CS 189
Introduction to Machine Learning

Notes

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Contents

1 Logistics

Homework is on a Wednesday-Wednesday cycle. The class textbook is ostensibly *Elements of Statistical Learning* by Tibshirani.

2 Introduction

The core of the class is to find patterns in data, then using the patterns to make predictions about new data. Models and statistics help us understand patterns. Optimization algorithms "learn" the patterns. Data drives everything, and you cannot learn much if the data is small or is poor-quality, but algorithms with lots of data are very successful.

There are many different machine learning tasks; one of the simplest and best is classification.

Definition 1 (Classifier). A *classifier* partitions data into several classes.

Example 2. Say we have training data $\{((x_i, y_i), z_i)\}_{i=1}^{m}$, where x_i is credit card balance, y_i is income, and z_i is whether the person has defaulted on their card (as, say, an indicator variable). We wish to predict the z value z_{pred} for new data points $(x_{\text{new}}, y_{\text{new}})$.

How do we solve this problem? We

- first, collect data,
- then, build a classifier based on the data,
- finally, classify any new points using the classifier.

One possible classifier is to take the k nearest neighboring points $\{(x_{n_i}, y_{n_i})\}_{i=1}^{k}$ for the new point $(x_{\text{new}}, y_{\text{new}})$ in Euclidean xy space, and average their z values, then round to get the predicted z value z_{pred}, so $z_{\text{pred}} = \text{round}\left(\sum_{i=1}^{k} z_{n_i}\right)$. Accordingly, this is called the *k-nearest-neighbor classifier*.

For small k, the k-nearest-neighbor classifier is prone to having really awkward decision boundaries.

Definition 3 (Overfitting). A classifier is *overfitting* when it does not does much more poorly on new data points than it does on old data points.

It's easy to see that, for example, 1-nearest-neighbors classifiers overfit on any noisy training data; on the other hand, for large k, the k-nearest-neighbor classifier does not overfit and the decision boundary is much more smooth, but it may degenerate into being a bad classifier with an incorrect decision boundary.

Another classifier is a *linear classifier*, which is somewhat of a misnomer. In a binary classification situation with a classification function $f \colon \mathbb{R}^d \to \{0, 1\}$, a linear classifier f is an $\mathbb{R}^{d-1}$-dimensional affine hyperplane. This classifier is a smooth solution which may oversimplify the real scenario, but will not overfit since the model is very constrained.

Definition 4 (Hyperparameter). A *hyperparameter* is a property of a machine learning model that is not explicitly learned from data.

Hyperparameters usually control the balance between overfitting and efficacy of the model.

To create a classifier model, given classified training data and test data, we:

- train a classifier on the training data, so it learns to distinguish classes from each other.
- test the classifier on the test data.

There are two kinds of errors associated with a model.

Definition 5 (Errors). The *training set error* is the fraction of misclassified data in the training set. The *test set error* is the fraction of misclassified data in the test set.

Definition 6 (Outliers). *Outliers* are points in the training data which are atypical in some way or just misclassified.

We don't really care about these outlier points very much; algorithms that overfit will sometimes weigh outliers a lot, and this is a way to create an overfitting model.

Hyperparameters generally control the balance between overfitting and underfitting. To select optimal hyperparameters, we do something called the validation process:

Definition 7 (Validation). The validation process produces a machine learning model with good hyperparameters. In the validation process, we:

- hold back a subset of the labeled data, called the validation set
- train the classifier multiple times with different hyperparameter settings
- choose the settings that work best on the validation set

Now there are three data sets:

- the training set, used to learn model weights.
- the validation set, which is used to tune hyperparameters and choose among different models.
- the test set, used as the final evaluation of the model.

There are two types of overarching problem classifications, and problems under them:

- *Supervised learning*, when the training data has labels
  - *Classification*: data labels are discrete and unordered
  - *Regression*: data labels are continous or ordered
- *Unsupervised learning*, when the training data has no labels
  - *Clustering*: observing clusters in (transformed) Euclidean space with respect to the data points, hinting at the data generation process.
  - *Dimensionality* reduction: finding projections of high dimensional data onto low dimensional manifolds.

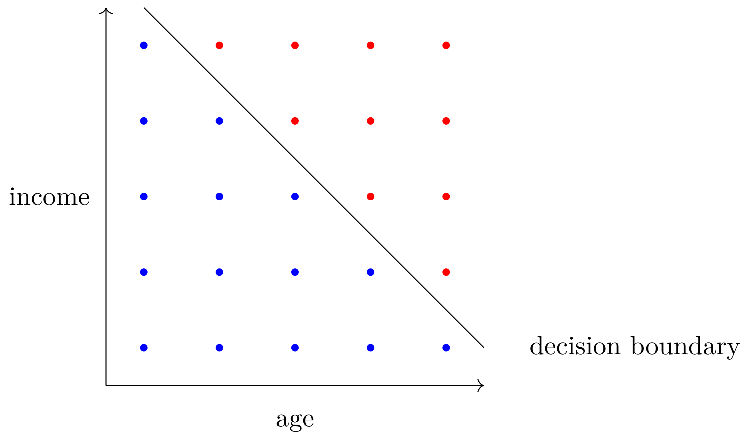
3 Linear Classifiers

We are given a dataset of n observations, each with d features. The reason why we use the letter d is that it reflects the dimension of our data points. Some observations belong to a class C; some do not, and belong to another class X.

Example 8. Observations can be bank loans, features can be income and age ($d = 2$). Some observations are in the class DEFAULTED, and some are not. The goal is to predict whether future borrowers will default, based on their income and age.

The way we think about the dataset is that we represent each observation as a point in a d-dimensional space. Each sample point is referred to as a feature vector, or an independent variable vector.

For the example, one may have the dataset



Definition 9 (Decision Boundary). The *decision boundary* is the boundary chosen by the classifier to separate items in the class C from those that do not.

Overfitting, in this case, refers to a sinuous decision boundary that fits sample points so well that it doesn't classify future points well.

For multiclass classifiers, some classifiers train a classification for each class and weight their output according to their returned probability. Others train an "*all-for-one*" method, which allows simultaneous probability computation for each class.

Definition 10 (Decision Function). A *decision function* is a function $f(x)$ that maps a sample point x to a scalar such that

$$f(x) > 0 \text{ if } x \in C, \quad f(x) \leq 0 \text{ otherwise}$$

This is also known as a *predictor function* or *discriminant function*.

For these classifiers, the *decision boundary* is $\left\{x \in \mathbb{R}^d : f(x) = 0\right\}$. Usually, this set is a $(d-1)$-dimensional manifold in $\mathbb{R}^d$.

Definition 11 (Isosurface and Isovalue). The set $\left\{x \in \mathbb{R}^d : f(x)\right\}$ is called an *isosurface* of f for the *isovalue* 0. In particular, f has other isosurfaces for other isovalues, e.g. $x \colon f(x) = 1$.

Sometimes there are needs for explicit nonzero isovalues.

Linear classifiers have linear decision boundaries, where the boundary manifold is a $(d-1)$-dimensional hyperplane $\{x \colon w \cdot x = \alpha\}$. Usually, linear classifiers also use a linear decision function.

Claim 12. Let $x, y \in H = \{x \colon w \cdot x = -\alpha\}$. Then $w \cdot (y - x) = 0$.

Proof. By computation,

$$w \cdot (y - x) = -\alpha - (-\alpha) = 0$$

as desired. □

In this case w is called the normal vector of H, because as the theorem shows, w is normal (perpendicular) to H. If w is a unit vector (i.e. $\|w\|_2 = 1$), then $w \cdot x + \alpha$ is the signed distance from x to H. In particular, $\text{sign}(w \cdot x + \alpha) > 0$ if w is on the same side of H as x, and 0 otherwise. If $\|w\|_2 \neq 1$, then the same concept holds, except we need to normalize w and α to find the distance.

Definition 13 (Weights). The coefficients in w, plus α, are called *weights* (or parameters or regression coefficients).

Sometimes we talk about when input data is linearly separable.

Definition 14 (Linearly Separable). The input data is *linearly separable* if there exists a hyperplane that separates all the sample points in class C from all the points not in class C.

Examples of Simple Linear Classifiers

Definition 15 (Centroid Method). A simple classifier is the centroid method. We compute the mean μ_C of all points in class C, and the mean μ_X of all points not in class C. The decision function is

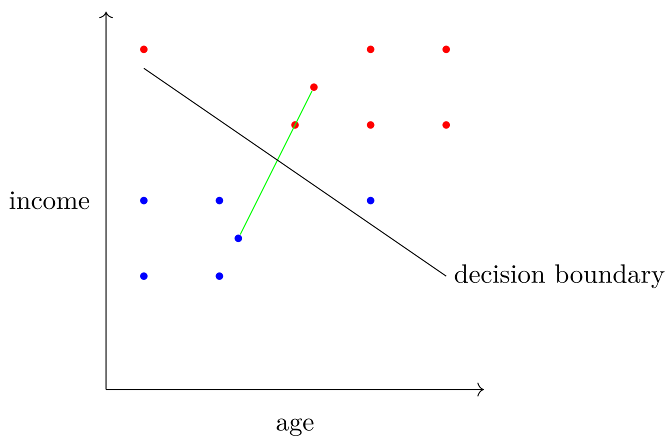
$$f(x) = \underbrace{(\mu_C - \mu_X)}_{\text{normal vector}} \cdot x - (\mu_C - \mu_X) \cdot \underbrace{\frac{\mu_C + \mu_X}{2}}_{\text{midpoint}(\mu_C, \mu_X)}$$

More explicitly, the algorithm for the centroid method is

Algorithm 1 The centroid method.

