requiring KS training runs. If data is particularly scarce, we set $S = N$, called the **leave-one-out** technique. Then we just choose the model with the best average test performance.

The following result shows that cross-validation (data splitting) leads to an estimator with risk nearly as good as the best model in the class.

Theorem 5.1 (Gyorfi, Kohler, Krzyak, Walk (2002))

Let $\mathcal{M} = \{m_h\}$ be a finite class of regression estimators indexed by a parameter h, with m being the true risk minimizer, $m_{\hat{h}}$ being the empirical risk minimizer over the whole dataset $\mathcal{D}$, and m_H being the empirical risk minimizer over the test set $\mathcal{D}_{\text{test}}$ for ordinary least squares loss.

$$m_H = \underset{m_h}{\text{argmin}} \frac{1}{N} \sum_{i \in \mathcal{D}_{\text{test}}} (y_i - m_h(x_i))^2 \tag{101}$$

$$m_{\hat{h}} = \underset{m_h}{\text{argmin}} \frac{1}{N} \sum_{i \in \mathcal{D}} (y_i - m_h(x_i))^2 \tag{102}$$

If the data Y_i and estimators are bounded by L, then for any $\delta > 0$, we have

$$\mathbb{E} \int |m_H(x) - m(x)|^2 \, d\mathbb{P}(x) \leq (1+\delta)\mathbb{E} \int |m_{\hat{h}}(x) - m(x)|^2 \, d\mathbb{P}(x) + \frac{C(1 + \log|M|)}{n} \tag{103}$$

where $c = L^2(16/\delta + 35 + 19\delta)$.

Code 5.1 (Minimal Example of Train Test Split in scikit-learn)

To implement this in scikit-learn, we want to use the `train_test_split` class. We can also set a random state parameter to reproduce results.

```
from sklearn.model_selection import train_test_split

# Split into training (80\%) and test (20\%) data
X_train, X_test, Y_train, Y_test = train_test_split(X, Y, test_size=0.2,
    random_state=66)
```

However, this process requires a lot of training runs and therefore may be computationally infeasible. Therefore, various **information criterion** has been proposed to efficiently select a model.

5.1 Leave 1 Out Cross Validation

5.1.1 Generalized (Approximate) Cross Validation

5.1.2 Cp Statistic

5.2 K Fold Cross Validation

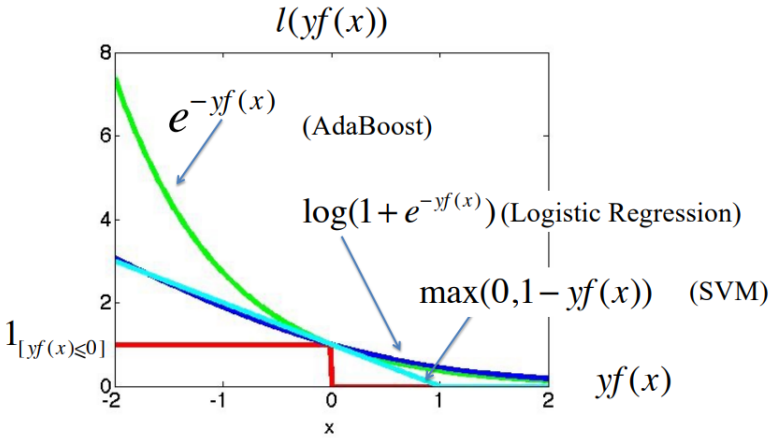
5.3 Data Leakage

5.4 Information Criterion

6 Linear Classification

6.1 Empirical Risk Minimizer

You literally just try to build a hyperplane to minimize the number of misclassifications, but this is not really differentiable and is hard. It's just a stepwise function. Therefore, you use a **surrogate loss function** to approximate the 0-1 loss function. The logistic uses some function, and the SVM uses the smallest convex function to approximate the 0-1 loss function. Here are some examples:



6.2 Perceptron

Definition 6.1 (Perceptron Model and Loss)

The simplest binary classification model is the **perceptron algorithm**. It is a discriminative parametric model that assigns

$$f_w(x) = \begin{cases} 1 & \text{if } w^T x + b \geq 0 \\ -1 & \text{if } w^T x + b < 0 \end{cases} \tag{104}$$

where we have chosen to label class $C_1 = 1$ and $C_2 = -1$. Note that unlike linear regression (and logistic regression, as we will see later), the perceptron is not a probabilistic model. It is a **discriminant function**, which just gives point estimates of the classes, not their respective probabilities. Like logistic regression, however, it is a linear model, meaning that the decision boundary it creates is always a linear (affine) hyperplane.

To construct the surrogate loss function, we would want a loss that penalizes not only if there is a misclassification, but how *far* that misclassified point is from the boundary. Therefore, if y and $\hat{y} = f_w(x)$ have the same sign, i.e. if $yf_w(x) > 0$, then the penalty should be 0, and if it is < 0, then the penalty should be proportional to the orthogonal distance of the misclassified point to the boundary, which is represented by $-wTxy$ (where the negative sign makes this cost term positive).

Definition 6.2 (Surrogate Loss for Perceptron)

Therefore, our cost functions would take all the points and penalize all the terms by 0 if they are correctly classified and by $-\mathbf{w}^T \boldsymbol{\phi}^{(n)} y^{(n)}$ if incorrectly classified.

$$L(y, \hat{y}) = \sum_{n=1} [-\mathbf{w}^T \boldsymbol{\phi}^{(n)} y^{(n)}]_+ \text{ where } [f(\mathbf{x})]_+ \coloneqq \begin{cases} f(\mathbf{x}) & \text{if } f(\mathbf{x}) > 0 \\ 0 & \text{else} \end{cases} \tag{105}$$

Note that this is a piecewise linear function and convex.

Code 6.1 (Perceptron in scikit-learn)

Let's implement this in scikit-learn, using two pipelines with different data standardization techniques to see the differences in the perceptron boundary.

```
from sklearn.pipeline import Pipeline
from sklearn.linear_model import Perceptron
from sklearn.preprocessing import QuantileTransformer, StandardScaler

pipe1 = Pipeline([
    ("scale", StandardScaler()),
    ("model", Perceptron())
])

pipe2 = Pipeline([
    ("scale", QuantileTransformer(n_quantiles=100)),
    ("model", Perceptron())
])
```

Figure 9

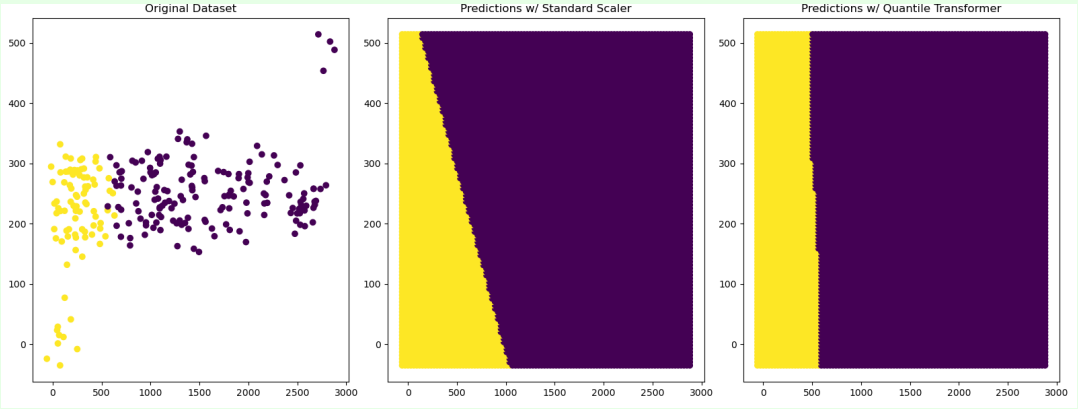


Figure 10: Perceptron Trained on Different Standardized Data

6.3 Logistic and Softmax Regression

We can upgrade from a discriminant function to a discriminative probabilistic model with **logistic regression**. In practice, we usually deal with **probabilistic models** where rather than giving a point estimate $\hat{y}$, we attempt to model the *distribution* $\mathbb{P}_{Y|X=\hat{x}}$. Even though in the end, we will just output the mean μ of this conditional distribution, modeling the distribution allows us to quantify uncertainty in our measurements.

Definition 6.3 (Logistic Regression)

The **logistic regression** model is a linear model of the form

$$f_w(x) = \sigma(w^T x) = \frac{1}{1+e^{-w^T x}}, \text{ where } \sigma(x) := \frac{1}{1+e^x} \tag{106}$$

It is different from linear regression in two ways:

1. In linear regression, we assumed that the targets are linearly dependent with the covariates as $y = w^T x + b$. However, this means that the hypothesis f_w is unbounded. Since we have two classes (say with labels 0 and 1), we must have some sort of *link function* σ that takes the real numbers and compresses it into the domain $[0, 1]$. Technically, we can choose any continuous, monotinically increasing function from $\mathbb{R}$ to $(0, 1)$. However, the following property of the sigmoid makes derivation of gradients very nice.

$$\sigma'(x) = \sigma(x)\big(1 - \sigma(x)\big) \tag{107}$$

2. Once this is compressed, we assume that the residual distribution is a Bernoulli.

Definition 6.4 (Binary Cross Entropy Loss as Surrogate Loss for Logistic Regression)

The surrogate loss for logistic regression is the **binary cross entropy loss**, which is defined as

$$L(y, \hat{y}) = -y \log \hat{y} - (1-y)\log(1-\hat{y}) \tag{108}$$

One important observation to make is that notice that the output of our hypothesis is used as a parameter to define our residual distribution.

1. In linear regression, the f_w was used as the *mean* μ of a Gaussian.
2. In logistic regression, the f_w is used also as the mean p of a Bernoulli.

The reason we want this sigmoid is so that we make the domains of the means of the residuals match the range of the outputs of our model. It's simply a manner of convenience, and in fact we could have really chose any function that maps $\mathbb{R}$ to $(0, 1)$.

Some questions may arise, such as "why isn't the variance parameter of the Gaussian considered in the linear model?" or "what about other residual distributions that have multiple parameters?" This is all answered by generalized linear models, which uses the output of a linear model as a *natural parameter* of the canonical exponential family of residual distributions.

Unfortunately, there is no closed form solution for logistic regression like the least squares solution in linear regression. Therefore, we can only resort to maximum likelihood estimation.

Theorem 6.1 (Maximum Likelihood Estimation for Logistic)

Given a dataset $\mathcal{D} = \{(x^{(i)}, y^{(i)})\}_{i=1}^N$, our likelihood is

$$L(\theta; \mathcal{D}) = \prod_{i=1}^n p(y^{(i)} \mid x^{(i)}; \theta) = \prod_{i=1}^N \left(h_\theta(x^{(i)})\right)^{y^{(i)}} \left(1 - h_\theta(x^{(i)})\right)^{1-y^{(i)}}$$

We can equivalently minimize its negative log likelihood, giving us the **binary cross entropy** loss function

$$\begin{aligned}\ell(\theta) &= -\log L(\theta) \\ &= -\sum_{i=1}^n y^{(i)} \log h_\theta(x^{(i)}) + (1 - y^{(i)}) \log(1 - h_\theta(x^{(i)}))\end{aligned}$$

Now taking the gradient for just a single sample $(x^{(i)}, y^{(i)})$ gives

$$\begin{aligned}\frac{\partial \ell}{\partial \theta} &= \left(\frac{y^{(i)}}{\sigma(\theta^T x^{(i)})} - \frac{1 - y^{(i)}}{1 - \sigma(\theta^T x^{(i)})}\right) \frac{\partial}{\partial \theta} \sigma(\theta^T x^{(i)}) \\ &= \frac{\sigma(\theta^T x^{(i)}) - y^{(i)}}{\sigma(\theta^T x^{(i)}) \left(1 - \sigma(\theta^T x^{(i)})\right)} \sigma(\theta^T x^{(i)}) \left(1 - \sigma(\theta^T x^{(i)})\right) x^{(i)} \\ &= \left(h_\theta(x^{(i)}) - y^{(i)}\right) x\end{aligned}$$

and summing it over some minibatch $M \subset \mathcal{D}$ gives

$$\nabla_\theta \ell_M = \sum_{(x,y) \in M} (y - h_\theta(x)) x$$

Therefore, the stochastic gradient descent algorithm is

$$\begin{aligned}\theta &= \theta - \eta \nabla_\theta \ell(\theta) \\ &= \theta - \eta \sum_{(x,y) \in M} (y - h_\theta(x)) x\end{aligned}$$

We would like to extend this to the multiclass case.

Definition 6.5 (Softmax Function)

The softmax function is defined

$$o(\mathbf{x}) = \frac{e^{\mathbf{x}}}{||e^{\mathbf{x}}||} = \frac{1}{\sum_j e^{x_j}} \begin{pmatrix} e^{x_1} \\ \vdots \\ e^{x_D} \end{pmatrix} \tag{109}$$

What makes the softmax so popular is that the total derivative turns out to simplify functions a lot. The total derivative of the softmax can be derived as such.

Lemma 6.1 (Derivative of Softmax)

The derivative of the softmax is

$$Do(\mathbf{x}) = \text{diag}(o(\mathbf{x})) - o(\mathbf{x}) \otimes o(\mathbf{x}) \tag{110}$$

where $\otimes$ is the outer product. That is, let y_i be the output of the softmax. Then, for the 4×4 softmax function, we have

$$Do(\mathbf{x}) = \begin{pmatrix} y_1(1-y_1) & -y_1y_2 & -y_1y_3 & -y_1y_4 \\ -y_2y_1 & y_2(1-y_2) & -y_2y_3 & -y_2y_4 \\ -y_3y_1 & y_3y_3 & y_3(1-y_3) & -y_3y_4 \\ -y_4y_1 & -y_4y_2 & -y_4y_3 & y_4(1-y_4) \end{pmatrix} \tag{111}$$

Proof.

We will provide a way that allows us not to use quotient rule. Given that we are taking the partial derivative of y_i with respect to x_j, we can use the log of it to get

$$\frac{\partial}{\partial x_j} \log(y_i) = \frac{1}{y_i} \frac{\partial y_i}{\partial x_j} \implies \frac{\partial y_i}{\partial x_j} = y_i \frac{\partial}{\partial x_j} \log(y_i)$$

Now the partial of the log term is

$$\begin{aligned} \log y_i &= \log \left(\frac{e^{x_i}}{\sum_l e^{x_l}} = x_i - \log \left(\sum_l e^{x_l} \right) \right. \\ \frac{\partial}{\partial x_j} \log(y_i) &= \frac{\partial x_i}{\partial x_j} - \frac{\partial}{\partial x_j} \log \left(\sum_l e^{x_l} \right) \\ &= 1_{i=j} - \frac{1}{\sum_l e^{x_l}} e^{x_j} \end{aligned}$$

and plugging this back in gives

$$\frac{\partial y_i}{\partial x_j} = y_i(1_{i=j} - y_j) \tag{112}$$

It also turns out that the sigmoid is a specific case of the softmax. That is, given softmax for 2 classes, we have

$$o \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = \frac{1}{e^{x_1} + e^{x_2}} \begin{pmatrix} e^{x_1} \\ e^{x_2} \end{pmatrix}$$

So, the probability of being in class 1 is

$$\frac{e^{x_1}}{e^{x_1} + e^{x_2}} = \frac{1}{1 + e^{x_2 - x_1}}$$

and the logistic sigmoid is just a special case of the softmax function that avoids using redundant parameters. We actually end up overparameterizing the softmax because the probabilities must add up to one.

Definition 6.6 (Softmax Regression Model)

The softmax regression of K classes assumes a model of the form

$$h_\theta(x) = o(\mathbf{W}\mathbf{x} + \mathbf{b}) \tag{113}$$

where $\mathbf{W} \in \mathbb{R}^{K \times D}, \mathbf{b} \in \mathbb{R}^D$. Again, we have a linear map followed by some link function (the softmax) which allows us to nonlinearly map our unbounded linear outputs to some domain that can be easily parameterized by a probability distribution. In this case, our residual distribution is a **multinomial distribution**

$$y \sim \text{Multinomial}\big(h_{\mathbf{w}}(\mathbf{x})\big) = \text{Multinomial}\big([h_{\mathbf{w}}(\mathbf{x})]_1, \dots, [h_{\mathbf{w}}(\mathbf{x})]_K\big) \tag{114}$$

Definition 6.7 (Multiclass Cross Entropy Loss as Surrogate Loss for Softmax)

The surrogate loss for softmax regression is the **multiclass cross entropy loss**, which is defined as

$$L(\theta; \mathcal{D}) = -\sum_{i=1}^N \sum_{k=1}^K y_k^{(i)} \log\left(h_\theta(\mathbf{x}^{(i)})\right)_k \tag{115}$$

Theorem 6.2 (Maximum Likelihood Estimation for Softmax)

Since a closed form solution is not available for logistic regression, it is clearly not available for softmax. Therefore, we one hot encode our target variables as $\mathbf{y}^{(i)}$ and write our likelihood as

$$L(\theta; \mathcal{D}) = \prod_{i=1}^N \prod_{k=1}^K p(C_k \mid \mathbf{x}^{(i)})^{\mathbf{y}_k^{(i)}} = \prod_{i=1}^N \prod_{k=1}^K \left(\mathbf{h}_{\mathbf{W}}(\mathbf{x}^{(i)})\right)_k^{\mathbf{y}_k^{(i)}} \tag{116}$$

Taking the negative logarithm gives us the **cross entropy** loss function

$$\ell(\boldsymbol{\theta}) = -\sum_{i=1}^N \sum_{k=1}^K y_k^{(i)} \log\left(\mathbf{h}_{\boldsymbol{\theta}}(\mathbf{x}^{(i)})\right)_k = -\sum_{i=1}^N \mathbf{y}^{(i)} \dot{\log}\big(\mathbf{h}_{\boldsymbol{\theta}}(\mathbf{x}^{(i)})\big) \tag{117}$$

where $\cdot$ is the dot product. The gradient of this function may seem daunting, but it turns out to be very cute. Let us take a single sample $(\mathbf{x}^{(i)}, \mathbf{y}^{(i)})$, drop the index i, and write

$$\begin{aligned} \mathbf{x} &\mapsto \mathbf{W}\mathbf{x} + \mathbf{b} = \mathbf{z} \\ \hat{\mathbf{y}} = \mathbf{a} &= o(\mathbf{z}) \\ L &= -\mathbf{y} \cdot \log(\mathbf{a}) = -\sum_{k=1}^K y_k \log(a_k) \end{aligned}$$

We must compute

$$\frac{\partial L}{\partial \mathbf{W}} = \frac{\partial L}{\partial \mathbf{a}} \frac{\partial \mathbf{a}}{\partial \mathbf{z}} \frac{\partial \mathbf{z}}{\partial \boldsymbol{\theta}}$$

We can compute $\partial L / \partial \mathbf{z}$ as such, using our derivations for the softmax derivative above. We compute

element wise.

$$\begin{aligned}\frac{\partial L}{\partial z_j} &= -\sum_{k=1}^{K} y_k \frac{\partial}{\partial z_j} \log(a_k) \\ &= -\sum_{k=1}^{K} y_k \frac{1}{a_k} \frac{\partial a_k}{\partial z_j} \\ &= -\sum_{k=1}^{K} \frac{y_k}{a_k} a_k (1_{\{k=j\}} - a_j) \\ &= -\sum_{k=1}^{K} y_k (1_{\{k=j\}} - a_j) \\ &= \left(\sum_{k=1}^{K} y_k a_j \right) - y_j \\ &= a_j \left(\sum_{k=1}^{K} y_k \right) - y_j \\ &= a_j - y_j\end{aligned}$$

and combining these gives

$$\frac{\partial L}{\partial \mathbf{z}} = (\mathbf{a} - \mathbf{y})^T \tag{118}$$

Now, computing $\partial \mathbf{z} / \partial \mathbf{W}$ gives us a 3-tensor, which is not ideal to work with. However, let us just compute this with respect to the elements again. We have

$$\begin{aligned}z_k &= \sum_{d=1}^{D} W_{kd} x_d + b_k \\ \frac{\partial z_k}{\partial W_{ij}} &= \sum_{d=1}^{D} x_d \frac{\partial}{\partial W_{ij}} W_{kd}\end{aligned}$$

where

$$\frac{\partial}{\partial W_{ij}} W_{kd} = \begin{cases} 1 & \text{if } i = k, j = d \\ 0 & \text{else} \end{cases} \tag{119}$$

Therefore, since d is iterating through all elements, the sum will only be nonzero if $k = i$. That is, $\frac{\partial z_k}{\partial W_{ij}} = x_j$ if $k = i$ and 0 if else. Therefore,

$$\frac{\partial \boldsymbol{z}}{\partial W_{ij}} = \begin{bmatrix} 0 \\ \vdots \\ 0 \\ x_j \\ 0 \\ \vdots \\ 0 \end{bmatrix} \leftarrow i\text{th element}$$

Now computing

$$\frac{\partial L}{\partial W_{ij}} = \frac{\partial L}{\partial \mathbf{z}} \frac{\partial \mathbf{z}}{\partial W_{ij}} = (\mathbf{a} - \mathbf{y}) \frac{\partial \mathbf{z}}{\partial W_{ij}} = \sum_{k=1}^{K} (a_k - y_k) \frac{\partial z_k}{\partial W_{ij}} = (a_i - y_i) x_j \tag{120}$$

To get $\partial L/\partial W_{ij}$ we want a matrix whose entry (i,j) is $(a_i - y_i)x_j$. This is simply the outer product as shown below. For the bias term, $\partial \mathbf{z}/\partial \mathbf{b}$ is simply the identity matrix.

$$\frac{\partial L}{\partial \mathbf{W}} = (\mathbf{a}-\mathbf{y})\mathbf{x}^T, \quad \frac{\partial L}{\partial \mathbf{b}} = \mathbf{a}-\mathbf{y} \tag{121}$$

Therefore, summing the gradient over some minibatch $M \subset [N]$ gives

$$\nabla_{\mathbf{W}} \ell_M = \sum_{i \in M} (\mathbf{h}_{\boldsymbol{\theta}}(\mathbf{x}^{(i)}) - \mathbf{y}^{(i)})(\mathbf{x}^{(i)})^T, \quad \nabla_{\mathbf{b}} \ell_M = \sum_{i \in M} (\mathbf{h}_{\boldsymbol{\theta}}(\mathbf{x}^{(i)}) - \mathbf{y}^{(i)}) \tag{122}$$

and our stochastic gradient descent algorithm is

$$\begin{aligned} \boldsymbol{\theta} = \begin{pmatrix} \mathbf{W} \\ \mathbf{b} \end{pmatrix} &= \begin{pmatrix} \mathbf{W} \\ \mathbf{b} \end{pmatrix} - \eta \begin{pmatrix} \nabla_{\mathbf{W}} \ell_M \\ \nabla_{\mathbf{b}} \ell_M \end{pmatrix} \\ &= \begin{pmatrix} \mathbf{W} \\ \mathbf{b} \end{pmatrix} - \eta \begin{pmatrix} \sum_{i \in M} (\mathbf{h}_{\boldsymbol{\theta}}(\mathbf{x}^{(i)}) - \mathbf{y}^{(i)})(\mathbf{x}^{(i)})^T \\ \sum_{i \in M} (\mathbf{h}_{\boldsymbol{\theta}}(\mathbf{x}^{(i)}) - \mathbf{y}^{(i)}) \end{pmatrix} \end{aligned}$$

6.3.1 Sparse Logistic Regression

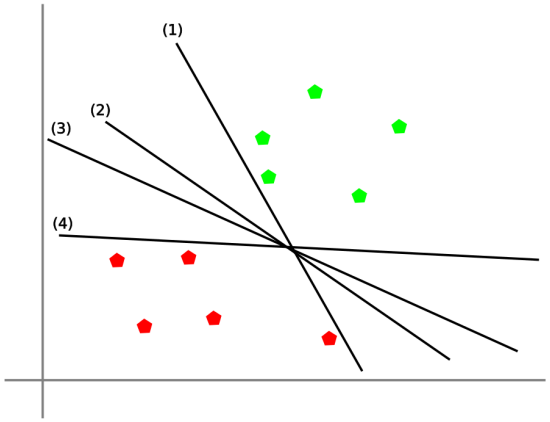
6.4 Support Vector Machines

Definition 6.8 (Hinge Loss)

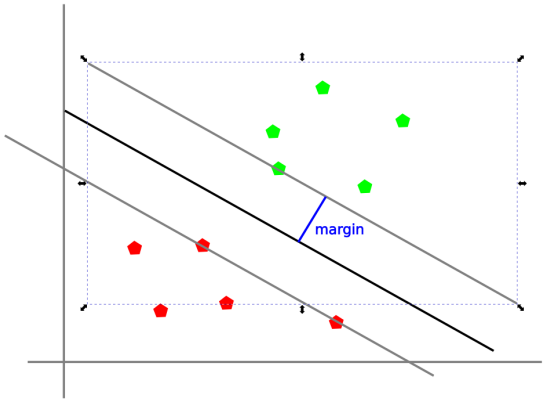
The **hinge loss** is a convex surrogate loss function for the 0-1 loss function. It is defined as

$$L(y, \hat{y}) = \max(0, 1 - y\hat{y}) \tag{123}$$

A support vector machine focuses only on the points that are most difficult to tell apart, whereas other classifiers pay attention all of the points. A SVM is a discriminative, non-probabilistic model. Let us first assume that our dataset $\mathcal{D} = \{\mathbf{x}_i, y_i\}$ is linearly separable with $y_i \in \{-1, +1\}$. Based on previous algorithms like the perceptron, it will find some separating hyperplane. However, there's an infinite number of separating hyperplanes as shown in Figure 11a. What support vector machines want to do is to find the best one, with the "best" defined as the hyperplane that maximizes the distance between either the closest positive or negative samples, shown in Figure 11*b*.



(a) Planes such as (1) and (4) are "too close" to the positive and negative samples.



(b) SVMs try to find the separating hyperplane with the best minimum margin.

Figure 11: Motivating problem

We want to formalize the concepts of these margins that we wish to maximize. To do this, we will define two terms.

Definition 6.9 (Geometric margin)

Given a point $\mathbf{x}_0$ and a hyperplane of equation $\mathbf{w} \cdot \mathbf{x} + b = 0$, the distance from $\mathbf{x}_0$ to the hyperplane, known as the **geometric margin**, can be computed with the formula

$$d = \frac{|\mathbf{x}_0 \cdot \mathbf{w} + b|}{||\mathbf{w}||} \tag{124}$$

Therefore, the geometric margin of the ith sample with respect to the hypothesis f is defined

$$\gamma_i = \frac{y_i \left(\mathbf{w} \cdot \mathbf{x}_i + b\right)}{||\mathbf{w}||} \tag{125}$$

We wish to optimize the parameters $\mathbf{w}, b$ in order to maximize the minimum of the geometric margins (the distance between the closest point and the hyperplane).

$$\underset{\mathbf{w},b}{\text{argmax}} \min_i \gamma_i = \underset{\mathbf{w},b}{\text{argmax}} \left\{ \frac{1}{||\mathbf{w}||} \min_i \left[y_i \left(\mathbf{w} \cdot \mathbf{x}_i + b\right)\right] \right\} \tag{126}$$

Direct solution of this optimization problem would be very complex, and so we convert this into an equivalent problem that is much easier to solve. Note that the solution to the above term is not unique. If there was a solution $(\mathbf{w}^*, b^*)$, then

$$\frac{y_i(\mathbf{w} \cdot \mathbf{x}_i + b)}{||\mathbf{w}||} = \frac{y_i(\lambda\mathbf{w} \cdot \mathbf{x}_i + \lambda b)}{||\lambda\mathbf{w}||} \tag{127}$$

That is, the geometric margin is not sensitive to scaling of the parameters of the hyperplane. Therefore, we can scale the numerator and the denominator by whatever we want and use this freedom to set

$$y_i(\mathbf{w} \cdot \mathbf{x}_i + b) = 1$$

for the point that is closest to the surface. In that case, all data points will satisfy the constraints

$$y_n(\mathbf{w} \cdot \mathbf{x}_i + b) \geq 1$$

In the case of data points for which the equality holds, the constraints are said to be *active*, whereas for the remainder they are *inactive*. Therefore, it will always be the case that $\min_i \left[y_i \left(\mathbf{w} \cdot \mathbf{x}_i + b\right)\right] = 1$, and the constraint problem reduces to

$$\underset{\mathbf{w},b}{\text{argmax}} \frac{1}{||\mathbf{w}||} = \underset{\mathbf{w},b}{\text{argmin}} \frac{1}{2}||\mathbf{w}||^2 \text{ subject to constraints } y_i(\mathbf{w} \cdot \mathbf{x}_i + b) \geq 1$$

This final step is the most significant step in this derivation and may be hard to wrap around the first time. So we dedicate the next subsubsection for this.

6.5 Functional and Geometric Margins

We could just work straight with this geometric margin, but for now, let's try to extend what we did with the perceptron into SVMs. We will find out that extending the concept of functional margins into SVMs

leads to ill-defined problems. In the perceptron, we wanted to construct a function $f(\mathbf{x}) = \mathbf{w} \cdot \mathbf{x} + b$ such that

$$y_i \, f(\mathbf{x}_i) \geq 0 \text{ for all } i = 1, 2, \dots, N$$

Definition 6.10 (Functional Margin)

The value of $y_i \, f(\mathbf{x}_i)$ gives us our confidence on our classification, and in a way it represents a kind of distance away from the separating hyperplane (if this value was 0, then we would be 50 50 split on whether to label it positive or negative). Therefore, we shall define

$$\hat{\gamma}_i = y_i f(\mathbf{x}_i)$$

as the **functional margin** of $(\mathbf{w}, b)$ with respect to the training sample $(\mathbf{x}_i, y_i)$. Therefore, the smallest of the function margins can be written

$$\hat{\gamma} = \min_i \gamma_i$$

called the **function margin**.

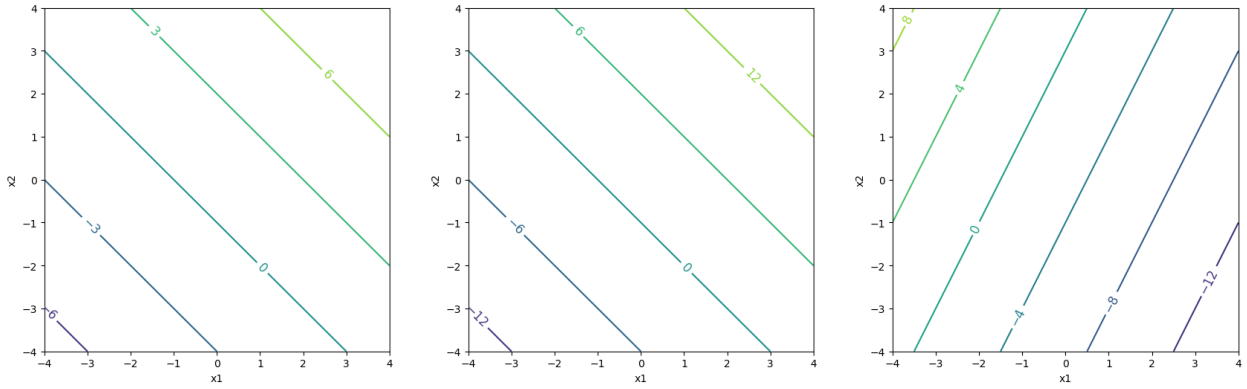
Note that the geometric margin and functional margin are related by a constant scaling factor. Given a sample $(\mathbf{x}_i, y_i)$, we have

$$\text{GeometricMargin} = \frac{y_i \, (\mathbf{w} \cdot \mathbf{x}_i + b)}{||\mathbf{w}||_2} = \frac{\text{FunctionalMargin}}{||\mathbf{w}||_2}$$

As we can see, the perceptron works with the functional margin, and since it does not care about how large the margin is (just whether it's positive or negative), we are left with an underdetermined system in which there exists infinite $(\mathbf{w}, b)$'s. Now what we want to do is impose a certain minimum margin $\gamma > 0$ and solve for $(\mathbf{w}, b)$ again, and keep increasing this γ until there is some unique solution. We can view this problem in two ways:

1. Take a specific minimum margin γ and find a $(\mathbf{w}, b)$, which may not exist, be unique, or exist infinitely that satisfies
$$y_i f(\mathbf{x}) = y_i(\mathbf{w} \cdot \mathbf{x} + b) \geq \gamma \text{ for all } i = 1, \dots, N$$
2. Take a specific $(\mathbf{w}, b)$ and calculate the maximum γ that satisfies the constraint equations above.

They're both equivalent problems, but both ill-posed if we look at (2). Since the samples are linearly separable by assumption, we can say that there exists some $\epsilon > 0$ such that $y_i f(\mathbf{x}_i) \geq \epsilon$ for all i. Therefore, if we just scale $(\mathbf{w}, b) \mapsto (\lambda \mathbf{w}, \lambda b)$ for some large λ, this leads to the solution for γ being unbounded. We can see in Figure 12 that we can increased confidence at no cost. Looking at (1), we can also see that if $(\mathbf{w}, b)$ does exist, then every other $(\lambda \mathbf{w}, \lambda b)$ for $\lambda > 1$ satisfies the property.



(a) $f(x) = x_1 + x_2 + 1$ (b) $f(x) = 2x_1 + 2x_2 + 2$ (c) $f(x) = -2x_1 + x_2 - 3$

Figure 12: From (a), you can see that simply multiplying everything by two automatically increases our confidence by 2, meaning that the functional margin can be scaled arbitrarily by scaing $(\mathbf{w}, b)$. There are still too many degrees of freedom in here and so extra constraints must be imposed.