Input: A set of data points $\{(X_i, y_i)\}_{i=1}^n$ where $X_i \in \{C_1, C_2\}$ and $y_i = 2\mathbb{1}(X_i \in C_1) - 1$.
Output: A decision function $f(x)$ that in the linearly separable case resolves to $f(x) = 2\mathbb{1}(x \in C_1) - 1$.
$\mu_{C_1} \leftarrow \frac{1}{|C_1|} \sum_{X \in C_1} X$
$\mu_{C_2} \leftarrow \frac{1}{|C_2|} \sum_{X \in C_2} X$
return $f(x) \overset{\text{def}}{=} (\mu_{C_1} - \mu_{C_2}) \cdot x - (\mu_{C_1} - \mu_{C_2}) \cdot \frac{\mu_{C_1} + \mu_{C_2}}{2}$

We want the decision boundary to go exactly between the mean vectors μ_C and μ_X; this is achieved when $x = 0$. The decision boundary is the hyperplane that bisects the line segment with endpoints μ_C and μ_X.



Question 16. Is it possible to design an dataset that the centroid method misclassifies every data point but one?

It turns out that it is possible.

Now we move to the perceptron algorithm, which uses gradient descent and is correct for linearly separated points.

Definition 17 (Perceptron Classifier). Consider n sample points $X_1, \ldots, X_n$. For each sample point, let the label $y_i = 1$ if $X_i \in C$ and $y_i = -1$ if $X_i \notin C$. For simplicity, consider only decision boundaries that pass through the origin. Then the goal is to find weights w such that $X_i \cdot w \geq 0$ if $y_i = 1$, and $X_i \cdot w \leq 0$ if $y_i = -1$. Putting these together, we get $y_i X_i \cdot w \geq 0$ for every i.

We may conceptualize hyperplanes in terms of x-space V, or feature space, and w-space, or weight space W. In particular, there is a natural injection between hyperplanes $H \in V$ and vectors $w \in W$

given by $\{x\colon w \cdot x = 0\} \mapsto w$. Correspondingly, there is a natural injection from hyperplanes $H \in W$ and vectors $x \in V$ given by $\{w\colon x \cdot w = 0\} \mapsto x$. If vector $x \in \{z\colon w \cdot z = 0\} \subseteq V$, then $w \cdot x = 0$, so $w \in \{y \cdot x \cdot y = 0\} \subseteq W$. If we want to enforce the inequality $x \cdot w \geq 0$, then

- in V, x should be on the same size of $\{z\colon w \cdot z = 0\}$ as w, and
- in W, w should be on the same side of $\{z\colon x \cdot z = 0\}$ as x.

Enforcing these constraints gives a set of feasible weight vectors, each of these giving a classifier.

How do we solve this optimization problem? The idea is that we define a risk function R that is positive if some constraints are violated, and zero otherwise. Then we use optimization to choose w that minimizes R.

Define the loss function

$$L(z, y_i) = \begin{cases} 0, & y_i z \geq 0 \\ -y_i z, & \text{otherwise} \end{cases} = -\min(0, y_i z)$$

where z is the classifier's prediction, and y_i is the training label. If $\operatorname{sign}(z) = \operatorname{sign}(y_i)$, the loss function is 0. If z has the wrong sign, the loss function is positive. Now define the risk function (also known as the objective function, or cost function) given by

$$R(w) = \sum_{i=1}^{n} L(X_i \cdot w, y_i) = \sum_{i \in V} -y_i X_i \cdot w$$

where $V = \{i\colon y_i X_i \cdot w < 0\}$ is the set of indices of misclassified sample points.

If w classifies all $X_1, \ldots, X_n$ correctly, then $R(w) = 0$. Otherwise, $R(w) > 0$, and we want to find a better w. Our goal is to solve this optimization problem. To solve this optimization problem, we use an optimization algorithm.

Gradient Descent

Algorithm 2 Regular gradient descent algorithm.

Input: A convex objective function $f_X(w)\colon \mathbb{R}^d \to \mathbb{R}$ to be minimized, where $f_X(w^*) = 0$, a step size $\varepsilon \in \mathbb{R}_{>0}$.
Output: The minimizer w^* of $\sum_{i=1}^n f_{X_i}(w)$.
  $w \leftarrow$ randomly initialized weight vector.
  while $\sum_{i=1}^n f_{X_i}(w) > 0$ **do**
    $w \leftarrow w - \varepsilon \boldsymbol{\nabla}_w \left(\sum_{i=1}^n f_{X_i}(w)\right)$
  return w

In the case of perceptrons, a random weight initialization is not always that good; sometimes we want w to be set at some $y_j X_j$, so that the starting weight classifies at least one point correctly.

Also, as in the case of perceptrons, this algorithm is really slow; in particular, if V is the set of misclassified points, then the perceptron algorithm training takes $\mathcal{O}(nd)$ time per iteration.

We amend this algorithm to account for this by only evaluating the loss function on one data point per iteration:

Algorithm 3 Stochastic gradient descent algorithm.

Input: A convex objective function $f_X(w)\colon \mathbb{R}^d \to \mathbb{R}$ to be minimized, where $\sum_{i=1}^n f_{X_i}(w^*) = 0$, a step size $\varepsilon \in \mathbb{R}_{>0}$.
Output: The minimizer w^* of $\sum_{i=1}^n f_{X_i}(w)$.
$w \leftarrow$ randomly initialized weight vector.
while $\exists$ (X_i, y_i) s.t. $f_{X_i}(w) > 0$ **do**
  $w \leftarrow w - \varepsilon \boldsymbol{\nabla}_w f_{X_i}(w)$
return w

If the separating hyperplanes are all affine, we can just add on an extra 1 entry to each data point X, so $X_{\text{new}} = \begin{bmatrix} X \\ 1 \end{bmatrix}$, and the w vector will learn the affine intercept naturally.

Note that for the perceptron, $\boldsymbol{\nabla}_w f_{X_i}(w) = -\min(0, y_i X_i)$, and inputting this into stochastic gradient descent yields the perceptron algorithm.

Algorithm 4 The perceptron algorithm, via stochastic gradient descent.

Input: A set of linearly separable sample points $\{(X_i, y_i)\}_{i=1}^n$ where $X_i \in \{C_1, C_2\}$ and $y_i = 2\,\mathbb{1}(X_i \in C_1) - 1$, and a step size $\varepsilon \in \mathbb{R}_{>0}$.
Output: A linear decision function $f(x)$ that in the linearly separable case reduces to $f(x) = 2\,\mathbb{1}(X_i \in C_1) - 1$.
$w \leftarrow y_j X_j$ for some $j \in \{1, \ldots, n\}$.
$V \leftarrow \{(X_i, y_i)\colon y_i X_i \cdot w < 0\}$
while $|V| > 0$ **do**
  $(X_i, y_i) \leftarrow$ entry of V
  $w \leftarrow w + \varepsilon \min(0, y_i X_i)$
  $V \leftarrow \{(X_i, y_i)\colon y_i X_i \cdot w < 0\}$
return $f(x) \overset{\text{def}}{=} \operatorname{sign}(w \cdot x)$

Support Vector Machines

The support vector machine is like a perceptron, except there is a notion of a "best" separating hyperplane, whereas a perceptron just tries to get any separating hyperplane. In particular, we wish to find the best weight vector for a separating hyperplane.

Definition 18 (Margin). Assume that $\{(X_i, y_i)\}_{i=1}^n$ is a set of linearly separable sample points. Also let the decision boundary be L. Then the *margin* is the distance from the decision boundary to the nearest sample point, that is, $m = \min_{X_i} \min_{\ell \in L} d(X_i, \ell)$.

For a successful classifier, we want to find a decision boundary with a maximized margin. We wish to have at least a margin of $c > 0$, so we enforce that $y_i\,(w \cdot X_i + \alpha) \geq c$ for all $i \in \{1, \ldots, n\}$. Since this constraint doesn't change when $(w, \alpha, c) \mapsto (\frac{w}{c}, \frac{\alpha}{c}, 1)$ (dividing both sides by c), it suffices to have the constraint $y_i\,(w \cdot X_i + \alpha) \geq 1$. If $\|w\| = 1$, then the signed distance from the hyperplane $H = \{x\colon w \cdot x = 0\}$ to X_i is $d(H, X_i) = w \cdot X_i + \alpha$. Otherwise,

$$d(H, X_i) = \frac{w}{\|w\|_2} \cdot X_i + \frac{\alpha}{\|w\|_2}$$

Hence the margin is

$$\min_i \frac{1}{\|w\|_2} |w \cdot X_i + \alpha| \geq \min_i \frac{1}{\|w\|_2} = \frac{1}{\|w\|_2}$$

In this manner there exists a *slab* of width $\frac{2}{\|w\|_2}$ which has no sample points. To maximize the margin, we have

$$\max_w \frac{1}{\|w\|_2} = \min_w \|w\|_2 = \min_w \|w\|_2^2$$

with the constraints $y_i (X_i \cdot w + \alpha) \geq 1$ and is called a quadratic program in $d+1$ dimensions. Since $\|w\|_2^2$ is convex, it has one unique solution, which gives us a maximum margin classifier, also known as a hard-margin support vector machine.

We now discuss soft-margin support vector machines, which are a modification of maximum-margin classifiers (hard-margin support vector machines). They solve two problems of hard-margin support vector machines:

- Hard-margin support vector machines fail if the data is not linearly separable; soft-margin support vector machines do not fail.
- Hard-margin support vector machines are very sensitive to outliers; soft margin support vector machines do not.

What we will do today is develop a support vector machine that violates the margin. We introduce the slack of a variable, ξ_i, as conceptually the amount that the data point (X_i, y_i) can violate the margin by; in particular, $d(X_i, H) = \frac{\xi_i}{\|w\|_2}$. We minimize the total amount of slack. The constraints now take the form $y_i (X_i \cdot w + \alpha) \geq 1 - \xi_i$. We also have to impose the constraint that the slack variables are nonnegative, so to avoid some data points having lots of slack and others having none, i.e. $\xi_i \geq 0$. When the signed distance $d(X_i, H) \leq \frac{1}{\|w\|_2}$, then (X_i, y_i) is said to violate the margin. In the soft-margin SVM, the margin is actually just defined as $\frac{1}{\|w\|_2}$. To prevent overfitting in the slack terms, we add a loss function of the slack to the objective function. The optimization problem becomes

$$\begin{aligned} \text{minimize } & \|w\|_2^2 + C \sum_{i=1}^n \xi_i \\ \text{subject to } & y_i (X_i \cdot w + \alpha) \geq 1 - \xi_i \ \forall i \in [1, n] \\ & \xi_i \geq 0 \ \forall i \in [1, n] \end{aligned}$$

The value of C is chosen by validation and is not trained.

This optimization problem is called a *quadratic program* in $d+n+1$ dimensions, where $w \in \mathbb{R}^d$, $\alpha \in \mathbb{R}$, and $\xi \in \mathbb{R}^n$, where $(\xi)_i = \xi_i$. There are $2n$ constraints. A quadratic program has a quadratic objective function and linear constraints. Most quadratic programs the Hessian is also positive semidefinite, which basically means that the program is convex in all dimensions. In this case the Hessian is $\boldsymbol{\nabla}^2_{w,\xi} \left(\|w\|_2^2 + C \sum_{i=1}^n \xi_i \right) = \begin{bmatrix} 2I_d & 0_n \\ 0_n & 0_d \end{bmatrix}$ which is clearly positive semidefinite. The value $C > 0$ is a scalar regularization hyperparameter that trades off:

- the desire to maximize the margin against the desire to keep all the slack variables small
- the tendency to underfit (via misclassifying training data) against the tendency to overfit (via converging to a hard margin SVM).
- the small effect of outliers against a large effect of outliers
- more flat, linear boundaries against more sinuous boundaries

The last item really only applies for the special cases of nonlinear decision boundaries.

We now consider how to turn linear classifiers (such as hard-margin SVMs) into nonlinear classifiers (like neural networks). The main idea is to make nonlinear features that lift points into a higher dimensional space. Then in this higher dimensional space, we can apply a standard linear classifier to obtain the classification function. This has the same effect as a low-dimensional nonlinear classifier.

Example 19 (Parabolic Lifting Map). We're given some sample points $\{(X_i, y_i)\}_{i=1}^n$. We define the parabolic lifting map as $\Phi\colon \mathbb{R}^d \to \mathbb{R}^{d+1}$, characterized as $\Phi(X) = \begin{bmatrix} X \\ \|X\|_2^2 \end{bmatrix}$. This lifts X onto the paraboloid $X_{d+1} = \|X\|_2^2$. A linear classifier in $\mathbb{R}^{d+1}$, or Φ space, then it induces a spherical classifier in $\mathbb{R}^d$, or X space, or feature space.

Claim 20. The lifted points $\Phi(X_1), \ldots, \Phi(X_n)$ are linearly separable if and only if $X_1, \ldots, X_n$ are separable by a hypersphere (including degenerate hyperspheres, which are hyperplanes).

Proof. Consider a hypersphere in $\mathbb{R}^d$ with center c and radius rho. Then the points x inside the hypersphere take the form

$$\begin{aligned}
\rho^2 &> \|x - c\|_2^2 \\
&> \|x\|_2^2 - 2c \cdot x + \|c\|_2^2 \\
\rho^2 - \|c\|_2^2 &> \begin{bmatrix} -2c^\top & 1 \end{bmatrix} \begin{bmatrix} x \\ \|x\|_2^2 \end{bmatrix}
\end{aligned}$$

where $\begin{bmatrix} -2c^\top & 1 \end{bmatrix}$ is the normal vector in $\mathbb{R}^{d+1}$ to the paraboloid $x_{d+1} = \|x\|_2^2$, and $\begin{bmatrix} x \\ \|x\|_2^2 \end{bmatrix} = \Phi(x)$. Thus all points separable by a hypersphere in $\mathbb{R}^d$ are linearly separable under the map Φ in $\mathbb{R}^{d+1}$.

All of these steps are reversible, so all points linearly separable in $\mathbb{R}^{d+1}$ under the map Φ are separable by a hypersphere in $\mathbb{R}^d$. $\square$

Example 21 (Axis-Aligned Ellipsoid/Hyperboloid Decision Boundaries). Axis-aligned ellipsoids in d dimensions have the equation

$$\sum_{i=1}^{d} \sum_{j=0}^{2} w_{3(i-1)+j} x_i^j + \alpha = 0$$

We obtain the map $\Phi\colon \mathbb{R}^d \to \mathbb{R}^{2d}$ where $\Phi(X) = \begin{bmatrix} X_1^2 & \cdots & X_d^2 & X_1 & \cdots & X_d \end{bmatrix}^\top$. The hyperplane is $w \cdot \Phi(x) + \alpha = 0$.

Example 22 (Ellipsoid/Hyperboloid Decision Boundaries). Ellipsoids in d dimensions have the equation

$$\sum_{j_1, \ldots, j_d = 0}^{2} w_{j_1, \ldots, j_d} \prod_{i=1}^{d} x_i^{j_i} + \alpha = 0$$

We obtain the map $\Phi\colon \mathbb{R}^d \to \mathbb{R}^{(d^2+3d)/2}$ by $\Phi(x) = \begin{bmatrix} X_1^2 & \cdots & X_d^2 & X_1X_2 & \cdots & X_{d-1}X_d & \cdots & X_1 & \cdots & X_d \end{bmatrix}^\top$. The hyperplane is $w \cdot \Phi(x) + \alpha = 0$.

The isosurface defined by this equation is called a quadric; when $d = 2$ the isosurfaces are conic sections.

Example 23 (Polynomial Decision Function). Let the degree of the polynomial we want be p. Then the mapping is $\Phi(X) = \begin{bmatrix} X_1^p & \cdots & X_d^p & \cdots \prod_{i=1}^d X_i^{j_i} & \cdots & X_1 & \cdots & X_d \end{bmatrix}^\top$. This mapping is $\Phi\colon \mathbb{R}^d \to \mathbb{R}^{\mathcal{O}(d^p)}$. This blows up, but we will use the "kernel trick" to compute these values later.

Example 24 (Edge Detection). Define an edge detector to be an algorithm for approximating grayscale/-color gradients in an image, i.e. top filter, Sibel filter, oriented Gaussian derivative filter. We collect the line orientations in local histograms (each having 12 orientation bins per region); then the histograms can be used as features, instead of raw features.

4 Abstractions

We can think of several different abstractions of machine learning. Most of the things we do resolve into four different layers of abstractions.

The top level is the application (i.e. the problem that we're trying to solve) and the data that we're given. The question we want to ask is is our data labeled (with a class or numerical score), or not?

- If the answer is yes, then the labels might be categorical (indicating a classification application) or quantitative (indicating a regression application).
- If the answer is no, then the problem is either identifying similarities within the data (indicating a clustering application) or relative positioning within the data (indicating a dimensionality reduction algorithm).

The second level is the model. A model is either parametric (a model can be characterized by a set of parameters, like weights) or non-parametric. A model consists of either:

- In a parametric model, there are decision functions (linear, polynomial, logistic, neural networks, etc.).
- In a non-parametric model, we make decisions based on data (nearest neighbors, decision trees, random forests, etc.).
- Features.
- Low vs. high capacity (which affects overfitting, underfitting, and inference).

The third level is the optimization problem. An optimization problem consists of variables, objective function, and constraints (for example, unconstrained optimization, a convex program, least squares regression, principal component analysis).

The fourth level is the optimization algorithm that solves the optimization problem. This can be gradient descent for differentiable problems, or the simplex method for programs, or the singular value decomposition.

We will discuss what optimization algorithms we have and which problems are prototypical in the space.

5 Optimization Algorithms

Unconstrained Optimization

We have a continuous objective function $f(w)$. Our goal is to find $w^* = \operatorname{argmin}_w f(w)$.

We have some definitions here for posterity. Call a function $f\colon \mathbb{R}^d \to \mathbb{R}$ Shewchuk-smooth if $f \in C^1$ (its first derivative is continuous). With respect to a function $f \in \mathbb{R}^d \to \mathbb{R}$, call x a global minimum if $f(x) \leq f(y)$ for each $y \in \mathbb{R}^d$, and call x a global minimum if there exists $\varepsilon > 0$ such that for every Δ with $\|\Delta\|_2 = \varepsilon$ we have $f(x) \leq f(x + \Delta)$.