6.5.1 Lagrange Duality

To minimize the equations with the constraint equations, we can use the method of Lagrange multipliers, which leads to to Lagrangian

$$\mathcal{L}(\mathbf{w}, b, \boldsymbol{\alpha}) = \frac{1}{2}||\mathbf{w}||^2 - \sum_i \alpha_i \big[y_i(\mathbf{w} \cdot \mathbf{x}_i + b) - 1 \big]$$

We can take the gradients with respect to $\mathbf{w}$ and b and set them to 0, which gives the two conditions

$$\mathbf{w} = \sum_i \alpha_i y_i \mathbf{x}_i$$
$$0 = \sum_i \alpha_i y_i \mathbf{x}_i$$

Now let's substitute our evaluated $\mathbf{w}$ back into $\mathcal{L}$, which gives the **dual representation** of the maximum margin problem in which we maximize

$$\begin{aligned} L &= \frac{1}{2}\Big(\sum_i \alpha_i y_i \mathbf{x}_i \Big)\Big(\sum_j \alpha_j y_j \mathbf{x}_j \Big) - \sum_i \alpha_i y_i x_i \cdot \Big[\sum_j \alpha_j y_j x_j \Big] - \sum_i \alpha_i y_i b + \sum_i \alpha_i \\ &= \sum_i \alpha_i - \frac{1}{2} \sum_{i,j} \alpha_i \alpha_j y_i y_j \, \mathbf{x}_i \cdot \mathbf{x}_j \end{aligned}$$

The summation with the b in it is 0 since we can pull the b out and the remaining sum is 0 from before. Now the optimization only depends on the dot product $\mathbf{x}_i \cdot \mathbf{x}_j$ of all pairs of sample vectors, which is very interesting. We will see more of this when we talk about kernel methods. Now, we need to solve the dual problem

$$\max_{\boldsymbol{\alpha}} \mathcal{L}(\boldsymbol{\alpha})$$

which can be done using some generic quadratic programming solver or some other method to get the optimum $\boldsymbol{\alpha}^*$, which gives us

$$\mathbf{w}^* = \sum_i \alpha_i^* y_i \mathbf{x}_i$$

6.6 Nonseparable Case

6.7 Gaussian/Linear Discriminant Analysis

6.7.1 Discriminative vs. Generative Models

Now we introduce our first example of a generative model, which introduces another division between models (in addition to parametric vs nonparametric, frequentist vs bayesian). Generally, there are two ways to model $\mathbb{P}_{Y|X=x}$.

Definition 6.11 (Discriminative Models)

Discriminative models attempt to do this directly by modeling only the conditional probability distribution $\mathbb{P}_{Y|X=x}$. We don't care about the underlying distribution of X, but rather we just want to try and predict Y given X. Essentially, we are trying to approximate the conditional expectation $h(X) = \mathbb{E}[Y \mid X]$, which is the best we can do. Given $X = x$, we use our model of $\mathbb{P}_{Y|X=x}$, and our hypothesis function will predict the its mean.

$$h(x) = \mathbb{E}[Y \mid X = x] \tag{128}$$

Definition 6.12 (Generative Models)

Generative models approximate this conditional probability by taking a more general approach. They attempt to model the joint probability distribution $\mathbb{P}_{X\times Y}$ (also called **inference**), which essentially gives everything we need about the data. Doing this allows us to *generate* more data (hence the name), which may be useful.
One way to approximate the joint distribution is to model the conditional distribution $\mathbb{P}_{X|Y=y}$, which gives the distribution of each labels. Now combined with the probability measure $\mathbb{P}_Y$, we can get the joint distribution. Usually in classification, the $\mathbb{P}_Y$ is easy to approximate (the MLE is simply the fequencies of the labels), so conventionally, modeling $\mathbb{P}_{X\times Y}$ and modeling $\mathbb{P}_{X|Y=y}$ are considered the same thing. Once we have these, we can calculate the joint distribution, but in high-dimensional spaces this tends to be computationally hard. Therefore, we usually resort to simply calculating $\mathbb{P}_{X|Y=y}$ and then using Bayes rule to approximate

$$\mathbb{P}_{Y|X} = \frac{\mathbb{P}_{X|Y}\mathbb{P}_Y}{\mathbb{P}_X} \tag{129}$$

where the normalizing term is computed using Monte Carlo simulations.

This is the first example of a generative model. In GDA, we basically write the likelihood as

$$\prod_{i=1}^{n} p(x_i, y_i) = \prod_i p(x_i \mid y_i)p(y_i) \tag{130}$$

where each $p(x_i \mid y_i)$ is Gaussian and $p(y_i)$ is Bernoulli. This specifies $p(x_i, y_i)$ and therefore is called a generative model. In logistic regression, we have

$$\prod_{i=1} p(x_i, y_i) = \left(\prod_i p(y_i \mid x_i)\right)\left(\prod_i p(x_i)\right) \tag{131}$$

and the first term is the logistic function and the second term is unknown. We only use the first part to classify, and this is a discriminative model. You can be agnostic about the data generating process and you can work with less data since there are less things to fit. Some people ask why should you model more unless you have to, so people tend to try to model the minimum, which is why logistic regression is more popular.

6.7.2 Construction

GDA assumes that $\mathbb{P}(x \,|y)$ is distributed according to a multivariate Gaussian distribution. Let us assume that the input space is d-dimensional and this is a binary classification problem. We set

$$\begin{aligned} y &\sim \text{Bernoulli}(\pi) \\ x \,|\, y = 0 &\sim \mathcal{N}_d(\mu_0, \Sigma) \\ x \,|\, y = 1 &\sim \mathcal{N}_d(\mu_1, \Sigma) \end{aligned}$$

This method is usually applied using only one covariance matrix Σ. The distributions are

$$\begin{aligned} p(y) &= \pi^y (1-\pi)^{1-y} \\ p(x \,|\, y=0) &= \frac{1}{(2\pi)^{d/2}|\Sigma|^{1/2}} \exp\left(-\frac{1}{2}(x-\mu_0)^T \Sigma^{-1}(x-\mu_0) \right) \\ p(x \,|\, y=1) &= \frac{1}{(2\pi)^{d/2}|\Sigma|^{1/2}} \exp\left(-\frac{1}{2}(x-\mu_1)^T \Sigma^{-1}(x-\mu_1) \right) \end{aligned}$$

Now, what we have to do is optimize the distribution parameters $\pi \in (0,1)\mathbb{R}, \mu_0 \in \mathbb{R}^d, \mu_1 \in \mathbb{R}^d, \Sigma \in \text{Mat}(d \times d, \mathbb{R}) \simeq \mathbb{R}^{d \times d}$ so that we get the best-fit model. Assuming that each sample has been picked independently, this is equal to maximizing

$$L(\pi, \mu_0, \mu_1, \Sigma) = \prod_{i=1}^{n} \mathbb{P}\big(x^{(i)}, y^{(i)} \,;\, \pi, \mu_0, \mu_1, \Sigma\big) \tag{132}$$

which is really just the probability that we get precisely all these training samples $(x^{(i)}, y^{(i)})$ given the 4 parameters. This can be done by optimizing its log-likelihood, which is given by

$$\begin{aligned} l(\pi, \mu_0, \mu_1, \Sigma) &= \log \prod_{i=1}^{n} \mathbb{P}(x^{(i)}, y^{(i)}; \pi, \mu_0, \mu_1, \Sigma) \\ &= \log \prod_{i=1}^{n} \mathbb{P}(x^{(i)} \,|\, y^{(i)}; \mu_0, \mu_1, \Sigma)\, \mathbb{P}(y^{(i)}; \pi) \\ &= \sum_{i=1}^{n} \log \left(\mathbb{P}(x^{(i)} \,|\, y^{(i)}; \mu_0, \mu_1, \Sigma)\, \mathbb{P}(y^{(i)}; \pi) \right) \end{aligned}$$

and therefore gives the maximum likelihood estimate to be

$$\begin{aligned} \pi &= \frac{1}{N} \sum_{n=1}^{N} 1\{y^{(n)} = 1\} \\ \boldsymbol{\mu}_0 &= \frac{\sum_{n=1}^{n} 1_{\{y^{(n)}=0\}} \mathbf{x}^{(n)}}{\sum_{n=1}^{N} 1_{\{y^{(n)}=0\}}} \\ \boldsymbol{\mu}_1 &= \frac{\sum_{n=1}^{n} 1_{\{y^{(n)}=1\}} \mathbf{x}^{(n)}}{\sum_{n=1}^{N} 1_{\{y^{(n)}=1\}}} \\ \boldsymbol{\Sigma} &= \frac{1}{N} \sum_{n=1}^{N} (\mathbf{x}^{(n)} - \mu_{y^{(n)}})(\mathbf{x}^{(n)} - \mu_{Y^{(i)}})^T \end{aligned}$$

A visual of the algorithm is below, with contours of the two Gaussian distributions, along with the straight line giving the decision boundary at which $\mathbb{P}(y = 1 \,|\, x) = 0.5$.

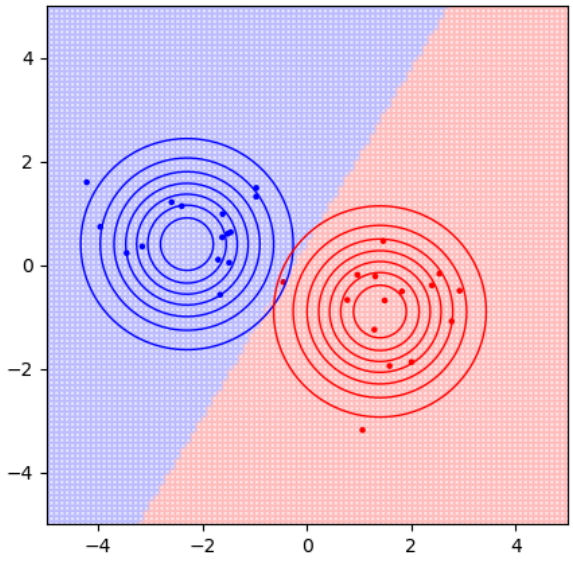


Figure 13: GDA of Data Generated from 2 Gaussisans centered at $(-2.3, 0.4)$ and $(1.4, -0.9)$ with unit covariance. The decision boundary is slightly off since MLE approximates the true means.

6.8 Fisher Linear Discriminant

7 Nonparametric Classification

7.1 K Nearest Neighbors

Question 7.1 (To Do)

Maybe similar like a kernel regression?

Given a bunch of points in a metric space $(\mathcal{X}, d)$ that have classification labels, we want to label new datapoints $\hat{\mathbf{x}}$ based on the labels of other points that already exist in our dataset. One way to look at it is to look for close points within the dataset and use their labels to predict the new ones.

Definition 7.1 (Closest Neighborhood)

Given a dataset $\mathcal{D} = \{\mathbf{x}^{(i)}, \mathbf{y}^{(i)}\}$ and a point $\hat{\mathbf{x}} \in (\mathcal{X}, d)$, let the **k closest neighborhood** of $\hat{\mathbf{x}}$ be $N_k(\hat{\mathbf{x}}) \subset [N]$ defined as the indices i of the k points in $\mathcal{D}$ that is closest to $\hat{\mathbf{x}}$ with respect to the distance metric $d_{\mathcal{X}}$.

Definition 7.2 (K Nearest Neighbors)

The **K Nearest Neighbors (KNN)** is a discriminative nonparametric supervised learning algorithm that doesn't have a training phase. Given a new point $\hat{\mathbf{x}}$, we look at all points in its k closest neighborhood, and $h(\hat{\mathbf{x}})$ will be equal to whatever the majority class will be in. Let us one-hot encode the labels $\mathbf{y}^{(i)}$ into $\mathbf{e}_i$'s, and the number of data point in the ith class can be stored in the

variable

$$a_i = \sum_{i \in N_k(\hat{\mathbf{x}})} 1_{\{\mathbf{y}^{(i)} = \mathbf{e}_i\}} \tag{133}$$

which results in the vector storing the counts of labels in the k closest neighborhood

$$\mathbf{a} = (a_1, a_2, \dots, a_{\mathcal{K}}) = \left(\sum_{i \in N_k(\hat{\mathbf{x}})} 1_{\{\mathbf{y}^{(i)} = \mathbf{e}_1\}}, \sum_{i \in N_k(\hat{\mathbf{x}})} 1_{\{\mathbf{y}^{(i)} = \mathbf{e}_2\}}, \dots, \sum_{i \in N_k(\hat{\mathbf{x}})} 1_{\{\mathbf{y}^{(i)} = \mathbf{e}_{\mathcal{K}}\}} \right) \tag{134}$$

and take the class with the maximum element as our predicted label.

The best choice of K depends on the data:

1. Larger values of K reduces the effect of noise on the classification, but make boundaries between classes less distinct. The number of misclassified data points (error) increases.
2. Smaller values are more sensitive to noise, but boundaries are more distinct and the number of misclassified data points (error) decreases.

Too large of a K value may increase the error too much and lead to less distinction in classification, while too small of a k value may result in us overclassifying the data. Finally, in binary (two class) classification problems, it is helpful to choose K to be odd to avoid tied votes.

This is an extremely simple algorithm that may not be robust. For example, consider $K \geq 3$, and we are trying to label a point $\hat{\mathbf{x}}$ that happens to be exactly where one point is on our dataset $\mathbf{x}^{(i)}$. Then, we should do $h(\hat{\mathbf{x}}) = y^{(i)}$, but this may not be the case if there are no other points with class $y^{(i)}$ in the k closest neighborhood of $\mathbf{x}^{(i)}$. Therefore, we want to take into account the distance of our new points from the others.

Definition 7.3 (Weighted Nearest Neighbor Classifier)

Let us define a monotinically decreasing function $\omega : \mathbb{R}_0^+ \mapsto \mathbb{R}_0^+$. Given a point $i \in N_k(\hat{\mathbf{x}})$, we can construct the weight of our matching label as inversely proportional to the distance: $\omega_i[d(\hat{\mathbf{x}}, \mathbf{x}^{(i)})]$ and store them as

$$\mathbf{a} = (a_1, a_2, \dots, a_{\mathcal{K}}) = \left(\sum_{i \in N_k(\hat{\mathbf{x}})} \omega_i 1_{\{\mathbf{y}^{(i)} = \mathbf{e}_1\}}, \sum_{i \in N_k(\hat{\mathbf{x}})} \omega_i 1_{\{\mathbf{y}^{(i)} = \mathbf{e}_2\}}, \dots, \sum_{i \in N_k(\hat{\mathbf{x}})} \omega_i 1_{\{\mathbf{y}^{(i)} = \mathbf{e}_{\mathcal{K}}\}} \right) \tag{135}$$

and again take the class with the maximum element.

One caveat of KNN is in high dimensional spaces, as its performance degrades quite badly due to the curse of dimensionality.

Example 7.1 (Curse of Dimensionality in KNN)

Consider a dataset of N samples uniformly distributed in a d-dimensional hypercube. Now given a point $x \in [0,1]^d$, we want to derive the expected radius r_k required to encompass its k nearest neighbors. Let us define this ball to be $B_{r_k} \coloneqq \{z \in \mathbb{R}^d \mid ||z - x||_2 \leq r_k\}$. Since thse N points are uniformly distributed, the expected number of points contained in $B_{r_k}(x)$ is simply the proportion of the volume that $B_{r_k}(x)$ encapsulates in the box, multiplied by N. Therefore, for some fixed x and r, let us denote $Y(x, y)$ as the random variable representing the number of points contained within $B_r(x)$. By linearity of expectation and summing over the expectation for whether each point will be in the ball, we have

$$\mathbb{E}[Y(x,r)] = N \cdot \frac{\mu(B_r(x) \cap [0,1]^d)}{\mu([0,1]^d)}$$

where μ is the Lebesgue measure of $\mathbb{R}^d$. Let us assume for not that we don't need to worry about cases where the ball is not fully contained within the cube, so we can just assume that Y is only dependent on r: $Y(r)$. Also, since the volume of the hypercube is 1, $\mu([0,1]^d) = 1$ and we get

$$\mathbb{E}[Y(r)] = N \cdot C_d \cdot r^d$$

which we set equal to k and evaluate for r. C_d is a constant such that the volume of the hypersphere of radius r can be derived as $V = C_d \cdot r^d$. We therefore get

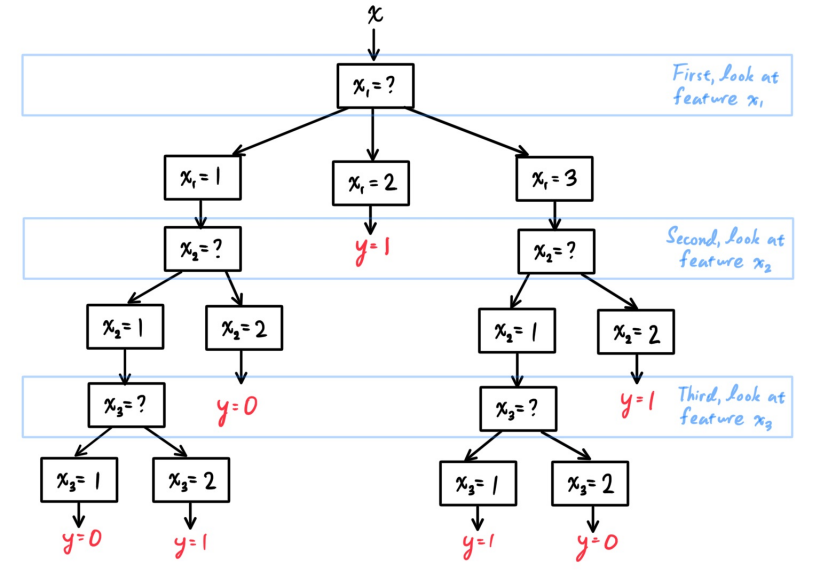
$$N \cdot C_d \cdot r_k^d = k \implies r_k = \left(\frac{k}{NC_d} \right)^{1/d}$$

It turns out that C_d decreases exponentially, so the radius r_k explodes as d grows. Another way of looking at this is that in high dimensions, the ℓ_2 distance between all the pairwise points are close in every single dimension, so it becomes harder to distinguish points that are close vs those that are far.

7.2 Classification Trees

Definition 7.4 (Decision Trees)

Like K nearest neighbors, **decision trees** are discriminative nonparametric classification algorithms that involves creating some sort of tree that represents a set of decisions using a given set of input data $\mathbf{x}^{(i)}$ with its given classification $\mathbf{y}^{(i)}$. When predicting the class of a new input $\hat{\mathbf{x}}$, we would look at its attributes in some order, e.g. $\hat{x_1}, \hat{x}_2, \hat{x}_3$, and make a decision on which class it is in.



The decision tree tries to take advantage of some nontrivial covariance between X and Y by constructing nested partitions of the dataset $\mathcal{D}$, and within a partition, it predicts the label that comprises the majority.

For now, let us assume that $\mathcal{X}$ is a Cartesian product of discrete sets, and we will extend them to continuous values later. Let us look at an example to gain some intuition.

Example 7.2 (Restaurant)

Consider the dataset

	OthOptions	Weekend	WaitArea	Plans	Price	Precip	Restaur	Wait	Crowded	Stay?
x_1	Yes	No	No	Yes	$$$	No	Mateo	0-5	some	Yes
x_2	Yes	No	No	Yes	$	No	Juju	16-30	full	No
x_3	No	No	Yes	No	$	No	Pizza	0-5	some	Yes
x_4	Yes	Yes	No	Yes	$	No	Juju	6-15	full	Yes
x_5	Yes	Yes	No	No	$$$	No	Mateo	30+	full	No
x_6	No	No	Yes	Yes	$$	Yes	BlueCorn	0-5	some	Yes
x_7	No	No	Yes	No	$	Yes	Pizza	0-5	none	No
x_8	No	No	No	Yes	$$	Yes	Juju	0-5	some	Yes
x_9	No	Yes	Yes	No	$	Yes	Pizza	30+	full	No
x_{10}	Yes	Yes	Yes	Yes	$$$	No	BlueCorn	6-15	full	No
x_{11}	No	No	No	No	$	No	Juju	0-5	none	No
x_{12}	Yes	Yes	Yes	Yes	$	No	Pizza	16-30	full	Yes

Let us denote $\mathcal{D}$ as the dataset, and say that $F_1, \dots, F_d$ were the features. This is a binary classification problem, and we can count that there are 6 positives and 6 negative labels.

The simplest decision tree is the trivial tree, with one node that predicts the majority of the dataset. In this case, the data is evenly split, so without loss of generality we will choose $h_0(\mathbf{x}) = 1$. We want to quantify how good our model is, and so like always we use a loss function.

Just like how a linear model is completely defined by its parameter $\boldsymbol{\theta}$, a decision tree is completely defined by the sequences of labels that it splits on. Therefore, training this is equivalent to defining the sequence, but we can't define this sequence unless we can compare how good a given decision tree is, i.e. unless we have defined a proper loss function. Depending on the training, we can use a greedy algorithm or not, and we have the flexibility to choose whether or not we can split on the same feature multiple times.

Definition 7.5 (Musclassification Error)

We will simply use the misclassification loss function.

$$L(h; \mathcal{D}) = \frac{1}{N} \sum_{i=1}^{N} 1_{\{y^{(i)} \neq h(x^{(i)})\}} = 1 - \text{accuracy} \tag{136}$$

Minimizing this maximizes the accuracy, so this is a reasonable one to choose. How do we train this? Unlike regression, this loss is not continuous, so the gradient is 0, and furthermore the model isn't even parametric, so there are no gradients to derive!

Fortunately, the nature of the decision tree only requires us to look through the explanatory variables $x_1, \dots, x_n$ and decide which one to split.

Let us take a decision tree h and model the accuracy of it as a random variable: $1_{\{Y = h_0(X)\}} \sim \text{Bernoulli}(p)$, where p is the accuracy. A higher accuracy of h corresponds to a lower entropy, and so the entropy of the random variable is also a relevant indicator.

$$H(1_{\{Y=h_0(X)\}}) = p \log p + (1-p) \log(1-p)$$

Therefore, when we are building a tree, we want to choose the feature x_i to split based on how much it lowers the entropy of the decision tree.

To set this up, let us take our dataset $\mathcal{D}$ and set X_i as the random variable representing the distribution (a

multinomial) of the $x_i^{(j)}$'s, and Y as the same for the $y^{(j)}$'s. This is our maximum likelihood approximation for the marginalized distribution of the joint measure $X \times Y = X_1 \times \ldots \times X_D \times Y$.

Given a single node, we are simply going to label every point to be whatever the majority class is in $\mathcal{D}$. Therefore, we start off with the entropy of our trivial tree $H(Y)$. Then, we want to see which one of the X_d features to split on, and so we can compute the conditional entropy $H(Y, X_d)$ to get the information gain $I(Y; X_d) = H(Y) - H(Y \mid X_d)$ for all $d = 1, \ldots, D$. We want to find a feature X_d that maximize this information gain, i.e. decreases the entropy as much as possible (a greedy algorithm), and we find the next best feature (with or without replacement), so that we have a decreasing sequence.

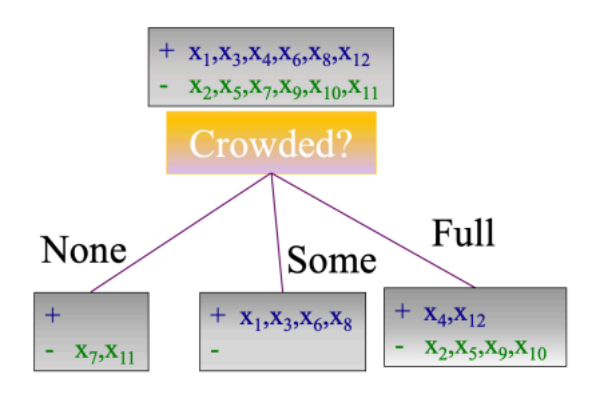
$$H(X) \geq H(X; Y) \geq H(X; Y, Z) \geq H(X; Y, Z, W) \geq \ldots \geq 0$$

Example 7.3 ()

Continuing the example above, since there are 6 labels of 0 and 1 each, we can model this $Y \sim$ Bernoulli(0.5) random variable, with entropy

$$H(Y) = \mathbb{E}[-\log_2 p(Y)] = \frac{1}{2}\big(-\log_2 \frac{1}{2}\big) + \frac{1}{2}\big(-\log_2 \frac{1}{2}\big) = 1$$

Now what would happen if we had branched according to how crowded it was, X_{crowded}. Then, our decision tree would split into 3 sections:



In this case, we can define the multinomial distribution X_{crowded} representing the proportion of the data that is crowded in a specific level. That is, $X_{\text{crowded}} \sim \text{Multinomial}(\frac{2}{12}, \frac{4}{12}, \frac{6}{12})$, with

$$\mathbb{P}(X_{\text{crowded}} = x) = \begin{cases} 2/12 & \text{if } x = \text{ none} \\ 4/12 & \text{if } x = \text{ some} \\ 6/12 & \text{if } x = \text{ full} \end{cases}$$

Therefore, we can now compute the conditional entropy of this new decision tree conditioned on how crowded the store is

$$\begin{aligned} H(Y \mid X_{\text{crowded}}) &= \sum_x \mathbb{P}(X_{\text{crowded}} = x) H(Y \mid X_{\text{crowded}} = x) \\ &= \frac{2}{12} H(\text{Bern}(1)) + \frac{4}{12} H(\text{Bern}(0)) + \frac{6}{12} H(\text{Bern}(1/3)) = 0.459 \\ I(Y; X_{\text{crowded}}) &= 0.541 \end{aligned}$$

We would do this for all the features and greedily choose the feature that maximizes our information gain.

Example 7.4 ()

The Ferrari F1 team hired you as a new analyst! You were given the following table of the past race history of the team. You were asked to use information gain to build a decision tree to predict race wins. First, you will need to figure out which feature to split first.

Rain	Good Strategy	Qualifying	Win Race
1	0	0	0
1	0	0	0
1	0	1	0
0	0	1	1
0	0	0	0
0	1	1	1
1	0	1	0
0	1	0	1
0	0	1	1
0	0	1	1

Let $X \sim \text{Bernoulli}(1/2)$ be the distribution of whether a car wins a race over the data. Then its entropy is

$$H(X) = \mathbb{E}[-\log_2 p(x)] = \frac{1}{2}\big(-\log_2 \frac{1}{2}\big) + \frac{1}{2}\big(-\log_2 \frac{1}{2}\big) = 1$$

Let $R \sim \text{Bernoulli}(4/10), G \sim \text{Bernoulli}(2/10), Q \sim \text{Bernoulli}(6/10)$ be the distribution of the features rain, good strategy, and qualifying over the data, respectively. Then, the conditional entropy of X conditioned on each of these random variables is

$$\begin{aligned}
H(X \mid R) &= \mathbb{P}(R=1)\, H(X \mid R=1) + \mathbb{P}(R=0)\, H(X \mid R=0) \\
&= \frac{4}{10} \cdot -\big(1 \cdot \log_2 1 + 0 \cdot \log_2 0\big) + \frac{6}{10} \cdot -\big(\frac{1}{6} \cdot \log_2 \frac{1}{6} + \frac{5}{6} \cdot \log_2 \frac{5}{6}\big) \approx 0.390 \\
H(X \mid G) &= \mathbb{P}(G=1)\, H(X \mid G=1) + \mathbb{P}(G=0)\, H(X \mid G=0) \\
&= \frac{2}{10} \cdot -\big(1 \cdot \log_2 1 + 0 \cdot \log_2 0\big) + \frac{8}{10} \cdot -\big(\frac{3}{8} \cdot \log_2 \frac{3}{8} + \frac{5}{8} \log_2 \frac{5}{8}\big) \approx 0.763 \\
H(X \mid Q) &= \mathbb{P}(Q=1)\, H(X \mid Q=1) + \mathbb{P}(Q=0)\, H(X \mid Q=0) \\
&= \frac{6}{10} \cdot -\big(\frac{4}{6} \cdot \log_2 \frac{4}{6} + \frac{2}{6} \cdot \log_2 \frac{2}{6}\big) + \frac{4}{10} \cdot -\big(\frac{1}{4} \log_2 \frac{1}{4} + \frac{3}{4} \log_2 \frac{3}{4}\big) \approx 0.875
\end{aligned}$$

Therefore, the information gain are

$$\begin{aligned}
I(X;R) &= 1 - 0.390 = 0.610 \\
I(X;G) &= 1 - 0.763 = 0.237 \\
I(X;Q) &= 1 - 0.875 = 0.125
\end{aligned}$$

And so I would split on R, the rain, which gives the biggest information gain.

Finally, we can use the Gini index of $X \sim \text{Bernoulli}(p)$, defined

$$G(X) = 2p(1-p) \tag{137}$$

Example 7.5 (Ferrari Example Continued)

We do the same as the Ferrari example above but now with the Gini reduction. Let $X \sim \text{Bernoulli}(1/2)$ be the distribution of whether a car wins a race over the data. Then its Gini index, which I will label with $\mathcal{G}$, is

$$\mathcal{G}(X) = 2 \cdot \frac{1}{2} \cdot \frac{1}{2} = \frac{1}{2}$$

Let $R \sim \text{Bernoulli}(4/10), G \sim \text{Bernoulli}(2/10), Q \sim \text{Bernoulli}(6/10)$ be the distribution of the features rain, good strategy, and qualifying over the data, respectively. Then we compute the conditional expectation

$$\begin{aligned}
\mathbb{E}[\mathcal{G}(X \mid R)] &= \mathbb{P}(R=1)\,\mathcal{G}(X \mid R=1) + \mathbb{P}(R=0)\,\mathcal{G}(X \mid R=0) \\
&= \frac{4}{10}\left[2 \cdot \frac{4}{4} \cdot \frac{0}{4}\right] + \frac{6}{10}\left[2 \cdot \frac{1}{6} \cdot \frac{5}{6}\right] \approx 0.167 \\
\mathbb{E}[\mathcal{G}(X \mid G)] &= \mathbb{P}(G=1)\,\mathcal{G}(X \mid G=1) + \mathbb{P}(G=0)\,\mathcal{G}(X \mid G=0) \\
&= \frac{2}{10}\left[2 \cdot \frac{2}{2} \cdot \frac{0}{2}\right] + \frac{8}{10}\left[2 \cdot \frac{3}{8} \cdot \frac{5}{8}\right] \approx 0.375 \\
\mathbb{E}[\mathcal{G}(X \mid Q)] &= \mathbb{P}(Q=1)\,\mathcal{G}(X \mid Q=1) + \mathbb{P}(Q=0)\,\mathcal{G}(X \mid Q=0) \\
&= \frac{6}{10}\left[2 \cdot \frac{4}{6} \cdot \frac{2}{6}\right] + \frac{4}{10}\left[2 \cdot \frac{1}{4} \cdot \frac{3}{4}\right] \approx 0.417
\end{aligned}$$

Therefore, the Gini reduction, which I'll denote as $I_{\mathcal{G}}$, is

$$\begin{aligned}
I_{\mathcal{G}}(X; R) &= 0.5 - 0.167 = 0.333 \\
I_{\mathcal{G}}(X; G) &= 0.5 - 0.375 = 0.125 \\
I_{\mathcal{G}}(X; Q) &= 0.5 - 0.417 = 0.083
\end{aligned}$$

Since branching across the feature R, the rain, gives the biggest Gini reduction, we want to split on the rain feature first.

7.2.1 Regularization

Given a dataset with D binary features, let $g(H, D)$ be the number of binary trees with depth at most H (including root node), with the restriction that the trees may not split on some variable multiple times within a path to a leaf node. Then, g can be defined recursively.

1. First, if $H = 1$, then $g(H, D) = 1$ always since we are just creating the trivial binary tree of one node.
2. If $D = 0$, then there are no features to split on and therefore we just have the single node $g(H, D) = 1$.
3. If $H > 1$ and $D > 0$, then say that we start with a node. We can either make this a leaf node by not performing any splitting at all, or split on one of the D variables. Then for each of the 2 nodes created on the split, we are now working with $D - 1$ features and a maximum height of $H - 1$ for each of the subtrees generated from the 2 nodes.

All this can be expressed as

$$g(H, D) = \begin{cases} 1 + D\left[g(H-1, D-1)\right]^2 & \text{if } H > 1, D > 0 \\ 1 & \text{if } H = 1 \text{ or } D = 0 \end{cases}$$

which is extremely large (in fact, NP hard). Therefore, some tricks like regularization must be implemented to limit our search space.

By defining the complexity of our decision tree $\Omega(h)$ as the number of nodes within the tree, we can modify our objective function to

$$L(h; \mathcal{D}) = \frac{1}{N}\sum_{i=1}^{N} 1_{\{y^{(i)} \neq h(x^{(i)})\}} + \lambda \Omega(h)$$

We can impose this constraint directly on the training algorithm, or we can calculate the regularized loss after the tree has been constructed, which is a method called **tree pruning**.

Given a large enough λ, we can in fact greatly reduce our search space by not considering any trees further than a certain point.

Theorem 7.1 ()

We describe a tree as a set of leaves, where leaf k is a tuple containing the logical preposition satisfied by the path to leaf k, denoted p_k, and the class label predicted by the leaf, denoted $\hat{y}_k$. For a dataset with d binary features, $p_k : \{0,1\}^d \to \{0,1\}$ is a function that returns 1 if a sample x_i satisfies the preposition, and 0 otherwise. That is, leaf k is $(p_k, \hat{y}_k)$, and a tree f with K leaves is described as a set $f = \{(p_1, \hat{y}_1), \dots, (p_K, \hat{y}_K)\}$. Assume that the label predicted by $\hat{y}_k$ is always the label for the majority of samples satisfying p_k. Finally, let $m_k = \sum_{i=1}^n p_k(x_i)$ denote the number of training samples "captured" by leaf k.
Given a (potentially optimal) tree

$$f = \{(p_1, \hat{y}_1), \dots, (p_\kappa, \hat{y}_\kappa), \dots, (p_K, \hat{y}_K)\},$$

the tree $f' = \{(p_1, \hat{y}_1), \dots, (p_{\kappa_1}, \hat{y}_{\kappa_1}), (p_{\kappa_2}, \hat{y}_{\kappa_2}), \dots, (p_K, \hat{y}_K)\}$ produced by splitting leaf $(p_\kappa, \hat{y}_\kappa)$ into two leaves $(p_{\kappa_1}, \hat{y}_{\kappa_1})$ and $(p_{\kappa_2}, \hat{y}_{\kappa_2})$ and any tree produced by further splitting $(p_{\kappa_1}, \hat{y}_{\kappa_1})$ or $(p_{\kappa_2}, \hat{y}_{\kappa_2})$ cannot be optimal if $m_\kappa < 2n\lambda$.