Definition 25 (Convexity). A set $S \in V$, where V is a vector space, is *convex* if $\forall x, y \in S$,

$$\alpha x + (1 - \alpha)\, y \in S.$$

A function $f\colon \mathbb{R}^d \to \mathbb{R}$ is convex if for every $x, y \in \mathbb{R}^d$,

$$f(\alpha x + (1 - \alpha)\, y) \geq \alpha f(x) + (1 - \alpha)\, f(y).$$

A convex function has either

- no minimum (for every $\varepsilon > 0$ there exists x such that $f(x) < -\varepsilon$), or
- just one local minimum, in which case it is also the global minimum, or
- a connected (and path connected) set S of local minima that are all gloabl minima.

If f is smooth, we can use the optimization methods:

- Gradient descent:
  - The blind algorithm found here: Section 3
  - With line search:
    - Secant method
    - Newton-Raphson method (which may need the Hessian matrix $\nabla_x^2 f(x)$)
  - Stochastic (blind) gradient descent, found here: Section 3
- Newton's method (needing the Hessian matrix $\nabla_x^2 f(x)$)
- Nonlinear conjugate gradient

If f is non-smooth, we can use the optimization methods:

- Gradient descent:
  - The blind algorithm found here: Section 3
  - With direct line search (e.g. golden section search)
- BFGS

We discussed line search a lot; line search picks the direction of steepest descent, then along this one-dimensional manifold we solve the optimization problem using one-dimensional methods.

Constrained Optimization

Like before, we have a continuous objective function $f(w)$. We also have a continuous constraint function $g(w) = 0$, which describes an isosurface.

One of the methods we can use is Lagrange multiplication, where we have $\nabla_w f(w) = \lambda \nabla_w g(w)$; solving for the optimal λ^* and then w^* finds the constrained optimum.

Another algorithm we can use is that of a linear program. A linear program has a linear objective function $f(w) = c^\top w$, and linear inequality constraints $Aw \leq b$, where $A \in \mathbb{R}^{n \times d}$ and $b \in \mathbb{R}^n$. Formally, we write the linear program as

$$\begin{aligned} \text{minimize } & c^\top x \\ \text{subject to } & Ax \leq b \end{aligned}$$

Each linear inequality $a_{:,i}^\top w \leq b_i$ separates the space into two half-spaces. The set of points w that satisfy all constraints is a convex polytope called the feasible region. We call the feasible region $\mathscr{F}$. The optimal $w \in \mathscr{F}$ is the $x \in \mathscr{F}$ furthest in the direction of c. The optimum w achieves equality for some constraints (called the active constraints) but not most.

Example 26. The support vector machine, which is a quadratic program, can be turned into a (crappy) linear program:

$$\begin{aligned} \text{maximize}_{w,\alpha} \ & 0 \\ \text{subject to } & y_i \left(w \cdot X_i + \alpha \right) \geq 1 \ \forall i \in [1, n] \end{aligned}$$

In this example, every feasible point (w, α) gives a linear classifier. The data are linearly separable if and only if $\mathcal{F} \neq \emptyset$. This is also true for the regular (quadratic) support vector machine.

Linear programs can be solved via simplex method, or interior point methods.

A quadratic program is the same as a linear program, except the objective function can be quadratic and convex. Formally, we write that

$$\begin{aligned} \text{minimize } & x^\top Q x + c^\top x \\ \text{subject to } & Ax \leq b \end{aligned}$$

where Q is a symmetric positive definite matrix (a positive definite matrix has $x^\mathsf{T} Q x > 0$ for all $x \neq 0$). This program has only one local minimum, and therefore a global minimum.

If Q is indefinite (has negative eigenvalues), then the problem is NP-hard. If Q is positive semidefinite, then the objective function has multiple local minima, but the problem is not too hard to solve.

Example 27. The hard-margin support vector machine is a quadratic program:

$$\begin{aligned} &\text{maximize } \|w\|_2^2 \\ &\text{subject to } y_i\left(w \cdot X_i + \alpha\right) \geq 1 \ \forall i \in [1, n] \end{aligned}$$

and so is the soft-margin support vector machine:

$$\begin{aligned} &\text{maximize } \|w\|_2^2 + C\sum_{i=1}^{n} \zeta_i \\ &\text{subject to } y_i\left(w \cdot X_i + \alpha\right) \geq 1 - \zeta_i \ \forall i \in [1, n] \\ &\zeta_i \geq 0 \ \forall i \in [1, n] \end{aligned}$$

There are simplex-like algorithms to solve quadratic programs, but there are special algorithms to solve support vector machines.

Also, the feasible regions in the linear program are equivalent to to the support vectors in the dual linear program.

6 Decision Theory

Our linear algorithms work well enough for "nice" data, but fails on real-world data. For example, we could have multiple sample points at the same Euclidean coordinate, but in different classes. To this end, we assume that the data comes from several different but overlapping distributions, one per class, and attempt to determine the distributions, which gives us a probabilistic classifier.

Example 28. Suppose some of the population has cancer ($Y = 1$) and the rest does not ($Y = -1$). Suppose we know $p_{X|Y}(x \mid y)$, where X is a random variable denoting the person's caloric intake. Recall that $p_Y(1) = \int_x p_{Y|X}(1 \mid x) p_X(x) \, \mathrm{d}x$; this gives us the probability that a person overall has cancer.

Theorem 29

Let X and Y be two random variables. Then

$$p_{Y|X}(y \mid x) = \frac{p_{X|Y}(x \mid y) p_Y(y)}{p_X(x)}$$

where p_X is the density of X, and so on. The density $p_{Y|X}(y \mid x)$ is the *posterior probability* of y given x; the density $p_Y(y)$ is the *prior probability* of y.

Theorem 29

Definition 30 (Loss Function). A *loss function* $L(x_c, x)$ specifies the penalty to the classifier if the classifier predicts x_c and the true class is x.

Usually $L(x, x) = 0$.

Definition 31 (Symmetric Loss Function). A *symmetric loss function* L has that there exists ℓ such that $L(x_c, x) = \ell$ for every x and every $x_c \neq x$ (that is, the penalty for a wrong guess is constant).

The most popular classification function is the *zero-one loss function*, which has $L(x_c, x) = \mathbb{1}(x_c \neq x)$.

Definition 32 (Risk). Let $r\colon \mathbb{R}^d \to \{-1, 1\}$ be a decision rule. Then the *risk* for r is the expected loss over all values of x and y:

$$R(r) = \mathrm{Ex}[L(r(X), Y)]$$

The *frequentist risk* is given by taking the expectation over the support of $p_{X,Y}(x, y)$:

$$R_{\mathrm{freq}}(r) = \mathrm{Ex}_{(X,Y)\sim p_{X,Y}(\cdot,\cdot)}[L(r(X), X)]$$

The *Bayesian risk* or *empirical risk* is given by taking the expectation over the data distribution:

$$R_{\mathrm{Bayes}}(r) = \mathrm{Ex}_{(X,Y)\sim p_{\mathrm{data}}(\cdot,\cdot)}[L(r(X), X)]$$

Definition 33 (Bayes Decision Rule). The Bayes decision rule, or the Bayes classifier, is the function r^* such that $r^* = \mathrm{argmin}_r\, R(r)$. Indeed,

$$r^*(x) = \operatorname*{argmax}_y \int_z L(y, z) p_{Y|X}(z \mid x)\, \mathrm{d}z\,.$$

When L is a symmetric loss function, we pick the class y with the biggest posterior probability, $p_{Y|X}(y \mid x)$.

The *Bayes classifier* has the optimal risk of any classifier.

Deriving and using r^* is called *risk minimization*. In the case where there are two classes $\{-1, 1\}$ and $L(y, y) = 0$, the Bayes classifier is

$$r^*(x) = \max\left(L(1, -1)p_{Y|X}(-1 \mid x), L(-1, 1)p_{Y|X}(1 \mid x)\right)$$

and

$$R_{\mathrm{Bayes}}(r^*) = \int_x \min_{y=\pm 1} L(-y, y) p_{X|Y}(x \mid y) p_Y(y)\, \mathrm{d}x$$

If L is the zero-one loss, then

$$R(r) = \mathrm{Pr}_{(X,Y)\in p_{X,Y}(\cdot,\cdot)}[r(x) \neq y]$$

and the Bayes optimal decision boundary is

$$\left\{x\colon\ \mathrm{Pr}_{(X,Y)\sim p_{X,Y}(\cdot,\cdot)}[Y = 1 \mid X = x]\right\} = \frac{1}{2}.$$

Note that this is an isocontour.

There are three ways to build classifiers:

- *Generative models* (e.g. linear discriminant analysis)
  - We assume that the sample points come from some probability distribution, and each class has its own probability distribution.
  - Guess the form of distribution (i.e. put a prior distribution on each class).
  - For each class C, we fit the distribution parameters to class C points, giving $p_{X|Y}(x \mid C)$.
  - We also estimate the prior distribution $p_Y(C)$.
  - Bayes' Theorem gives $p_{Y|X}(C \mid x)$.
  - If the loss is zero-one loss, we pick $C = \mathrm{argmax}_c\, p_{Y|X}(c \mid x) = \mathrm{argmax}_c\, p_{Y|X}(c \mid x) p_Y(c)$
- *Discriminative models* (e.g. logistic regression)
  - Model $p_{Y|X}(C \mid x)$ directly.
- Find the decision boundary (e.g. SVM)
  - Model $r(x)$ directly (no posterior distribution).