Proof.

Let c be the number of misclassifications in leaf $(p_\kappa, \hat{y}_\kappa)$. Since a leaf classifies according to the majority of m_κ, we must have

$$c \leq \frac{m_\kappa}{2} < n\lambda$$

By splitting leaf $(p_\kappa, \hat{y}_\kappa)$ into leaves $(p_{\kappa_1}, \hat{y}_{\kappa_1})$ and $(p_{\kappa_2}, \hat{y}_{\kappa_2})$, assume that we have reduced the number of misclassifications by $b \leq c$. Then, we have

$$\ell(f', \mathbf{X}, \mathbf{y}) = \ell(f, \mathbf{X}, \mathbf{y}) - \frac{b}{n}$$

However, we have increased the number of leaves by 1, and so

$$\lambda s(f') = \lambda s(f) + \lambda$$

Combining the last two equations, we have obtained

$$R(f', \mathbf{X}, \mathbf{y}) = R(f, \mathbf{X}, \mathbf{y}) + \lambda - \frac{b}{n}$$

However, we know that

$$\begin{aligned} b \leq c &\implies \frac{b}{n} \leq \frac{c}{n} < \frac{n\lambda}{n} = \lambda \\ &\implies -\frac{b}{n} > -\lambda \\ &\implies \lambda - \frac{b}{n} > \lambda - \lambda = 0 \end{aligned}$$

and so $R(f', \mathbf{X}, \mathbf{y}) > R(f, \mathbf{X}, \mathbf{y})$. This means that f' cannot be optimal according to our regularized objective. We have also proved that further splitting $(p_{\kappa_1}, \hat{y}_{\kappa_1})$ or $(p_{\kappa_2}, \hat{y}_{\kappa_2})$ cannot be optimal since we can just set $f = f'$, and apply the same argument.

8 Generalized Linear Models

Remember the linear model looked like this, where we use the conventional β notation to represent parameters.

$$Y = X^T\beta + \epsilon, \quad \epsilon \sim N(0, \sigma^2 I) \tag{138}$$

which implies that $Y \mid X \sim N(X^T\beta, \sigma^2 I)$. Basically, given x, I assume some distribution of Y, and the value of x will help me guess what the mean of this distribution is. Note that we in here assume that only the mean depends on X. I could potentially have something crazy, like

$$Y \mid X \sim N(X^T\beta, (X^T\gamma)(XX^T + I))$$

where the covariance will depend on X, too, but in this case we only assume that that mean is dependent on X.

$$Y \mid X \sim N(\mu(X), \sigma^2 I)$$

where in the linear model, $\mu(X) = X^T\beta$. So, there are three assumptions we are making here:

1. $Y \mid X$ is Gaussian.
2. X only affects the mean of $Y \mid X$, written $\mathbb{E}[Y \mid X] = \mu(X)$.
3. X affects the mean in a linear way, such that $\mu(X) = X^T\beta$.

So the two things we are trying to relax are:

1. **Random Component**: the response variable $Y \mid X$ is continuous and normally distributed with mean $\mu = \mu(X) = \mathbb{E}[Y \mid X]$.
2. **Link**: I have a link that explains the relationship between the X and the μ, and this relationship is $\mu(X) = X^T\beta$.

So when talking about GLMs, we are not changing the fact that we have a linear function $X \mapsto X^T\beta$. However, we are going to assume that $Y \mid X$ now comes from a broader **family of exponential distributions**. Second, we are going to assume that there exists some **link function** g

$$g(\mu(X)) = X^T\beta$$

Admittedly, this is not the most intuitive way to think about it, since we would like to have $\mu(X) = f(X^T\beta)$, but here we just decide to call $f = g^{-1}$. Therefore, if I want to give you a GLM, I just need to give you two things: the conditional distribution $Y \mid X$, which can be any distribution in the exponential family, and the link function g.

We really only need this link function due to compatibility reasons. Say that $Y \mid X \sim \text{Bern}(p)$. Then, $\mu(X) = \mathbb{E}[Y \mid X]$ always lives in $[0, 1]$, but $X^T\beta$ always lives in $\mathbb{R}$. We want our model to be realistic, and we can clearly see the problem shown in Figure 14.

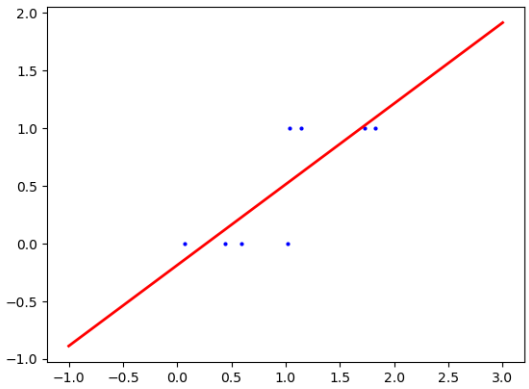


Figure 14: Fitting a linear model for Bernoulli random variables will predict a mean that is outside of $[0, 1]$ when getting new datapoints.

If $Y \mid X$ is some exponential distribution, then its support is always positive and so $\mu(X) > 0$. But if we stick to the old form of $\mu(X) = X^T\beta$, then $\text{Im}(\mu) = \mathbb{R}$, which is not realistic when we predict negative values. Let's take a couple examples:

Example 8.1 (Disease Epidemic)

In the early stages of a disease epidemic, the rate at which new cases occur can often increase exponentially through time. Clearly, $\mu(X) = \mathbb{E}[Y \mid X]$ should be positive and we should have some sort of exponential trend. Hence, if $\mu(x)$ is the expected number of cases on data x, a model of the form

$$\mu(x) = \gamma \exp(\delta x) \tag{139}$$

seems appropriate, where γ and δ are simply scaling factors. Clearly, $\mu(X)$ is not of the form $f(X^T\beta)$. So what I do is to transform μ in such a way that I can get something that is linear.

$$\log(\mu(X)) = \log(\gamma) + \delta X \tag{140}$$

which is now linear in X, of form $\beta_0 + \beta_1 X$. This will have some effects, but this is what needs to be done to have a genearlized linear model. Note that what I did to μ was take the log of it, and so the link function is $g = \log$, called the **log-link**. Now that we have chosen the g, we still need to choose what the conditional distribution $Y \mid X$ would be. This is determined by speaking with industry professionals, experience, and convenience. In this case, Y is a count, and since this must be a discrete distribution. Since it is not bounded above, we think Poisson.

Example 8.2 (Prey Capture Rate)

The rate of capture of preys, Y, by a hunting animal, tends to increase with increasing density of prey X, but eventually level off when the predator is catching as much as it can cope with. We want to find a perhaps concave function that levels off, and suitable model might be

$$\mu(X) = \frac{\alpha X}{h + X} \tag{141}$$

where α represents the maximum capture rate, and h represents the prey density at which the capture rate is half the maximum rate. Again, we must find some transformation g that turns this into a

linear function of X, and what we can do it use the **reciprocal-link**.

$$\frac{1}{\mu(X)} = \frac{h+X}{\alpha X} = \frac{h}{\alpha}\frac{1}{X} + \frac{1}{\alpha} \tag{142}$$

The standard deviation of capture rate might be approximately proportional to the mean rate, suggesting the use of a Gamma distribution for the response.

Example 8.3 (Kyphosis Data)

The Kyphosis data consist of measurements on 81 children following corrective spinal surgery. The binary response variable, Kyphosis, indicates the presence or absence of a postoperative deforming. The three covariates are: age of the child in months, number of the vertebrae involved in the operation, and the start of the range of the vertebrae involved. The response variable is binary so there is no choice: $Y \mid X$ is Bernoulli with expected value $\mu(X) \in (0,1)$. We cannot write $\mu(X) = X^T\beta$ because the right hand side ranges through $\mathbb{R}$, and so we find an invertible function that squishes $\mathbb{R}$ to $(0,1)$, and so we can choose basically any CDF.

For clarification, when writing a distribution like Bernoulli(p), or Binomial(n,p), Poisson(λ), or $N(\mu,\sigma^2)$, the hyperparameters that we usually work with we will denote as $\boldsymbol{\theta}$, and the space that this $\boldsymbol{\theta}$ lives in will denote Θ. For example, for the Bernoulli, $\Theta = [0,1]$, and for Poisson, $\Theta = [0,+\infty)$.

Ultimately, a GLM consists of three steps:

1. The observed input X enters the model through a linear function $\beta^T X$.
2. The conditional mean of response, is represented as a function of the linear combination

$$\mathbb{E}[Y \mid X] = \mu = f(\beta^T X) \tag{143}$$

3. The observed response is drawn from an exponential family distribution with conditional mean μ.

8.1 Exponential Family

We can write the pdf of a distribution as a function of the input x and the hyperparameters θ, so we can write $P_\theta(x) = p(\theta, x)$. For now, let's think that both $x, \theta \in \mathbb{R}$. Think of all the functions that depend on θ and x. There are many of them, but we want θ and x to interact in a certain way. The way that I want them to interact with each other is that they are multiplied within an exponential term. Now clearly, this is not a very rich family, so we are just slapping some terms that depend only on θ and only on x.

$$p_\theta(x) = \exp(\theta x)h(x)c(\theta)$$

But now if $\theta \in \mathbb{R}^k$ and $x \in \mathbb{R}^q$, then we cannot simply take the product nor the inner product, but what we can do is map both of them into a space that has the same dimensions, so I can take the inner product. That is, let us map $\boldsymbol{\theta} \mapsto \boldsymbol{\eta}(\boldsymbol{\theta}) \in \mathbb{R}^k$ and $\mathbf{x} \mapsto \mathbf{T}(\mathbf{x}) \in \mathbb{R}^k$, and so our exponential distribution form would be generalized into something like

$$p_{\boldsymbol{\theta}}(\mathbf{x}) = \exp\big[\boldsymbol{\eta}(\boldsymbol{\theta}) \cdot \mathbf{T}(\mathbf{x})\big]h(\mathbf{x})c(\boldsymbol{\theta})$$

We can think of $c(\boldsymbol{\theta})$ as the normalizing term that allows us to integrate the pdf to 1.

$$\int_{\mathcal{X}} p_{\boldsymbol{\theta}}(\mathbf{x}) = c(\boldsymbol{\theta}) \int \exp\big[\boldsymbol{\eta}(\boldsymbol{\theta}) \cdot \mathbf{T}(\mathbf{x})\big]h(\mathbf{x})\, d\mathbf{x}$$

We can just push the $c(\boldsymbol{\theta})$ term into the exponential by letting $c(\boldsymbol{\theta}) = e^{-\log(c(\boldsymbol{\theta}))^{-1}}$ to get our definition.

Definition 8.1 (Exponential Family)

A **k-parameter exponential family** is a family of distributions with pdf/pmf of the form

$$p_{\boldsymbol{\theta}}(\mathbf{x}) = \exp\left[\boldsymbol{\eta}(\boldsymbol{\theta}) \cdot \mathbf{T}(\mathbf{x}) - B(\boldsymbol{\theta})\right] h(\mathbf{x})$$

The h term, as we will see, will not matter in our maximum likelihood estimation, so we keep it outside the exponential.

1. $\boldsymbol{\eta}$ is called the **canonical parameter**. Given a distribution parameterized by the regular hyperparameters $\boldsymbol{\theta}$, we would like to parameterize it in a different way $\boldsymbol{\eta}$ under the function $\boldsymbol{\eta} : \Theta \to \mathbb{R}$
2. $\mathbf{T}(\mathbf{x})$ is called the **sufficient statistic**.
3. $h(\mathbf{x})$ is a nonnegative scalar function.
4. $B(\boldsymbol{\theta})$ is the normalizing factor.

Let's look at some examples.

Example 8.4 (Gaussian)

If we put the coefficient into the exponential and expand the square term, we get

$$p_\theta(x) = \exp\left(\frac{\mu}{\sigma^2} \cdot x - \frac{1}{2\sigma^2} \cdot x^2 - \frac{\mu^2}{2\sigma^2} - \log(\sigma\sqrt{2\pi})\right)$$

where

$$\boldsymbol{\eta}(\boldsymbol{\theta}) = \begin{pmatrix} \mu/\sigma^2 \\ -1/2\sigma^2 \end{pmatrix},\ T(x) = \begin{pmatrix} x \\ x^2 \end{pmatrix},\ B(\theta) = \frac{\mu^2}{2\sigma^2} + \log(\sigma\sqrt{2\pi}),\ h(x) = 1$$

This is not a unique representation since we can take the $\log(\sqrt{2\pi})$ out of the exponential, but why bother to do this when we can just stuff everything into B and keep h simple.

Example 8.5 (Gaussian with Known Variance)

If we have known variance, we can write the Gaussian pdf as

$$p_\theta(x) = \exp\left[\frac{\mu}{\sigma} \cdot \frac{x}{\sigma} - \frac{\mu^2}{2\sigma^2}\right] \cdot \frac{1}{\sigma\sqrt{2\pi}} e^{x^2/2\sigma^2}$$

where

$$\eta(\theta) = \frac{\mu}{\sigma},\ T(x) = \frac{x}{\sigma},\ B(\theta) = \frac{\mu^2}{2\sigma^2},\ h(x) = \frac{1}{\sigma\sqrt{2\pi}} e^{x^2/2\sigma^2}$$

Example 8.6 (Bernoulli)

The pmf of a Bernoulli with θ is

$$\begin{aligned} p_\theta(x) &= \theta^x (1-\theta)^{(1-x)} \\ &= \exp\left[x \log(\theta) + (1-x)\log(1-\theta)\right] \\ &= \exp\left(x \log\left[\frac{\theta}{1-\theta}\right] - \log\left[\frac{1}{1-\theta}\right]\right) \end{aligned}$$

where

$$\eta(\theta) = \log\left[\frac{\theta}{1-\theta}\right],\ T(x) = x,\ B(\theta) = \log\left[\frac{1}{1-\theta}\right],\ h(x) = 1$$

Example 8.7 (Binomial with Known Number of Trials)

We can transform a binomial with known N as

$$\begin{aligned} p_\theta(x) &= \binom{N}{x}\theta^x(1-\theta)^{1-x} \\ &= \exp\left[x\ln\left(\frac{\theta}{1-\theta}\right) + \ln(1-\theta)\right] \cdot \binom{N}{x} \end{aligned}$$

where

$$\eta(\theta) = \ln\left(\frac{\theta}{1-\theta}\right),\ T(x) = x,\ B(\theta) = \ln(1-\theta),\ h(x) = \binom{N}{x}$$

Example 8.8 (Poisson)

The pmf of Poisson with θ can be expanded

$$\begin{aligned} p_\theta &= \frac{\theta^{-x}}{x!}e^{-\theta} \\ &= \exp\big[-\theta + x\log(\theta) - \log(x!)\big] \\ &= \exp\big[x\log(\theta) - \theta\big]\,\frac{1}{x!} \end{aligned}$$

where

$$\eta(\theta) = \log(\theta),\ T(x) = x,\ B(\theta) = \theta,\ h(x) = \frac{1}{x!}$$

However, the uniform is not in here. In fact, any distribution that has a support that does not depend on the parameter is not an exponential distribution.

Let us now focus on one parameter families where $\theta \in \Theta \subset \mathbb{R}$, which do not include the Gaussian (with unknown mean and variance, Gamma, multinomial, etc.), which has a pdf written in the form

$$p_\theta(x) = \exp\big[\eta(\theta)\,T(x) - B(\theta)\big]\,h(x)$$

8.1.1 Canonical Exponential Family

Now a common strategy in statistical analysis is to reparamaterize a probability distribution. Suppose a family of probability distributions $\{P_\theta\}$ is parameterized by $\theta \in \Theta \subset \mathbb{R}$. If we have an invertible function $\eta : \Theta \to \mathcal{T} \subset \mathbb{R}$, then we can paramaterize the same family with η rather than θ, with no loss of information. Typically, it is the case that η is invertible for exponential families, so we can just reparameterize the whole pdf and write

$$p_\eta(x) = \exp\big[\eta\,T(x) - \phi(\eta)\big]\,h(x)$$

where $\phi = B \circ \eta^{-1}$.

Definition 8.2 (Canonical One-Parameter Exponential Family)

A family of distributions is said to be in **canonical one-parameter exponential family** if its density is of form

$$p_\eta(x) = \exp\big[\eta\,T(x) - \phi(\eta)\big]\,h(x)$$

which is a subfamily of the exponential family. The function ψ is called the **cumulant generating function**.

Before we move on, let us just provide a few examples.

Example 8.9 (Poisson)

The Poisson can be represented as

$$p_\theta(x) = \exp\left[x \log \theta - \theta\right] \frac{1}{x!}$$

Now let $\eta = \log \theta \implies \theta = e^\eta$. So, we can reparamaterize the density as

$$p_\eta(x) = \exp\left[x\eta - e^\eta\right] \frac{1}{x!}$$

where $P_\eta = \text{Poisson}(e^\eta)$ for $\eta \in \mathcal{T} = \mathbb{R}$, compared to $P_\theta = \text{Poisson}(\theta)$ for $\theta \in \Theta = \mathbb{R}^+$.