The advantage of generative and discriminative models is that $p_{Y|X}(C \mid x)$ tells us the probability that we are correct, which can be useful. Generative models give us a great way to diagnose outliers, with $p_X(x) \ll 1$ being an indicator of the outlier. However, it's often really hard to estimate distributions accurately, and real distributions rarely match the standard distributions we impose as priors.

7 Discriminant Analysis

Gaussian Discriminant Analysis

In this section, we assume that each class is distributed normally, and the distribution for each class C is different.

The density for the multivariate Gaussian is as follows. If $X \mid Y \sim \text{Normal}(\mu_Y, \Sigma_Y)$, then

$$p_{X|Y}(x \mid C) = \frac{1}{\left(\sqrt{2\pi \det(\Sigma_C)}\right)^d} \exp\left(-\frac{1}{2}(x-\mu_C)^\top \Sigma_C^{-1}(x-\mu_C)\right)$$

If $\Sigma_C = \sigma_C^2 I$ (an *isotropic* Gaussian), then

$$p_{X|Y}(x \mid C) = \left(\sqrt{2\pi\sigma_C^2}\right)^{-d} \exp\left(-\frac{\|x-\mu_C\|^2}{2\sigma_C^2}\right)$$

For each class $C \in \mathcal{C}$, suppose we estimate the mean $\hat{\mu}_C = \mathrm{Ex}_{(X,C)\sim p_{\text{data}}}[X]$, variance $\hat{\sigma}_C^2 = \mathrm{Ex}_{(X,C)\sim p_{\text{data}}}[x]$, and prior $\hat{\pi}_C = p_Y(C)$. Also assume that the risk function is symmetric. Then the Bayes decision rule gives

$$\begin{aligned}
r^*(x) &= \operatorname*{argmax}_{C\in\mathcal{C}} \frac{p_{X|Y}(x \mid C)\hat{\pi}_C}{p_Y(C)} \\
&= \operatorname*{argmax}_{C\in\mathcal{C}} p_{X|Y}(x \mid C)\hat{\pi}_C \\
&= \operatorname*{argmax}_{C\in\mathcal{C}} \log\left(p_{X|Y}(x \mid C)\right) + \log(\hat{\pi}_C) \\
&= \operatorname*{argmax}_{C\in\mathcal{C}} -\frac{\|x-\mu_C\|_2^2}{2\sigma_C^2} - d\log(\sigma_C) + \log(\hat{\pi}_C)
\end{aligned}$$

Suppose there are only two classes $\mathcal{C} = \{C, D\}$. Then if we define

$$Q_A(x) = -\frac{-\|x-\mu_A\|_2^2}{2\sigma_A^2} - d\log(\sigma_A) + \log(\hat{\pi}_A)$$

the Bayes classifier is

$$r^*(x) = \begin{cases} C, & Q_C(x) > Q_D(x) \\ D, & Q_C(x) < Q_D(x) \end{cases}$$

To recover the posterior probabilities, we use Bayes theorem. In particular, we have

$$p_{Y|X}(C \mid x) = \frac{p_{X|Y}(x \mid C)p_Y(C)}{\sum_{A\in\mathcal{C}} p_{X|Y}(x \mid A)p_Y(A)} = \frac{\mathrm{e}^{Q_C(x)}/\sqrt{2\pi}^d}{\sum_{A\in\mathcal{C}} \mathrm{e}^{Q_A(x)}/\sqrt{2\pi}^d} = \frac{\mathrm{e}^{Q_C(x)}}{\sum_{A\in\mathcal{C}} \mathrm{e}^{Q_A(x)}}$$

Again let $C = \{C, D\}$. Then

$$p_{Y|X}(C \mid x) = \frac{\mathrm{e}^{Q_C(x)}}{\mathrm{e}^{Q_C(x)} + \mathrm{e}^{Q_D(x)}} = \frac{1}{1+\mathrm{e}^{Q_D(x)-Q_C(x)}} = \sigma(Q_C(x) - Q_D(x))$$

where $\sigma(x) = \frac{1}{1+\mathrm{e}^{-x}}$.

Linear Discriminant Analysis

The linear discriminant analysis is a variant of Gaussian discriminant analysis. The additional assumption is that all the class Gaussians have the same variance σ^2. In this case it's harder to overfit because there are fewer parameters. Indeed, in the two-class case,

$$Q_C(x) - Q_D(x) = \underbrace{\frac{\langle \mu_C - \mu_D | x \rangle}{\sigma^2}}_{\langle w|x \rangle} - \underbrace{\frac{\|\mu_C\|^2 - \|\mu_D\|^2}{2\sigma^2} + \log(\hat{\pi}_C) - \log(\hat{\pi}_D)}_{\alpha}$$

Now it's a linear classifier. The linear discriminant function is

$$L_C(x) = \frac{\langle \mu_C | \sigma^2 \rangle}{\sigma^2} - \frac{\|\mu_C\|^2}{2\sigma^2} + \log(\hat{\pi}_C)$$

Then the classifier is $r(x) = \operatorname{argmax}_{C \in \mathcal{C}} L_C(x)$. In the two-class case, the decision boundary is $\langle w|x \rangle + \alpha = 0$ and the posterior distribution is $p_{Y|X}(C \mid x) = \sigma(\langle w|x \rangle + \alpha)$.

The linear discriminant analysis has a geometric description in the form of Voronoi diagrams; a point is classified to the closest μ_C for $C \in \mathcal{C}$. Also, in the two-class case, if $\hat{\pi}_C = \hat{\pi}_D = \frac{1}{2}$, then by simple algebraic manipulation the linear discriminant rule degenerates to the centroid classifier (Section 3).

It's important to know that $e^{Q_C(x)} \propto p_{X,Y}(x, C)$, and in a sense we're picking the most likely class for the data x.

8 Parameter Estimation

We use maximum likelihood estimation for parameters.

Definition 34 (Maximum Likelihood Estimation). Given a process, we want to estimate a parameter Y given an outcome $X = x$. Then $\mathrm{MLE}(Y \mid X) = \operatorname{argmax}_y p_{X|Y}(X \mid y)$.

Since the density is smooth, it's usually easy to optimize $p_{X|Y}$ via calculus methods.

Example 35 (Gaussian Fitting). Given sample points $X_1, \ldots, X_n$, we want to find the best fit normal distribution. Then

$$\begin{aligned}
\mathrm{MLE}(\mu, \sigma \mid X_1, \ldots, X_n) &= \operatorname*{argmax}_{\mu,\sigma} p_{X_1,\ldots,X_n|\mu,\sigma^2}\left(X_1, \ldots, X_n \,\middle|\, \mu, \sigma^2\right) \\
&= \operatorname*{argmax}_{\mu,\sigma} \prod_{i=1}^{n} p_{X_i|\mu,\sigma^2}\left(X_i \,\middle|\, \mu, \sigma^2\right) \\
&= \operatorname*{argmax}_{\mu,\sigma} \sum_{i=1}^{n} \log\left(p_{X_i|\mu,\sigma^2}\left(X_i \,\middle|\, \mu, \sigma^2\right)\right) \\
&= \sum_{i=1}^{n} \left(-\frac{\|X_i - \mu\|^2}{2\sigma^2} - d\log\left(\sqrt{2\pi}\right) - d\log(\sigma)\right)
\end{aligned}$$

We want to set $\boldsymbol{\nabla}_\mu \mathrm{MLE}(\mu, \sigma^2 \mid X_1, \ldots, X_n) = 0$ and $\boldsymbol{\nabla}_\sigma \frac{\partial \mathrm{MLE}\left(\mu, \sigma^2 \,\middle|\, X_1, \ldots, X_n\right)}{\partial \sigma^2} = 0$. From the first equation we have

$$\begin{aligned}
\boldsymbol{\nabla}_\mu \mathrm{MLE}\left(\mu, \sigma^2 \,\middle|\, X_1, \ldots, X_n\right) &= \sum_{i=1}^{n} \frac{X_i - \mu}{\sigma^2} \\
&\overset{\text{set}}{=} 0\hat{\mu} && = \frac{1}{n}\sum_{i=1}^{n} X_i
\end{aligned}$$

and from the second equation we have

$$\frac{\partial \operatorname{MLE}(\mu, \sigma^2 \mid X_1, \dots, X_n)}{\partial \sigma} = \sum_{i=1}^{n} \frac{\|X_i - \mu\|_2^2 - d\sigma^2}{\sigma^3}$$

$$\stackrel{\text{set}}{=} 0\hat{\sigma}^2 \qquad = \frac{1}{dn}\sum_{i=1}^{n} \|X_i - \mu\|_2^2$$

We don't know μ exactly, so in practice we substitute $\hat{\mu}$.

For QDA, we estimate the conditional mean $\hat{\mu}_C$ and conditional variance $\hat{\sigma}_C^2$ for each class C separately, and estimate the prior $\hat{\pi}_C = \frac{|\{X_i\}|}{|\{X_i \in \mathcal{C}\}|}$.

For LDA, we use the same means and priors as QDA, but we estimate the one variance for all classes:

$$\hat{\sigma}^2 = \frac{1}{dn}\sum_{C \in \mathcal{C}} \sum_{\{i \colon Y_i = C\}} \|X_i - \hat{\mu}_C\|^2$$

when the inner sum is a constant multiple of the pooled within-class variance.