Example 8.10 (Gaussian)

Recall that the Gaussian with known parameter σ^2 and unknown $\theta = \mu$ is in the exponential family, since we can expand it as

$$p_\theta(x) = \exp\left[\frac{\mu}{\sigma^2} \cdot x - \frac{\mu^2}{2\sigma^2}\right] \cdot \frac{1}{\sigma\sqrt{2\pi}} e^{x^2/2\sigma^2}$$

We can perform the change of parameter $\eta = \mu^2/2\sigma^2 \implies \mu = \sigma^2\eta$, and substituting this in will give the canonical representation

$$p_\eta(x) = \exp\left[\eta x - \frac{\sigma^2\eta^2}{2}\right] \cdot \frac{1}{\sigma\sqrt{2\pi}} e^{x^2/2\sigma^2}$$

where now $P_\eta = N(\sigma^2\eta, \sigma^2)$ for $\eta \in \mathcal{T} = \mathbb{R}$, compared to $P_\theta = N(\theta, \sigma^2)$ for $\theta \in \Theta = \mathbb{R}$, which is basically the same space.

Example 8.11 (Bernoulli)

The Bernoulli has an exponential form of

$$p_\theta(x) = \exp\left[x \log\left(\frac{\theta}{1-\theta}\right) + \log(1-\theta)\right]$$

Now setting $\eta = \log\left(\frac{\theta}{1-\theta}\right) \implies \theta = \frac{1}{1+e^{-\eta}}$, and so $B(\theta) = -\log(1-\theta) = -\log\left(\frac{e^{-\eta}}{1+e^{-\eta}}\right) = \log(1+e^\eta) = \psi(\eta)$, and so the canonical paramaterization is

$$p_\eta(x) = \exp\left[x\eta - \log(1+e^\eta)\right]$$

We present two useful properties of the exponential family.

Theorem 8.1 (Moments)

Let random variable X be in the canonical exponential family P_η

$$p_\eta(x) = e^{\eta T(x) - \psi(\eta)} h(x)$$

Then, the expectation and variance are encoded in the cumulant generating function in the following way

$$\mathbb{E}[T(X)] = \psi'(\eta) \qquad \text{Var}[T(X)] = \psi''(\eta)$$

Proof.

Example 8.12 ()

We show that this is consistent with the Poisson, normal, and Bernoulli distributions.

1. In the Poisson, $\psi(\eta) = e^\eta$, and so $\psi'(\eta) = e^\eta = \theta = \mathbb{E}[X]$. Taking the second derivative gives $\psi''(\eta) = e^\eta = \theta = \text{Var}[X]$, too.
2. In the Normal with known variance σ^2, we have $\psi(\eta) = \frac{1}{2}\sigma^2\eta^2$. So

$$\begin{aligned} \mathbb{E}[X] &= \psi'(\eta) = \sigma^2\eta = \mu \\ \text{Var}[X] &= \psi''(\eta) = \sigma^2 \end{aligned}$$

3. In the Bernoulli, we have $\psi(\eta) = \log(1 + e^{-\eta})$. Therefore,

$$\begin{aligned} \mathbb{E}[X] &= \psi'(\eta) = \frac{x^\eta}{1+x^\eta} = \frac{1}{1+e^{-\eta}} = \theta \\ \text{Var}[X] &= \psi''(\eta) = -\left(\frac{1}{1+e^{-\eta}}\right)^2 e^{-\eta} \cdot -1 = \theta^2 \cdot \frac{1-\theta}{\theta} = \theta(1-\theta) \end{aligned}$$

Theorem 8.2 (Convexity)

Consider a canonical exponential family with density

$$p_\eta(x) = e^{\eta T(x) - \psi(\eta)} h(x)$$

and natural parameter space $\mathcal{T}$. Then, the set $\mathcal{T}$ is convex, and the cumulant generating function ψ is convex on $\mathcal{T}$.

Proof.

This can be proven using Holder's inequality. However, from the theorem above, note that $\text{Var}[T(X)] = \psi''(\eta)$ must be positive since we are talking about variance. This implies that the second derivative of ψ is positive, and therefore must be convex.

We will look at a subfamily of the exponential family. Now remember that we introduce the functions $\boldsymbol{\eta}$ and $\mathbf{T}$ so that we can capture a much broader range of distributions, but if we have one parameter $k = 1$, then we can just set $\boldsymbol{\eta}(\boldsymbol{\theta})$ to be the new parameter θ. The **canonical exponential family** for $k = 1, y \in \mathbb{R}$, is defined to have the pdf

$$f_\theta(y) = \exp\left(\frac{y\theta - b(\theta)}{\phi} + c(y, \phi)\right) \tag{144}$$

where

$$h(y) = \exp\big(c(y, \phi)\big) \tag{145}$$

If ϕ is known, this is a one-parameter exponential family with θ being the **canonical parameter**, and if ϕ is unknown, the $h(y)$ term will not depend on θ, which we may not be able to split up into the exponential pdf form. In this case ϕ is called the **dispersion parameter**. For now, we will always assume that ϕ is known.

We can prove this for all other classes, too. We can think of the $c(y, \phi)$ as just a term that we stuff every other term into. What really differentiates the different distributions of the canonical exponential family is the $b(\theta)$. The form of b will determine whether this distribution is a Gaussian, or a Bernoulli, or etc. This b will capture information about the mean, the variance, the likelihood, about everything.

8.2 Cumulant Generating Function

Definition 8.3 (Score)

The **score** is the gradient of the log-likelihood function with respect to the parameter vector. That is, given that $L(\boldsymbol{\theta})$ is the likelihood, then

$$s(\boldsymbol{\theta}) \coloneqq \frac{\partial \log L(\boldsymbol{\theta}; \mathbf{x})}{\partial \boldsymbol{\theta}}$$

which gives a row covector.

Now, remember that the score also depends on the observations $\mathbf{x}$. If we rewrite the likelihood as a probability density function $L(\boldsymbol{\theta}; \mathbf{x}) = f(\mathbf{x}; \boldsymbol{\theta})$, then we can say that the expected value of the score is equal to 0, since

$$\begin{aligned}
\mathbb{E}[s(\boldsymbol{\theta})] &= \int_{\mathcal{X}} f(\mathbf{x}; \boldsymbol{\theta}) \frac{\partial}{\partial \boldsymbol{\theta}} \log L(\boldsymbol{\theta}; \mathbf{x}) \, d\mathbf{x} \\
&= \int_{\mathcal{X}} f(\mathbf{x}; \boldsymbol{\theta}) \frac{1}{f(\mathbf{x}; \boldsymbol{\theta})} \frac{\partial f(\mathbf{x}; \boldsymbol{\theta})}{\partial \boldsymbol{\theta}} \, dx \\
&= \frac{\partial}{\partial \boldsymbol{\theta}} \int_{\mathcal{X}} f(\mathbf{x}; \boldsymbol{\theta}) \, d\mathbf{x} \\
&= \frac{\partial}{\partial \boldsymbol{\theta}} 1 = 0
\end{aligned}$$

where we take a leap of faith in switching the derivative and integral in the penultimate line. Furthermore, we can get the second identity

$$\mathbb{E}\left[\frac{\partial^2 \ell}{\partial \theta^2}\right] + \mathbb{E}\left[\frac{\partial \ell}{\partial \theta}\right]^2 = 0$$

We can apply these two identities as follows. Since

$$\ell(\theta) = \frac{Y\theta - b(\theta)}{\phi} + c(Y; \phi)$$

therefore

$$\frac{\partial \ell}{\partial \theta} = \frac{Y - b'(\theta)}{\phi}$$

which yields

$$0 = \mathbb{E}\left[\frac{\partial \ell}{\partial \theta}\right] = \frac{\mathbb{E}[Y] - b'(\theta)}{\phi} \implies \mathbb{E}[Y] = \mu = b'(\theta)$$

On the other hand, we have

$$\frac{\partial^2 \ell}{\partial \theta^2} + \left(\frac{\partial \ell}{\partial \theta}\right)^2 = -\frac{b''(\theta)}{\phi} + \left(\frac{Y - b'(\theta)}{\phi}\right)^2$$

and from the previous result, we get

$$\frac{Y - b'(\theta)}{\phi} = \frac{Y - \mathbb{E}[Y]}{\phi}$$

together with the second identity, yields

$$0 = -\frac{b''(\theta)}{\phi} + \frac{\mathrm{Var}(Y)}{\phi^2} \implies \mathrm{Var}(Y) = \phi\,''(\theta)$$

Since variance is always positive, this implies that $b'' > 0$ and therefore b must be convex.

8.3 Link Functions

Now let's go back to GLMs. In linear models, we said that the conditional expectation of Y given $X = \mathbf{x}$ must be a linear function in x

$$\mathbb{E}[Y \mid X = \mathbf{x}] = \mu(\mathbf{x}) = \mathbf{x}^T\beta$$

But if the conditional distribution takes values in some subset of $\mathbb{R}$, such as $(0, 1)$, then it may not make sense to write this as a linear function, since $X^T\beta$ has an image spanning $\mathbb{R}$. So what we need is a link function that relates, i.e. transforms the restricted subset of μ, onto the real line, so that now you can express it of the form $X^T\beta$.

$$g\big(\mu(X)\big) = X^T\beta$$

Again, it is a bit more intuitive to talk about g^{-1}, which takes our $X^T\beta$ and transforms it to the values that I want, so we will talk about both of them simultaneously. If g is our link function, we want it to satisfy 3 requirements:

1. g is continuously differentiable
2. g is strictly increasing
3. $\text{Im}(g) = \mathbb{R}$, i.e. it spans the entire real line

This implies that g^{-1} exists, which is also continuously differentable and is strictly increasing.

Example 8.13 ()

If I have a conditional distribution...

1. that is Poisson, then we want our μ to be positive, and so we need a link function $g : \mathbb{R}^+ \to \mathbb{R}$. One choice would be the logarithm

$$g(\mu(X)) = \log\big(\mu(X)\big) = X^T\beta$$

2. that is Bernoulli, then we want our μ to be in $(0, 1)$ and we need a link function $g : (0, 1) \to \mathbb{R}$. There are 2 natural choices, which may be the **logit** function

$$g(\mu(X)) = \log\left(\frac{\mu(X)}{1 - \mu(X)}\right) = X^T\beta$$

or the **probit** function

$$g(\mu(X)) = \Phi^{-1}\big(\mu(X)\big) = X^T\beta$$

where Φ is the CDF of a standard Gaussian. The two functions can be seen in Figure 15.

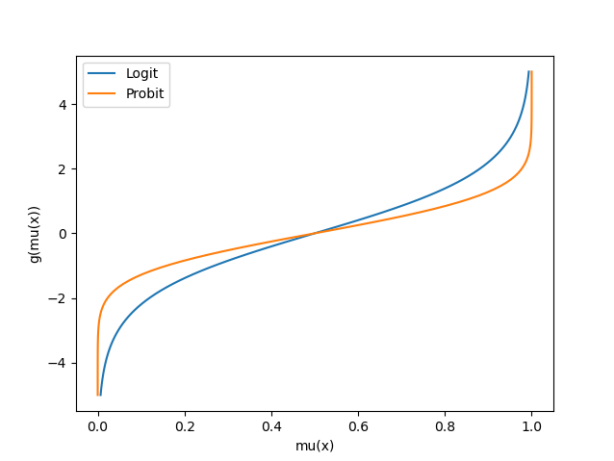


Figure 15: Logit and Probit Functions

Now there are many choices of functions we can take. In fact, if μ lives in $(0, 1)$, then we can really just take our favorite distribution that has a density that is supported everywhere in $\mathbb{R}$ and take the inverse cdf as our link. So far, we have no reason to prefer one function to another, but in the next section, we will see that there are more natural choices.

8.3.1 Canonical Link Functions

Now let's summarize what we have. We assume that the conditional distribution $Y \mid X = x$ follows a distribution in the exponential family, which we can completely characterize by the cumulant generating function ψ. For different values of x, the conditional distribution will be paramaterized by different $\eta(x)$, and the resulting distribution P_η will have some mean $\mu(x)$, which is usually not the natural parameter η. Now, let's forget about our knowledge that $\psi'(\eta) = \mu$, but we know that there is some relationship between $\eta \leftrightarrow \mu$.

Given an x, I need to use the linear predictor $x^T\beta$ to predict $\mu(x)$, which can be done through the link function g.

$$g\big(\mu(x)\big) = x^T\beta$$

Now what would be a natural way of choosing this g? Note that our natural parameter η for this canonical family takes value on the entire real line. I must construct a function g that maps μ onto the entire real line, and so why not make it map to η. Therefore, we have

$$\eta(x) = g\big(\mu(x)\big) = x^T\beta$$

Definition 8.4 (Canonical Link)

The function g that links the mean μ to the canonical parameter θ is called the **canonical link**.

$$g(\mu) = \theta$$

Now using our knowledge that $\psi'(\eta) = \mu$, we can see that

$$g = (\psi')^{-1}$$

This is indeed a valid link function.

1. $\psi'' > 0$ since it models the variance, and so ψ' is strictly increasing and so $g = (\psi')^{-1}$ is also strictly increasing.
2. The domain of ψ' is the real line since it takes in the natural parameter η which exists over $\mathbb{R}$, so $\text{Im}(g) = \mathbb{R}$.

So, given our cumulant generating function ψ and our link function g, both satisfying

$$\psi'(\eta) = \mu \text{ and } g(\mu) = x^T\beta$$

we can combine them to get

$$(g \circ \psi')(\eta) = g(\mu) = x^T\beta$$

and so, even though the mean of the response variable is not linear with respect to x, the value of $(g \circ \psi')(\eta)$ is indeed linear. In fact, if we choose the canonical link, then the equation

$$\eta = x^T\beta$$

means that the natural parameter of our conditional distribution in the exponential family is linear with respect to x! From this we can find the conditional mean $\mu(x)$.

The reason we focus on canonical link functions is because, when the canonical link is used, the components of the model (the parameters of the linear predictor) have an additive effect on the response variable in the

transformed (linked) scale, which makes the interpretation of the results easier. It's also worth noting that while using the canonical link function has some desirable properties, it is not always the best or only choice, and other link functions may be used if they provide a better fit for the data or make more sense in the context of the problem at hand.

Let us evaluate some canonical link functions.

Example 8.14 ()

The Bernoulli has the canonical exponential form of

$$p_\eta(x) = \exp\big[x\eta - \log(1+e^\eta)\big]$$

where $\eta = \log\left(\frac{\theta}{1-\theta}\right)$. Since we have prior knowledge that $\theta = \mu$ (i.e. the expectation of a Bernoulli is the hyperparameter θ itself), we have a function that maps $\mu \mapsto \eta$.

$$\eta = g(\mu) = \log\left(\frac{\mu}{1-\mu}\right)$$

which gives us our result. We can also take the inverse of $\psi' = \frac{e^\eta}{1+e^\eta}$ to get our result

$$g(\mu) = (\psi')^{-1}(\mu) = \log\left(\frac{\mu}{1-\mu}\right)$$

8.4 Likelihood Optimization

Now let us have a bunch of data points $\{(x_n, y_n)\}_{n=1}^N$. By our model assumption, we know that the conditional distribution $Y \mid X = x_n$ is now of an exponential family with parameter $\eta_n = \eta(x_n)$ and density

$$p_{\eta_n}(y_n) = \exp\big[y_n\eta_n - \psi(\eta_n)\big]h(y_n)$$

Now we want to do likelihood optimization on β (not η or μ), and to do this, we must rewrite the density function in a way so that it depends on β. Given a link function g, note the following relationship between β and η:

$$\begin{aligned}\eta_n = \eta(x_n) &= (\psi')^{-1}(\mu(x_n)) \\ &= (\psi')^{-1}\big(g^{-1}(x_n^T\beta)\big) \\ &= h(x_n^T\beta)\end{aligned}$$

where for shorthand notation, we define $h \coloneqq (g \circ \psi')^{-1}$. Subtituting this into the above likelihood, taking the product of all N samples, and logarithming the equation gives us the following log likelihood to optimize over β.

$$\ell(\beta) = \log \prod_{n=1}^N p_{\eta_n}(y_n) = \sum_{n=1}^N y_n h(x_n^T\beta) - \psi(h(x_n^T\beta))$$

where we dropped the $h(y_n)$ term at the end since it is a constant and does not matter. If g was the canonical link, then h is the identity, and we should have a linear relationship between $\eta(x_n) = x_n^T\beta$. This means that the η_n reduces only to $x_n^T\beta$, which is much more simple to optimize.

$$\ell(\beta) = \log \prod_{n=1}^N p_{\eta_n}(y_n) = \sum_{n=1}^N y_n x_n^T\beta - \psi(x_n^T\beta)$$

Note that the first term is linear w.r.t β, and ψ is convex, so the entire sum must be concave w.r.t. β. With this, we can bring in some tools of convex optimization to solve.