9 Anisotropic Multivariate Gaussians

Some linear algebraic facts to know:

- If v is an eigenvector of A with eigenvalue λ, then v is an eigenvector of A^k with eigenvalue λ^k.
- If A is invertible and v is an eigenvector of A with eigenvalue λ, then v is an eigenvector of A^{-1} with eigenvalue λ^{-1}.
- Every real, symmetric $n \times n$ matrix has real eigenvalues and n eigenvectors that are mutually orthogonal (this is the Spectral Theorem). In general a matrix can have more than n eigenvectors if its eigenspaces are not orthogonal and there exists a plane of eigenvectors in their intersection.

One of the more useful ways to visualize a symmetric matrix is via quadratic forms. Take the function $f(z) = \|z\|_2^2 = z^\mathsf{T} z$; this is quadratic and isotropic, where the isosurfaces are hyperspheres. More to the point, the function $f(x) = x^\mathsf{T} A^{-2} x = \|A^{-1}x\|_2^2$ is the quadratic form of the matrix A^{-2} (assuming that A is symmetric). This quadratic form is anisotropic, and the isosurfaces are ellipsoids. In particular, the canonical isosurface representation of the quadratic form is $\|A^{-1}x\|_2^2 = 1$. The axes of this quadratic form are the eigenvectors of A, and the lengths of the axes are the corresponding eigenvalues of A (because if v_i axis has length λ_i, $\|A^{-1}v_i\|_2^2 = \left\|\frac{1}{\lambda_i} v_i\right\|_2^2 = 1$, so v_i lies on the ellipsoid). The sign of the product of the eigenvalues determines the handedness of the coordinate system. Correspondingly, if A is diagonal, then the eigenvectors are the coordinate axes (and the isosurface ellipsoids are axis aligned).

Recall that if A is symmetric and has all positive eigenvalues then A is *positive definite*, and $x^\mathsf{T} M x > 0$ for all $x \neq 0$. If A has non-negative eigenvalues then A is *positive semi-definite*, and $x^\mathsf{T} A x \geq 0$ for all x. If A has at least one positive and at least one negative eigenvalue, then A is *indefinite*. If A has no zero eigenvalue then it is invertible in any case.

Quadratic forms $f(x) = x^\mathsf{T} A x$ with A positive definite have one minimum x^*; if A is positive semidefinite then there are infinitely many minima which lie on an affine hyperplane with number of parameters equal to the number of indices i such that $\lambda_i = 0$; if A is indefinite than the quadratic form has no minimum value (and can grow arbitrarily negative).

We've been dealing with the quadratic form $f(x) = x^\mathsf{T} M x$ (with M some PD/PSD/ID matrix) instead of $f(x) = x^\mathsf{T} A^{-2} x$, which generates the ellipse as an isocontour. It should be easy to see that if the original quadratic from is $x^\mathsf{T} M x$ then $M = A^{-2}$ and $A = M^{-1/2}$, which means that M has the same eigenvectors as A so $v_i(A) = v_i(M)$ but $\lambda_i(A) = \frac{1}{\sqrt{\lambda_i(M)}}$. Therefore M is PD/PSD/ID if and only if A is PD/PSD/ID respectively.

We now cover eigendecomposition of symmetric A, which is trivial so I won't write it here.

Given a symmetric PSD matrix $\Sigma = U\Lambda U^\top$, we can find the symmetric square root $\Sigma^{1/2} = U\Lambda^{1/2}U^\top$.

Finally, we begin discussing anisotropic Gaussians. Let $X \sim \text{Normal}(\mu, \Sigma)$ have an anisotropic distribution over $\mathbb{R}^d$. Then

$$p_X(x) = \frac{1}{\left(\sqrt{2\pi}\right)^d \sqrt{\det(\Sigma)}} \exp\left(-\frac{(x-\mu)^\top \Sigma^{-1} (x-\mu)}{2}\right)$$

where Σ is the $d \times d$ symmetric positive definite covariance matrix. Correspondingly, Σ^{-1} is the $d \times d$ symmetric positive definite *precision* matrix. Let $q(x) = (x-\mu)^\top \Sigma^{-1} (x-\mu)$; we understand this function, since it is a quadratic form. The isosurfaces of $q(x)$ are the same as $p_X(x)$ since the rest of the function is monotonic $\mathbb{R} \to \mathbb{R}$.

The covariance matrix Σ has eigenvalues that are the variances along the eigenvectors. The square root $\Sigma^{1/2}$ maps spheres to ellipsoids; the eigenvalues of $\Sigma^{1/2}$ are Gaussian widths/ellipsoid axis radii/standard deviations along the axes.

Since $\Sigma = U\Lambda U^\top$, $\Sigma^{-1} = U\Lambda^{-1}U$.

We're dealing with anisotropic Gaussians, so the parameter estimation might be different.

Let $X_1, \ldots, X_n$ be sample points wiht classes $y_1, \ldots, y_n$.

For quadratic discriminant analysis, we have that the estimated covariance for class C is

$$\hat{\Sigma}_C = \frac{1}{|\{i : y_i = C\}|} \sum_{i : y_i = C} (X_i - \hat{\mu}_C)(X_i - \hat{\mu}_C)^\top = \frac{\left(X_C - 1\mu_C^\top\right)\left(X_C - 1\mu_C^\top\right)^\top}{|\{i : y_i = C\}|}$$

where X_C is the matrix of data points that are class C. For completeness,

$$\hat{\mu}_C = \frac{1}{|\{i : y_i = C\}|} \sum_{i : y_i = C} X_i$$

and

$$\hat{\pi}_C = \frac{|\{i : y_i = C\}|}{n}$$

For linear discriminant analysis, we have that the estimated total covariance is just

$$\hat{\Sigma} = \frac{1}{n} \sum_{C \in \mathcal{C}} \sum_{i : y_i = C} (X_i - \hat{\mu}_C)(X_i - \hat{\mu}_C)^\top = \frac{1}{n} \sum_{C \in \mathcal{C}} \left(X_C - 1\hat{\mu}_C^\top\right)\left(X_C - 1\hat{\mu}_C^\top\right)^\top$$

which is the *pooled-within-class* covariance matrix.

Choosing the C that maximizes the estimated $p_{X,Y}(x, C)$ is equivalent to maximizing the *quadratic discriminant function*

$$Q_C(x) = \log\left(\left(\sqrt{2\pi}\right)^d p_{X|Y}(x \mid C)\hat{\pi}_C\right) = -\frac{1}{2}(x - \hat{\mu}_C)^\top \hat{\Sigma}_C^{-1} (x - \hat{\mu}_C) - \frac{1}{2}\log\left(\det\left(\hat{\Sigma}_C\right)\right) + \log(\hat{\pi}_C)$$

In the case of $|\mathcal{C}| = 2$ the Bayes decision boundary is a quadric.

In the case of linear discriminant analysis where the Gaussians have the same covariance, the *linear discriminant function* is

$$L_C(x) = \hat{\mu}_C^\top \hat{\Sigma}^{-1} x - \frac{1}{2}\hat{\mu}_C^\top \hat{\Sigma}^{-1} \hat{\mu}_C + \log(\pi_C)$$

Sometimes LDA (in a two-class classification scheme) is inteprreted as projecting points onto the normal w, where $w^\top = (\hat{\mu}_C - \hat{\mu}_D)^\top \Sigma^{-1}$.

LDA only has $d + 1$ parameters (in the two-class case), whereas QDA has $\frac{d(d+3)}{2} + 1$ parameters. QDA is more likely to overfit.

10 Regression

In classification, given a point x, we want to predict a class (often a binary decision problem). In regression, given a point x, we wish to predict a numerical value. We want to choose a form of the regression function $h_\theta(x)$, where h is a hypothesis on the regression function form, parameterized by θ. This regression function is like a decision function in classification. We choose a cost function (objective function) to optimize; usually this is a sum of loss functions that evaluate the loss at one data point at a time.

Some regression functions are:

- Linear regression: $h_\theta(x) = \theta^\top x$ (x is usually augmented with a 1 vector to find an affine regressor).
- Polynomial regression, which is linear regression with polynomial features.
- Logistic regression: $h_\theta = \sigma\left(\theta^\top x\right)$, where $\sigma(x) = \frac{1}{1+e^{-x}}$, and x is usually augmented.

Let y be the true label for point x. Some loss functions are:

- Squared error: $L(h_\theta(x), y) = (h_\theta(x) - y)^2$.
- Absolute error: $L(h_\theta(x), y) = |h_\theta(x) - y|$.
- Logistic error, or cross-entropy: $L(h_\theta(x), y) = -y \log(h_\theta(x)) - (1-y)\log(1 - h_\theta(x))$.

Some cost functionals are

- Mean loss: $J(h_\theta) = \frac{1}{n}\sum_{i=1}^n L(h_\theta(X_i), y_i)$.
- Maximum loss: $J(h_\theta) = \max_{1 \le i \le n} L(h_\theta(X_i), y_i)$.
- Weighted loss: $J(h_\theta) = \sum_{i=1}^n w_i L(h_\theta(X_i), y_i)$.
- ℓ^2-regularized mean loss: $J(h_\theta) = \lambda\|\theta\|_2^2 + \frac{1}{n}\sum_{i=1}^n L(h_\theta(X_i), y_i)$
- ℓ^1-regularized mean loss: $J(h_\theta) = \lambda\|\theta\|_1 + \frac{1}{n}\sum_{i=1}^n L(h_\theta(X_i), y_i)$

Some famous regression methods are:

- Least-squares linear regression: linear regression function, squared error, mean loss.
- Weighted least-squares linear regression: linear regression function, squared error, weighted sum loss.
- Ridge regression: linear regression function, squared error, ℓ^2-regularized mean loss.
- LASSO regression: linear regression function, squared error, ℓ^1-regularized mean loss.
- Logistic regression: logistic regression function, cross-entropy error, mean loss.
- Least absolute deviation regression: linear regression function, absolute error, mean loss.
- Chebyshev criterion regression: linear regression function, absolute error, maximum loss.

The first three regression methods (least-squares linear regression, weighted least-squares linear regression, and ridge regression) give convex quadratic cost functions, and closed form solutions are possible. LASSO regression is often framed as a quadratic program, usually with an exponential number of constraints, and solved using those methods. Logistic regression has a convex cost function, and we minimize it via gradient descent. Least absolute deviation regression and Chebyshev criterion regression are formulated as linear programs and solved that way.

Linear Regression

Least-squares linear regression uses a linear regression function, squared loss function, and a mean loss cost functional. Without augmenting the data matrix$X$, the optimization problem is

$$\begin{aligned}(\theta_1^*, \theta_2^*) &= \operatorname*{argmin}_{\theta_1, \theta_2} \sum_{i=1}^n L(h_{\theta_1,\theta_2}(X_i), y_i) \\ &= \operatorname*{argmin}_{\theta_1, \theta_2} \sum_{i=1}^n \left(\theta_1^\top X_i + \theta_2 - y_i\right)^2\end{aligned}$$

$$
\begin{aligned}
&= \operatorname*{argmin}_{\theta_1, \theta_2} \sum_{i=1}^{n} \left(\begin{bmatrix} \theta_1^\mathsf{T} & \theta_2^\mathsf{T} \end{bmatrix} \begin{bmatrix} X_i \\ 1 \end{bmatrix} \right)^2 \\
&= \operatorname*{argmin}_{\theta_1, \theta_2} \left\| \begin{bmatrix} X & 1 \end{bmatrix} \begin{bmatrix} \theta_1 \\ \theta_2 \end{bmatrix} - y \right\|_2^2 \\
&\overset{\text{set}}{=} \operatorname*{argmin}_{\theta_1, \theta_2} \operatorname{RSS}\left(\begin{bmatrix} \theta_1 \\ \theta_2 \end{bmatrix} \right)
\end{aligned}
$$

Define $\theta = \begin{bmatrix} \theta_1 \\ \theta_2 \end{bmatrix}$ and augment X, so $X = \begin{bmatrix} X & 1 \end{bmatrix}$. Then

$$
\begin{aligned}
\theta^* &= \operatorname*{argmin}_{\theta} \operatorname{RSS}(\theta) \\
\nabla_\theta \operatorname{RSS}(\theta) &= 2X^\mathsf{T} X\theta - 2X^\mathsf{T} y \\
&\overset{\text{set}}{=} 0 \\
X^\mathsf{T} X \theta^* &= X^\mathsf{T} y
\end{aligned}
$$

If $X^\mathsf{T} X$ is singular, then the problem is underconstrained, so we can use Cholesky decomposition, LU decomposition, conjugate gradient method, etc. that solves for θ. Otherwise, we can do $\theta^* = \left(X^\mathsf{T} X\right)^{-1} X^\mathsf{T} y$. If X is very large, we can solve the implied linear system instead of worrying about the inverse. The term $X^+ = \left(X^\mathsf{T} X\right)^{-1} X^\mathsf{T}$ is the *left pseudoinverse* of X, because $X^+ X = I$ when X is full rank. The matrix $H = XX^+$ is called the *hat matrix*, because $\hat{y} = XX^+ y = Hy$. If $n > d + 1$ then H is singular.

The matrix $H = XX^+$ can be interepreted as an orthogonal projection from $\mathbb{R}^n$ onto $\mathbb{R}^{d+1}$, giving the normal equations $X^\mathsf{T} (X\theta - y) = 0$.

Logistic Regression

Logistic regression has the regression function $h_\theta = \sigma\left(\theta^\mathsf{T} x\right)$. It fits probabilities in the range $(0, 1)$, so it's used to fit a distribution. Usually it's used for classification; the input y_i's can be probabilities, but usually they're either 0 or 1.

Using the augmented X and θ, the optimization problem is

$$
\begin{aligned}
\theta^* &= \operatorname*{argmin}_{\theta} J(h_\theta) \\
&= -\operatorname*{argmin}_{\theta} \sum_{i=1}^{n} \left[y_i \log(h_\theta(X_i)) + (1 - y_i) \log(1 - h_\theta) \right]
\end{aligned}
$$

This cost function is convex, so we can solve it via gradient descent. First, note that $\nabla_x \sigma(x) = \sigma(x)(1 - \sigma(x))$. Then

$$
\begin{aligned}
\nabla_\theta \sum_{i=1}^{n} y_i \log(h_\theta(X_i)) + (1 - y_i) \log(h_\theta(X_i)) &= \sum_{i=1}^{n} y_i \log\left(\sigma\left(\theta^\mathsf{T} X_i\right)\right) + (1 - y_i) \log\left(\sigma\left(\theta^\mathsf{T} X_i\right)\right) \\
&= \sum_{i=1}^{n} \left(\frac{y_i}{\sigma(\theta^\mathsf{T} X_i)} - \frac{1 - y_i}{1 - \sigma(\theta^\mathsf{T} X_i)} \right) \sigma\left(\theta^\mathsf{T} X_i\right) \left(1 - \sigma\left(\theta^\mathsf{T} X_i\right)\right) X_i \\
&= \sum_{i=1}^{n} \left(y_i - \sigma\left(\theta^\mathsf{T} X_i\right) \right) X_i \\
&= X^\mathsf{T} (y - \sigma(X\theta))
\end{aligned}
$$

(In $\sigma(X\theta)$, the σ is applied componentwise.)

The gradient descent rule is $\theta \leftarrow \theta + \varepsilon X^\top (y - \sigma(X\theta))$.

If we want to incorporate polynomial features, we can add columns as features that are polynomial functions of the original features. We can also add non-polynomial features in this matter. Otherwise, the process is just like linear or logistic regression. Logistic regression and quadratic features in fact models quadratic discrimiinant analysis. Higher degree polynomials have very high possibility to overfit (because of the VC-dimension, but of course that won't be mentioned).

Another modification to least-squares regression is to weight each sample point, in weighted least-squares regression. We assign each sample point x_i a weight ω_i and collect them in $\Omega = \operatorname{diag}(\omega) \in \mathbb{R}^{n\times n}$. A greater value of w_i biases $(\hat{y}_i - y_i)^2$ to be smaller, where $\hat{y} = Xw$. The optimization problem is

$$w^* = \min_w (Xw - y)^\top \Omega (Xw - y) = \sum_{i=1}^{n} \omega_i (X_i \cdot w - y_i)^2$$

and the normal equations are $X^\top \Omega X w = X^\top \Omega y$.

Newton's Method

Newton's method is an iterative optimization method for a C^2 (twice differentiable) function $J(w)$ that works well for logistic regression, and in low-dimensional space works much faster than gradient descent. The basic idea is to approximate $J(w)$ near w by a quadratic function, then jump to its unique critical point. We use the Taylor quadratic approximation:

$$\boldsymbol{\nabla}_w J(w) = \boldsymbol{\nabla}_v J(v) + \left(\boldsymbol{\nabla}_v^2 J(v)\right)(w - v) + o\left(\|w - v\|_2^2\right)$$

Finding the critical point w sets $\boldsymbol{\nabla}_w J(w) = 0$, so $w = v - \left(\boldsymbol{\nabla}_v^2 J(v)\right)(\boldsymbol{\nabla}_v J(v))$

Algorithm 5 Newton's method.

Input: A convex twice-differentiable function $f(w)\colon \mathbb{R}^d \to \mathbb{R}$ to be minimized.
Output: A minimizer w^* of f.

```
w ← randomly initialized weight vector.
while ∇_w J(w) ≠ 0 do
    w ← w − (∇²_w J(w))^{−1} (∇_w J(w))
return w
```

Alternatively, if $\boldsymbol{\nabla}_w^2 J(w)$ is not invertible, then we have

Algorithm 6 Non-invertible Newton's method.

Input: A convex twice-differentiable function $f(w)\colon \mathbb{R}^d \to \mathbb{R}$ to be minimized.
Output: A minimizer w^* of f.

```
w ← randomly initialized weight vector.
while ∇_w J(w) ≠ 0 do
    e ← a "good" solution to the linear system (∇²_w J(w)) e = −∇_w J(w)
    w ← w + e
return w
```

The Newton's method doesn't know the difference between minima, maxima, and saddle points. The caveat is that the starting point must be "close enough" to the desired critical point.

Newton's method works specifically well for logistic regression. Recall that $\sigma(\gamma) = \sigma(\gamma)(1 - \sigma(\gamma))$ and define for convenience $s_i = \sigma\left(X_i^\top w\right)$ and $s = \begin{bmatrix} s_1 \\ \vdots \\ s_n \end{bmatrix}$. Then $\nabla_w J(w) = -\sum_{i=1}^n (y_i - s_i) X_i = -X^\top (y - s)$ and $\nabla_w^2 J(w) = \sum_{i=1}^n s_i (1 - s_i) X_i X_i^\top = X^\top \Omega X$ where $\Omega = \operatorname{diag}(s \otimes (1 - s))$. Clearly Ω is positive definite, so $X^\top \Omega X$ is positive semidefinite, so $J(w)$ is convex. This problem is weighted least squares, but since Ω changes on every iteration, this problem is iteratively weighted least squares. This penalizes points with $s_i \approx \frac{1}{2}$ and ignores points near 0 or 1. By contrast, even though the posteriors of discriminant analysis (LDA, QDA) are themselves logistic functions, LDA and QDA weight each point equally.