9 Boosting

9.1 AdaBoost

Definition 9.1 (Exponential Loss)

The **exponential loss** is a loss function that is used in boosting algorithms. Given a prediction $f(x)$ and a true label $y \in \{-1, 1\}$, the exponential loss is defined as

$$L(y, f(x)) = e^{-yf(x)} \tag{146}$$

9.2 Gradient Boosting

9.3 Random Forests

10 Bagging

The bias variance noise decomposition gives us a very nice way of explaining overfittting. That is, the bias (expectation of the squared difference between the true $\mathbb{E}[Y \mid X]$ and the expected trained hypothesis function $h_{\boldsymbol{\theta};\mathcal{D}}$) reduces, but the variance in this overfitted model increases. Therefore, if we had a slightly different dataset $\mathcal{D}$ sampled from $(X \times Y)^N$, then we might have a very different trained hypothesis since it's so sensitive to the data.

A way to treat this is through **ensemble learning**, where we train *multiple* models over slightly different datasets, and then average their predictions in order to decrease the variance. Even though each model is trained over a smaller dataset, resulting it being more noisy, the average of all these slightly more noisy models will hopefully bring down the variance more than what we have added. There are two similar techniques: bagging and bootstrapping.

Definition 10.1 (Bootstrap Aggregating)

Given a dataset $\mathcal{D}$ of N samples and a model $\mathcal{M}$, **bagging** is an ensemble method done with two steps:

1. Sample $\tilde{N}$ data points with replacement from $\mathcal{D}$ to get a dataset $\mathcal{D}_1$, and do this M times to get
$$\mathcal{D}_1, \mathcal{D}_2, \dots, \mathcal{D}_M \subset \mathcal{D}$$
2. For each sub dataset $\mathcal{D}_m$, train our model to get the optimal hypothesis $h^*_{\mathcal{D}_m}$. We should have M different hypothesis functions, each trained on each sub dataset.
$$h^*_{\mathcal{D}_1}, h^*_{\mathcal{D}_2}, \dots, h^*_{\mathcal{D}_M}$$

To predict the output on a new value $\hat{\mathbf{x}}$, we can evaluate all the $h^*_{\mathcal{D}_m}(\hat{\mathbf{x}})$.

11 Clustering and Density Estimation

11.1 K Means

11.2 Mixture Models

Gaussian mixture models.

We've talked about the theory and implementation behind all these models, but in practice, how do we even use them? If we are trying to predict lung cancer in a patient, do we use linear regression, a nonparametric model, or something else? It's not clear at all what to do with the data. Unfortunately, this just comes with domain expertise and experience with data, but we can provide some general pointers.

As stated before, we have the flexibility to choose whatever model to train on. So how do we choose which form is the best? Well this is just an assumption that most researchers make, and this is called **model selection**.

Example 14.1 (Polynomial Regression)

The number of terms M, i.e. the degree $M-1$ of the polynomial

$$h_{\boldsymbol{\theta}}(x) = w_0 + w_1 x + w_2 x^2 + \ldots + w_{M-1} x^{M-1}$$

in polynomial regression gives us models with different complexities, where $\mathcal{M}_M$ determines the model with a $M-1$th degree polynomial.

Example 14.2 ()

Suppose I have data sampled data $x^{(1)}, \dots, x^{(N)}$ on age at death for N people from an unknown distribution X. Then, possible models that model the distribution are

1. $\mathcal{M}_1$: the exponential distribution $p(x \mid \lambda) = \lambda e^{-\lambda y}$ with parameter $\theta = \lambda$.
2. $\mathcal{M}_2$: the gamma distribution $p(y \mid a, b) = (b^a/\Gamma(a))y^{a-1}e^{-by}$ with parameter $\boldsymbol{\theta} = (a, b)$.
3. $\mathcal{M}_3$: the log-normal distribution with $X \sim N(\mu, \sigma^2)$ where $\boldsymbol{\theta} = (\mu, \sigma^2)$.

Example 14.3 ()

A mixture of Gaussians model

$$p(\mathbf{y}) = \sum_{m=1}^{M} \pi_m N(\mathbf{y} \mid \boldsymbol{\mu}_m, \boldsymbol{\Sigma}_m)$$

has submodels where we must determine the number of Gaussians M.

Now if we assume that the actual true distribution X or the true regressor $\mathbb{E}[Y \mid X]$ is contained within our model $\mathcal{M}$, then we say our model is **well-specified**. But since researchers have no idea what the data generating process is, so $\mathbb{E}[Y \mid X] \notin \mathcal{M}$. Hence there is the saying that saying that "all models are wrong," since we never know what the true data generating process is, and thus the quantity

$$\mathbb{E}[Y \mid X] - h^*_{\boldsymbol{\theta}}(X)$$

where $h^*_{\boldsymbol{\theta}}(X)$ is the optimized hypothesis functions within $\mathcal{M}$, will always be nonzero. How close we can get this quantity to 0 determines how useful the model is, and a misspecified model is fundamentally a convenient (or even necessary) assumption on the distribution underlying the data, which may only be a reasonable approximation.

14.2 Feature Engineering

This is also very domain specific.

14.3 Data Preprocessing

14.3.1 Feature Extraction

The simplest linear function for regression is simply

$$h_{\mathbf{w}}(\mathbf{x}) = w_0 + w_1 x_1 + \ldots + w_D x_D$$

This is called linear regression not because h is a linear function of $\mathbf{x}$. It is a linear function of $\mathbf{w}$. Therefore, we can fix nonlinear functions $\phi_j(\mathbf{x})$ and consider linear combinations of them.

$$h_{\mathbf{w}}(\mathbf{x}) = w_0 + \sum_{j=1}^{M-1} w_j \phi_j(\mathbf{x})$$

We usually choose a dummy basis function $\phi_0(\mathbf{x}) = 1$ for notational convenience, so that if $\boldsymbol{\phi}$ is the vector of the function ϕ_j, then we can write $h_{\mathbf{w}}(\mathbf{x}) = \mathbf{w}^T \boldsymbol{\phi}(\mathbf{x})$. This mapping from the original variables $\mathbf{x} \in \mathbb{R}^D$ to the basis functions $\{\phi_j(\mathbf{x})\}$, which span a linear function space of dimension M, is called **preprocessing** or **feature extraction** of the data.

Example 14.4 ()

Here are some examples of how we can extract features.

1. The mapping from a single variable x to its powers

$$x \mapsto (1, x, x^2, \dots, x^{M-1}) \tag{147}$$

2. The mapping from a configuration of K atoms with their momenta in $\mathbb{R}^{6K}$ to their atomic cluster expansion polynomials.
3. The Legendre polynomials, which form an orthonormal basis in the space of polynomials.
4. Using equally spaced Gaussian basis functions over the dataset.

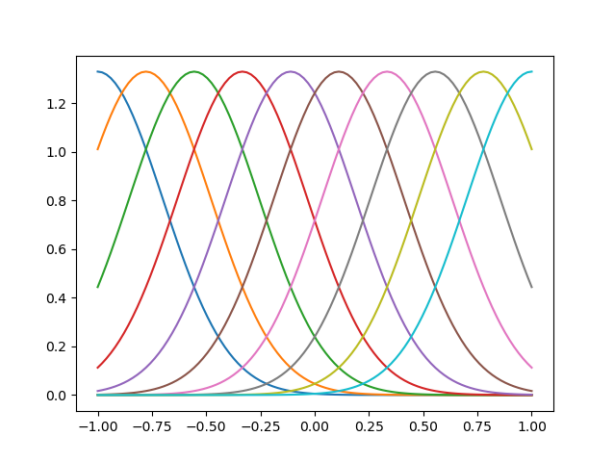


Figure 16: Gaussian basis functions over the interval $[-1, 1]$ with standard deviation of 0.3

Changing the input space from D dimensions to M dimensions (i.e. extracting our M features) gives the design matrix

$$\mathbf{X} = \begin{pmatrix} \mathbf{x}^{(1)} \\ \mathbf{x}^{(2)} \\ \mathbf{x}^{(3)} \\ \vdots \\ \mathbf{x}^{(n)} \end{pmatrix} \implies \mathbf{\Phi} = \begin{pmatrix} — & \phi(\mathbf{x}^{(1)}) & — \\ — & \phi(\mathbf{x}^{(2)}) & — \\ \vdots & \vdots & \vdots \\ — & \phi(\mathbf{x}^{(n)}) & — \end{pmatrix} \tag{148}$$

We have shown that the `PolynomialFeatures` transformer converts our features to a polynomial basis. We can do this for an arbitrary number of features, for example if we map $D = 2$ to a second degree polynomial, we would have the transformation

$$(x_1, x_2) \mapsto (1, x_1, x_2, x_1^2, x_1 x_2, x_2^2)$$

```
>>> import numpy as np
>>> from sklearn.preprocessing import PolynomialFeatures
>>> X = np.arange(6).reshape(3, 2)
>>> X
array([[0, 1],
       [2, 3],
       [4, 5]])
>>> poly = PolynomialFeatures(2)
>>> poly.fit_transform(X)
array([[ 1.,  0.,  1.,  0.,  0.,  1.],
```

```
        [ 1.,  2.,  3.,  4.,  6.,  9.],
        [ 1.,  4.,  5., 16., 20., 25.]])
```

Sometimes, we are only worried about the interaction terms among features, so we can set the parameter `interaction_only=True`, which would, in the third degree case, transform the features

$$(x_1, x_2, x_3) \mapsto (1, x_1, x_2, x_3, x_1x_2, x_1x_3, x_2x_3, x_1x_2x_3)$$

Spline transformers are piecewise polynomials, which is also built in. We notice that it is cumbersome to transform the dataset `X` with the transformer, store it into another variable, and train the model on that. We can "combine" the transforming (even multiple layers of transformers) and the model by implementing a "pipeline," which is initialized by inputting a list of tuples (name and the object) and has the same methods as the model.

```
from sklearn.pipeline import Pipeline
model = Pipeline([("poly_transform", PolynomialFeatures(degree=2)),
                  ("lin_regression", LinearRegression())
                  ])
model.fit(X, y)
```

Now, let's talk about how we can implement a custom transformer. We basically have to create a new subclass that implements the `fit` (which always returns `self`) and the `transform` (which returns the transformed matrix) methods. Here we show for Gaussian basis functions.

```
from sklearn.base import BaseEstimator, TransformerMixin

class GaussianFeatures(BaseEstimator, TransformerMixin):
    """Uniformly spaced Gaussian features for one-dimensional input"""

    def __init__(self, N, width_factor=2.0):
        self.N = N
        self.width_factor = width_factor

    def fit(self, X, y=None):
        # create N centers spread along the data range
        self.centers_ = np.linspace(X.min(), X.max(), self.N)
        self.width_ = self.width_factor * (self.centers_[1] - self.centers_[0])
        return self

    def transform(self, X):
        transformed_rows = []
        for mu in self.centers_:
            transformed_rows.append(stats.norm.pdf(X, mu, self.width_))

        return np.hstack(tuple(transformed_rows))

model = Pipeline([("gauss_transform", GaussianFeatures(20)),
                  ("lin_regression", LinearRegression())
                  ])

N = 60
X = np.random.uniform(-1, 1, size=(N, 1))
Y = true_func(X) + np.random.normal(0, 0.3, size=(N, 1))

model = Pipeline([("gauss_transform", GaussianFeatures(10)),
              ("lin_regression", LinearRegression())
```

```
                ])
model.fit(X, Y)
```

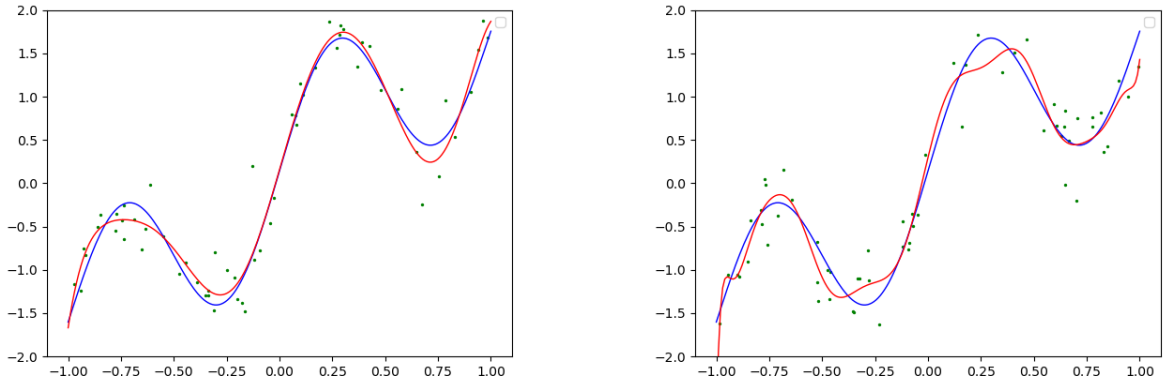
If we would like to impelment the fourier expansion of a function of form

$$f(x) = \frac{1}{2}a_0 + \sum_{n=1}^{N} a_n \cos(nx) + \sum_{n=1}^{N} b_n \sin(nx)$$

Then we would create the basis functions according to

```
class FourierFeatures(BaseEstimator, TransformerMixin):
    "Fourier Expansion for one-dimensional input"

    def __init__(self, N):
        self.N = N

    def fit(self, X, Y=None):
        return self

    def transform(self, X):
        transformed_columns = []
        transformed_columns.append(np.ones(shape=X.shape))

        for n in range(self.N):
            transformed_columns.append(np.sin(n * X))
            transformed_columns.append(np.cos(n * X))

        print(np.hstack(tuple(transformed_columns)).shape)
        return np.hstack(tuple(transformed_columns))
```

and both of them would give the following fits to our original function $f(x) = \sin(2\pi x) + 2\cos(x - 1.5)$.



(a) Fitting with 10 Gaussian basis functions.

(b) Fitting with 10 Fourier basis functions.

Figure 17

14.3.2 Standardizing Data

Standardizing typically meanss that our featuers will be rescaled to have the properties of a standard normal distribution with mean of 0 and a standard deviation of 1. Here are a few methods to scale our data,

with their results shown on a dataset of 30 points in $\mathbb{R}^2$.

1. **StandardScaler**: This is probably the most used method for standardizing data. It standardizes features by removing the mean and scaling to unit variance. The standard score of a sample $x^{(n)}$ is $(x - \bar{x})/S$ where $\bar{x}$ is the mean of the training samples and S is the standard deviation of the training samples.

```
from sklearn.preprocessing import StandardScaler
scaler = StandardScaler()
scaled_data = scaler.fit_transform(data)
```

2. **MinMaxScaler**: While not technically "standardization," MinMaxScaler is another preprocessing method for scaling. It transforms features by scaling each feature to a given range, typically between zero and one, or so that the maximum absolute value of each feature is scaled to unit size.

```
from sklearn.preprocessing import MinMaxScaler
scaler = MinMaxScaler()
scaled_data = scaler.fit_transform(data)
```

3. **MaxAbsScaler**: This scaler works similarly to the MinMaxScaler but scales in a way that the training data lies within the range $[-1, 1]$ by dividing through the largest maximum value in absolute value. It is meant for data that is already centered at zero or sparse data.

```
from sklearn.preprocessing import MaxAbsScaler
scaler = MaxAbsScaler()
scaled_data = scaler.fit_transform(data)
```

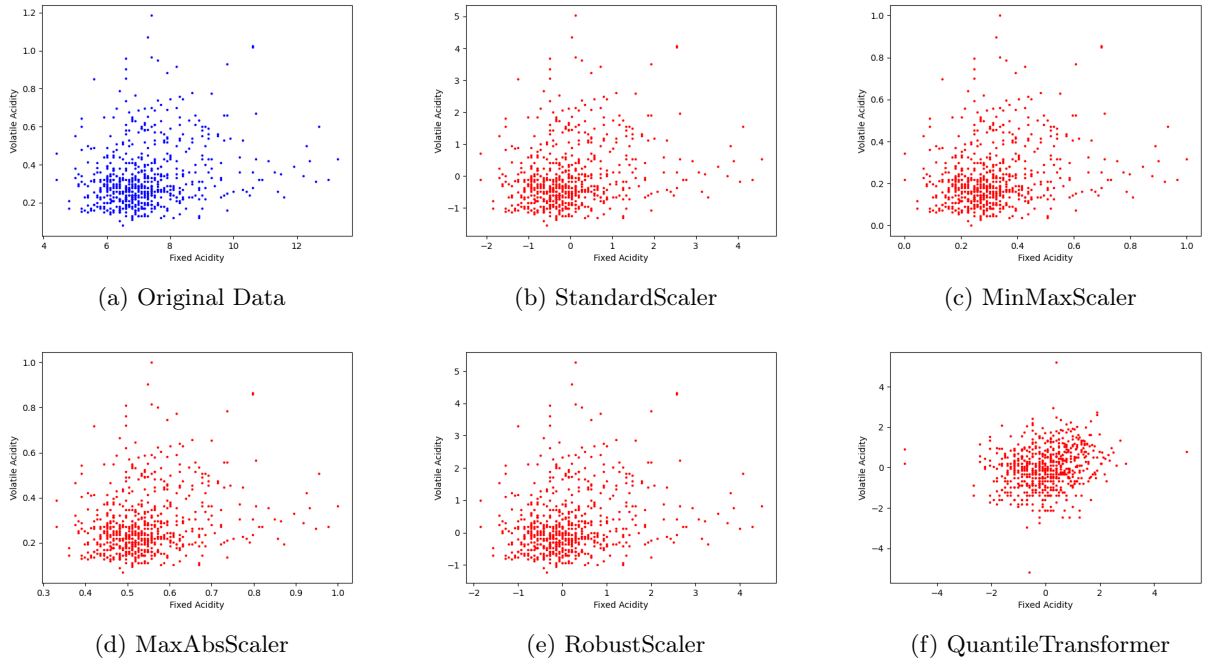
4. **RobustScaler**: This scaler removes the median and scales the data according to the quantile range (defaults to IQR: Interquartile Range). It's robust to outliers, which makes it a good choice if you have data with possible outliers.

```
from sklearn.preprocessing import RobustScaler
scaler = RobustScaler()
scaled_data = scaler.fit_transform(data)
```

5. **QuantileTransformer**: Note that the presence of outliers messes with our scaling. More generally for skewed distributions (like an exponential), a linear transformation does not take care of these outliers, so we would like some nonlinear preprocessing algorithm. One common one is the QuantileTransformer, which takes the quantiles (percentiles) of the dataset and transforms then so that those are equidistant from each other. By default, it divides up the data into 1000 quantiles.

```
from sklearn.preprocessing import QuantileTransformer
transformer = QuantileTransformer(n_quantiles = 100, output_distribution='normal')
transformed_data = transformer.fit_transform(data)
```

Let's talk about how these scalers will work on some data. We take a wine data with the two variables representing fixed acidity and volatile acidity.



(a) Original Data (b) StandardScaler (c) MinMaxScaler

(d) MaxAbsScaler (e) RobustScaler (f) QuantileTransformer

Figure 18: The StandardScaler simply standardizes the data to have 0 mean and unit variance.

It's important to note that whether you should standardize your data and how you should do it depends on the specific characteristics of your data and the machine learning algorithm you're using. For example, some algorithms, like many in deep learning, assume that all features are on the same scale. Others, like Decision Trees and Random Forests, do not require feature scaling at all.

14.4 Data Augmentation

15 Archive

15.1 Bayesian Probability

Now this book puts a heavy emphasis on Bayesian probabilistic models. For now, we will denote $p(X)$ to be the distribution of a random variable X. We capture our assumptions about the model parameter $\mathbf{w}$ with a prior distribution $p(\mathbf{w})$. Our likelihood $p(\mathcal{D} \mid \mathbf{w})$ is the conditional distribution of getting the data $\mathcal{D}$ from our model with parameter $\mathbf{w}$. Therefore, Bayes theorem is expressed

$$p(\mathbf{w} \mid \mathcal{D}) = \frac{p(\mathcal{D} \mid \mathbf{w})\, p(\mathbf{w})}{p(\mathcal{D})}$$

The denominator $p(\mathcal{D})$ is a normalizing term equal to $\int p(\mathcal{D} \mid \mathbf{w})\, p(\mathbf{w})\, d\mathbf{w}$, and for high dimensional $\mathcal{W}$ it may not be feasible to compute this integral without monte carlo sampling. Therefore, we focus on the numerator terms and remember the rule

$$\text{posterior} \propto \text{likelihood} \times \text{prior}$$

For clarification, $\mathcal{D}$ can represent different things depending on the problem:

1. In a density estimation problem, where we have a single dataset $\mathbf{X}$, $\mathcal{D} = \mathbf{X}$ since this data tells us information about which distribution it could come from.

2. In a regression problem, $\mathcal{D} = \mathbf{Y}$, that is, $\mathcal{D}$ will always be the output data, not the input data $\mathbf{X}$. We can think of the input data $\mathbf{X}$ as always being fixed, and it is upon observation of the *outputs* $\mathbf{Y}$ on these inputs that gives us information.

In both the frequentist and Bayesian settings, the likelihood $p(\mathcal{D} \mid \mathbf{w})$ plays a central role. In the frequentist setting, the process is divided into two steps:

1. We optimize $\mathbf{w}$ with some **estimator**, with a popular one being the **maximum likelihood estimator**. A popular estimator is **maximum likelihood**, which seeks to maximize $p(\mathcal{D} \mid \mathbf{w})$ w.r.t. $\mathbf{w}$.
2. We optimize $\mathbf{w}$ with some **estimator**, with a popular one being the **maximum likelihood estimator**. A popular estimator is **maximum likelihood**, which seeks to maximize $p(\mathcal{D} \mid \mathbf{w})$ w.r.t. $\mathbf{w}$.
3. We fix the optimized $\mathbf{w}^*$ and error bars on this estimate are obtained by considering the distribution of possible datasets $\mathcal{D}$. One approach is **bootstrapping**, which goes as follows. Given our original dataset $\mathbf{X} = \{x^{(1)}, \dots, x^{(N)}\}$, we can create a new dataset $\mathbf{X}'$ by sampling N points at random from $\mathbf{X}$, with replacement, so that some points in $\mathbf{X}$ may be replicated in $\mathbf{X}'$, whereas other points in $\mathbf{X}$ may be absent in $\mathbf{X}'$. This process is repeated L times to generate L different datasets. Then, we can look at the variability of prediction between the different bootstrap data sets.

In a Bayesian setting, there is only a single dataset $\mathcal{D}$ and the uncertainity in the parameters is expressed through a probability distribution over $\mathbf{w}$. It also includes prior knowledge naturally in the form of prior distributions.

15.2 Density Estimation

15.2.1 Frequentist Approach

As a start, let us have a dataset of observations $\mathbf{X} = \{x^{(1)}, \dots, x^{(n)}\}$ assuming that they are all iid from $X \sim N(0, 1)$ distribution. Since this is iid, we can look at the joint distribution X^N on $\mathbb{R}^N$ and get the likelihood of form

$$p(\mathbf{X} \mid \mu, \sigma^2) = \prod_{n=1}^{N} p_X(x^{(n)} \mid \mu, \sigma^2)$$

which in turn gives the log-likelihood as

$$\ln p(\mathbf{X} \mid \mu, \sigma^2) = -\frac{1}{2\sigma^2} \sum_{n=1}^{N} (x_n - \mu)^2 - \frac{N}{2} \ln \sigma^2 - \frac{N}{2} \ln(2\pi)$$

This is a function of two variables, μ and σ^2 and we can optimize it to get the maximum likelihood estimates of

$$\mu_{ML} = \frac{1}{N} \sum_{n=1}^{N} x_n \text{ and } \sigma^2_{ML} = \frac{1}{N} \sum_{n=1}^{N} (x_n - \mu_{ML})^2$$

However, as we saw in the previous section, the estimate for σ^2 is biased by a factor of $(N-1)/N$, and this is an intrinsic flaw in the frequentist approach.

15.2.2 Bayesian Approach

In the Bayesian approach, we want to model

$$p(x \mid \mathcal{D}) = \int p(x \mid \mathbf{w})\, p(\mathbf{w} \mid \mathcal{D})\, d\mathbf{w}$$

15.3 Regression with Regularization

15.3.1 Frequentist's Maximum Likelihood Approach

Now given the hypothesis function $h_{\mathbf{w}}$, researchers assume that the relationship between the X and Y values are captured by

$$Y = h_{\mathbf{w}}(X) + \epsilon$$

where ϵ is some residual noise, also a random variable. Researchers assume that this random variable has a nice form. One popular choice is that $\epsilon \sim N(0, \sigma^2)$ since if we assume that this error is due to a large number of weakly dependent unknown factors, then by CLT we can assume that their sum is Gaussian. But ultimately this is just another assumption. With this Gaussian assumption, we can assume that each input output pair $(x^{(n)}, y^{(n)})$ is generated by form $y^{(n)} = h_{\mathbf{w}}(x^{(n)}) + \epsilon$ and so the conditional distribution of $y^{(n)}$ given $X^{(n)}$ is

$$Y \mid X = x^{(n)} \sim N(h_{\mathbf{w}}(x^{(n)}), \sigma^2)$$

and therefore, the probability of getting $y^{(n)}$ given $x^{(n)}$ is modeled by the conditional pdf

$$p_{Y|X=x^{(n)}}(y^{(n)}) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{[y^{(n)} - h_{\mathbf{w}}(x^{(n)})]^2}{2\sigma^2} \right)$$

Extending this to the dataset $\mathcal{D} = \mathbf{Y}$ coming from the N-fold joint distribution of X, by independence this distribution is a multivariate Gaussian

$$Y^n \mid X^n = \mathbf{X} \sim N(h_{\mathbf{w}}(\mathbf{X}), \sigma^2 \mathbf{I})$$

where by abuse of notation, $h_{\mathbf{w}}(\mathbf{X})$ is $h_{\mathbf{w}}$ operated element-wise on the vector $\mathbf{X}$, and $\mathbf{I}$ is the $N \times N$ identity matrix. The pdf is

$$\begin{aligned} p_{Y^n|X^n=\mathbf{X}}(\mathbf{Y}) &= \prod_{n=1}^{N} p_{Y|X=x^{(n)}}(y^{(n)}) \\ &= \prod_{n=1}^{N} \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{[y^{(n)} - h_{\mathbf{w}}(x^{(n)})]^2}{2\sigma^2} \right) \end{aligned}$$

The two parameters of interest here that we would like to maximize are $\mathbf{w}$ and σ^2. We can take the log of this function to maximize this, which gives us

$$\ell(\mathbf{w}, \sigma^2) = -\frac{1}{\sigma^2} E_D(\mathbf{w}) - \frac{N}{2} \ln \sigma^2 - \frac{N}{2} \ln(2\pi)$$

and here we can see that maximizing the likelihood w.r.t. $\mathbf{w}$ is equal to minimizing the sum-of-squares error function $E_D(\mathbf{w}) = -\frac{1}{2} \sum_{n=1}^{N} [y^{(n)} - h_{\mathbf{w}}(x^{(n)})]^2$. Therefore, a maximum likelihood estimation under a Gaussian residual assumption implies minimization of the sum-of-squares error function! To maximize with respect to both $\mathbf{w}$ and σ^2, we can use the fact that this function is C^1 (continuously differentiable), and so we just need to find where the partials are 0. Ultimately, we can just optimize for $\mathbf{w}$ first and then solve for σ^2. If $h_{\mathbf{w}}$ was linear (not necessarily in $\mathbf{x}$, but with $\mathbf{w}$), then we can transform the x_d values, get the proper design matrix $\mathbf{\Phi}$, and compute

$$\mathbf{w}_{ML} = (\mathbf{\Phi}^T \mathbf{\Phi})^{-1} \mathbf{\Phi}^T \mathbf{Y}$$

If we add a ridge penalty term to get $E(\mathbf{w}) = E_D(\mathbf{w}) + \frac{\lambda}{2} ||\mathbf{w}||_2^2$, then this results in solving the matrix equation

$$\mathbf{w}_{ML} = (\mathbf{\Phi}^T \mathbf{\Phi} + \lambda \mathbf{I})^{-1} \mathbf{\Phi}^T \mathbf{Y}$$

With these optimized parameters, we have a **probabilistic model** in which given a new value $\hat{\mathbf{x}}$, we can predict the conditional distribution of $\hat{y}$ to be

$$p(y' \mid \hat{\mathbf{x}}, \mathbf{w}_{ML}, \sigma_{ML}^2) = N(\hat{y} \mid h_{\mathbf{w}_{ML}}(\mathbf{x}'), \sigma_{ML}^2)$$

15.3.2 Bayesian Approach

We will now demonstrate how having a normal $\alpha\mathbf{I}$ prior around the origin in a Bayesian setting is equivalent to having a ridge penalty of $\lambda = \sigma^2/\alpha^2$ in a frequentist setting. If we have a Gaussian prior of form

$$p(\mathbf{w} \mid \alpha^2) = N(\mathbf{w} \mid \mathbf{0}, \alpha^2\mathbf{I}) = \left(\frac{1}{2\pi\alpha^2}\right)^{M/2} \exp\left(-\frac{1}{2\alpha^2}||\mathbf{w}||_2^2\right)$$

We can use Bayes rule to compute

$$\begin{aligned} p(\mathbf{w} \mid \mathbf{X}, \mathbf{Y}, \alpha^2, \sigma^2) &\propto p(\mathbf{Y} \mid \mathbf{w}, \mathbf{X}, \alpha^2, \sigma^2)\, p(\mathbf{w} \mid \mathbf{X}, \alpha^2, \sigma^2) \\ &= \left[\prod_{n=1}^{N} p(y^{(n)} \mid \mathbf{w}, \mathbf{x}^{(n)}, \alpha^2, \sigma^2)\right] p(\mathbf{w} \mid \mathbf{X}, \alpha^2, \sigma^2) \\ &= \left[\prod_{n=1}^{N} \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{(y^{(n)} - h_{\mathbf{w}}(x^{(n)}))^2}{2\sigma^2}\right)\right] \cdot \left(\frac{1}{2\pi\alpha^2}\right)^{M/2} \exp\left(-\frac{1}{2\alpha^2}||\mathbf{w}||_2^2\right) \end{aligned}$$

and taking the negative logarithm gives us

$$\ell(\mathbf{w}) = \frac{1}{2\sigma^2}\sum_{n=1}^{N}\left(y^{(n)} - h_{\mathbf{w}}(\mathbf{x}^{(n)})\right)^2 + \frac{N}{2}\ln\sigma^2 + \frac{N}{2}\ln(2\pi) - \frac{M}{2}\ln(2\pi\alpha^2) + \frac{1}{2\alpha^2}||\mathbf{w}||_2^2$$

taking out the constant terms relative to $\mathbf{w}$ and multiplying by $2\sigma^2$ (which doesn't affect optima) gives us the ridge penalized error with a penalty term of $\lambda = \sigma^2/\alpha^2$.

$$E(\mathbf{w}) = \frac{1}{2}\sum_{n=1}^{N}\left(y^{(n)} - h_{\mathbf{w}}(\mathbf{x}^{(n)})\right)^2 + \frac{\sigma^2}{\alpha^2}||\mathbf{w}||_2^2$$

But minimizing this still gives a point estimate of $\mathbf{w}$, which is not the full Bayesian treatment. In a Bayesian setting, we are given the training data $(\mathbf{X}, \mathbf{Y})$ along with a new test point $\mathbf{x}'$ and want to evaluate the predictive distribution $p(y \mid \mathbf{x}', \mathbf{X}, \mathbf{Y})$. We can do this by integrating over $\mathbf{w}$.

$$\begin{aligned} p(y \mid \mathbf{x}', \mathbf{X}, \mathbf{Y}) &= \int p(y \mid \mathbf{x}', \mathbf{w}, \mathbf{X}, \mathbf{Y})\, p(\mathbf{w} \mid \mathbf{x}', \mathbf{X}, \mathbf{Y})\, d\mathbf{w} \\ &= \int p(y \mid \mathbf{x}', \mathbf{w})\, p(\mathbf{w} \mid \mathbf{X}, \mathbf{Y})\, d\mathbf{w} \end{aligned}$$

where we have omitted the irrelevant variables, along with α^2 and σ^2 to simplify notation. By substituting the posterior $p(\mathbf{w} \mid \mathbf{X}, \mathbf{Y})$ with a normalized version of our calculation above and by noting that

$$p(y \mid \mathbf{x}', \mathbf{w}) = N(y \mid h_{\mathbf{w}}(\mathbf{x}'), \sigma^2) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{\left(y - h_{\mathbf{w}}(\mathbf{x}')\right)^2}{2\sigma^2}\right)$$

Now this integral may or may not have a closed form, but if we consider the polynomial regression with the hypothesis function of form

$$h_{\mathbf{w}}(x) = w_0 + w_1 x + w_2 x^2 + \ldots + w_{M-1}x^{M-1}$$

then this integral turns out to have a closed form solution given by

$$p(y \mid \mathbf{x}', \mathbf{X}, \mathbf{Y}) = N\big(y \mid m(x'), s^2(x')\big)$$

where

$$\begin{aligned} m(x') &= \frac{1}{\sigma^2}\boldsymbol{\phi}(x')^T\mathbf{S}\left(\sum_{n=1}^{N}\boldsymbol{\phi}(x^{(n)})y^{(n)}\right) \\ s^2(x') &= \sigma^2 + \boldsymbol{\phi}(x')^T\mathbf{S}\boldsymbol{\phi}(x') \\ \mathbf{S}^{-1} &= \alpha^{-2}\mathbf{I} + \frac{1}{\sigma^2}\sum_{n=1}^{N}\boldsymbol{\phi}(x^{(n)})\boldsymbol{\phi}(x')^T \end{aligned}$$

and $\boldsymbol{\phi}(x)$ is the vector of functions $\phi_i(x) = x^i$ from $i = 0, \ldots, M-1$.

References

[1] L. Györfi, M. Kohler, A. Krzyzak, and H. Walk. *A Distribution-Free Theory of Nonparametric Regression.* Springer Series in Statistics. Springer New York, 2002.

[2] Daniel Hsu, Sham M. Kakade, and Tong Zhang. Random design analysis of ridge regression, 2014.