It's worthwhile to compare the two methods.

- Advantages of LDA:
  - For well-separated classes, LDA is stable; logistic regression is surprisingly unstable.
  - LDA and QDA extends easily and elegantly to multiple classes; logistic regression needs modifying (softmax regression).
  - LDA is more accurate when the conditional densities of the data are normal, especially if n is small.
- Advantages of logistic regression:
  - It puts more emphasis on the decision boundary, and creates the decision boundary around the variances in the points near to it. Therefore it's less sensitive to outliers far from the decision boundary.
  - It's more robust on some non-Gaussian distribution (one with skew).
  - Naturally fits labels between 0 and 1.

Normally, our binary classification boundary is where the probability of a point on the boundary being in either class is $\frac{1}{2}$. As we vary that, we can obtain new, possibly better, classifiers. In binary classification problems, the ROC curve plots the false positive rate $\text{FP} = \frac{|\{y_i : y_i = -1, f(X_i) = -1\}|}{|\{y_i : y_i = -1\}|}$ on the x-axis, against the true positive rate $\text{TP} = \frac{|\{y_i : y_i = 1, f(X_i) = 1\}|}{|\{y_i : y_i = 1\}|}$. The false negative rate is $\text{FN} = 1 - \text{TP}$ and the true negative rate is $\text{FN} = 1 - \text{FP}$. The sensitivity is the true positive rate and the false negative rate is the specificity. The points $(0, 0)$ and $(1, 1)$ are on the curve, representing the classifier that classifies any point as -1 and the classifier that classifies any point as 1. Any point (x, x) on the straight line line between $(0, 0)$ and $(1, 1)$ represents a classifier that randomly classes the proportion x of sample points as 1 and the rest -1. A good metric of the efficacy of your classifier is the area under the ROC curve.

Bias-Variance Decomposition

A typical data distribution model is that

- The sample X-values come from some unkown probability distribution: $X_i \sim \mathcal{D}$, for $\mathcal{D}$ a distribution.
- The Y-values are the sum of an unknown, non-random function, and random noise:

  $$Y_i = g(X_i) + \varepsilon_i$$

  where $g\colon \mathbb{R}^d \to \mathbb{R}$ and $\varepsilon_i \sim \mathcal{N}$, a noise distribution with 0 expectation.

The goal of regression is to find the $\hat{g}$ that best estimates g. The ideal approach is $\hat{g}(x) = \text{Ex}_{X \sim \mathcal{D}}[Y \mid X = x]$; this estimator is unbiased, since

$$\begin{aligned}
\hat{g}(X) &= \text{Ex}_{X \sim \mathcal{D}}[Y \mid X = x] \\
&= \text{Ex}_{X \sim \mathcal{D}}[g(X_i) + \varepsilon \mid X = x]
\end{aligned}$$

$$
\begin{aligned}
&= \mathrm{Ex}_{X\sim\mathcal{D}}[g(X_i) \mid X = x] + \mathrm{Ex}_{X\sim\mathcal{D}}[\varepsilon \mid X = x] \\
&= g(X)
\end{aligned}
$$

Of course, we don't have $\mathcal{D}$ to take the expectation over.

Suppose $\mathcal{N} = \mathrm{Normal}(0, \sigma^2)$, i.e. our noises are normally distributed. Then $Y_i \mid X_i \sim \mathrm{Normal}(g(X_i), \sigma^2)$. Then

$$
\begin{aligned}
p_{Y|X}(y \mid x) &= \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{(y_i - g(x_i))^2}{2\sigma^2}\right) \\
\log\left(p_{Y|X}(y \mid x)\right) &= -\frac{(y_i - g(x_i))^2}{2\sigma^2} - C && \text{(C is some constant.)} \\
\ell(g \mid (X_i, Y_i)_{i=1}^n) &= \log\left(\prod_{i=1}^n p_{Y|X}(y_i \mid x_i)\right) \\
&= \sum_{i=1}^n \log\left(p_{Y|X}(y_i \mid x_i)\right) \\
&= -\frac{1}{2\sigma^2} \sum_{i=1}^n (y_i - g(x_i))^2 - C'
\end{aligned}
$$

where C and C' are some constants that are irrelevant in the optimization problems that follow. The takeaway is that assuming normal noise, the maximum likelihood estimator $\hat{g}$ of g is a linear function.

Logistic regression also has a motivation via maximum likelihood. Indeed, imagine that each X_i has β copies, where $Y_i\beta$ copies are in class C and $(1 - Y_i)\beta$ copies are in class D. Then the likelihood is

$$
\mathcal{L}(\hat{g}; (X_i, Y_i)_{i=1}^n) = \prod_{i=1}^n \hat{g}(X_i)^{Y_i\beta} (1 - \hat{g}(X_i))^{(1-Y_i)\beta}
$$

and the log-likelihood is

$$
\begin{aligned}
\ell(\hat{g}) &= \log(\mathcal{L}(\hat{g}; (X_i, Y_i)_{i=1}^n)) \\
&= \beta \sum_{i=1}^n [Y_i \log(\hat{g}(X_i)) + (1 - Y_i)\log(1 - \hat{g}(X_i))] \\
&= -\beta \sum_{i=1}^n L(\hat{g}(X_i), Y_i) && \text{(Logistic loss function.)} \\
\max_{\hat{g}} \ell(\hat{g}) &= \max_{\hat{g}} \sum_{i=1}^n L(\hat{g}(X_i), Y_i)
\end{aligned}
$$

There are two sources of error in a hypothesis $\hat{g}$:

- *bias*: the error due to inability of hypothesis $\hat{g}$ to fit g perfectly, $\mathrm{Ex}_{\mathcal{D}}[\hat{g}(X)] - g(X)$.
- *variance*: the error due to fitting random noise in the data, $\mathrm{Ex}_{\mathcal{D}}\left[(g(X) - \hat{g}(X))^2\right]$.

Indeed, take some point $z \in \mathbb{R}^d$ and draw ε from $\mathcal{N}$ at random. Define $\gamma = \hat{g}(z) + \varepsilon$. Then $\mathrm{Ex}_{\mathcal{D}}[\gamma] = \mathrm{Ex}_{\mathcal{D}}[\hat{g}(z)]$ and $\mathrm{Var}_{\mathcal{D}}[\gamma] = \mathrm{Var}_{\mathcal{D}}[\varepsilon]$.

Then

$$
\begin{aligned}
R(\hat{g}) &= \mathrm{Ex}_{\mathcal{D},\gamma}[L(\hat{g}(z), \gamma)] \\
&= \mathrm{Ex}\left[(\hat{g}(z) - \gamma)^2\right] \\
&= \mathrm{Ex}_{\mathcal{D}}\left[\hat{g}(z)^2\right] + \mathrm{Ex}_{\mathcal{D},\gamma}\left[\gamma^2\right] - 2\,\mathrm{Ex}_{\mathcal{D},\gamma}[\gamma\hat{g}(z)]
\end{aligned}
$$

$$
\begin{aligned}
&= \mathrm{Var}_{\mathcal{D}}[\hat{g}(z)] + \mathrm{Ex}_{\mathcal{D}}[h(z)]^2 + \mathrm{Var}_{\mathcal{D},\gamma}[\gamma] + \mathrm{Ex}_{\mathcal{D},\gamma}[\gamma]^2 - 2\,\mathrm{Ex}_{\mathcal{D},\gamma}[\gamma]\,\mathrm{Ex}_{\mathcal{D}}[\hat{g}(z)] \\
&= (\mathrm{Ex}_{\mathcal{D}}[h(z)] - \mathrm{Ex}_{\mathcal{D},\gamma}[\gamma])^2 + \mathrm{Var}_{\mathcal{D}}[\hat{g}(z)] + \mathrm{Var}_{\mathcal{D},\gamma}[\gamma] \\
&= (\mathrm{Ex}_{\mathcal{D}}[\hat{g}(z)] - g(z))^2 + \mathrm{Var}_{\mathcal{D}}[\hat{g}(z)] + \mathrm{Var}[\varepsilon] \\
&= \underbrace{\mathrm{Bias}(\hat{g})^2}_{\text{squared bias}} + \underbrace{\mathrm{Var}_{\mathcal{D}}[\hat{g}(z)]}_{\text{variance}} + \underbrace{\mathrm{Var}[\varepsilon]}_{\text{irreducible error}}
\end{aligned}
$$

This is the pointwise version of the bias-variance decomposition. The general version takes $z \sim \mathcal{D}$ and takes the expectation over z, obtaining the expected squared bias and the expected variance. Some implications are:

- Underfitting indicates a lot of bias.
- Overfitting is caused by high variance.
- Training error reflects the bias but not the variance; the test error reflects both.
- For many distributions, variance goes to 0 as $n \to \infty$.
- If $\hat{g}$ can fit g exactly, for many "nice" distributions the bias goes to 0 as $n \to \infty$.
- If $\hat{g}$ cannot fit g well, the bias is large at "most" points.
- Adding a good feature reduces bias; adding a bad feature rarely increases it.
- Adding a feature usually increases variance.
- It's not possible to reduce the irreducible error.
- Noise in test sets affects only the irreducible error; noise in the training set affects only the bias and variance.
- For real-world data, g is rarely knowable.
- But we can test learning algorithms by choosing g and making synthetic data.