USC CSCI 467: Introduction to Machine Learning
Lecture Notes

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Contents

Chapter 1

Linear Regression

We wil begin our exploration of supervised learning with linear regression. Recall that a **regression** problem is one where we are trying to predict a real-valued quantity. Some examples of regression problems include:

- Predicting the tomorrow's high temperature given information about temperatures, precipitation, etc. today.
- Predicting the sale price of a house given the house's area, number of bedrooms, etc.
- Predicting the future price of a stock given current information about the company.

1.1 Setup

Our goal is to learn a function f that maps inputs x (e.g., information about houses) to outputs y (e.g., prices). In linear regression, we make the key design decision to model y with a **linear** function of the input x. Based on patterns in the **training data**, we will try to find the linear function f that best approximates y. The figure below shows a one-dimensional case, where we want to fit a line to the available data.

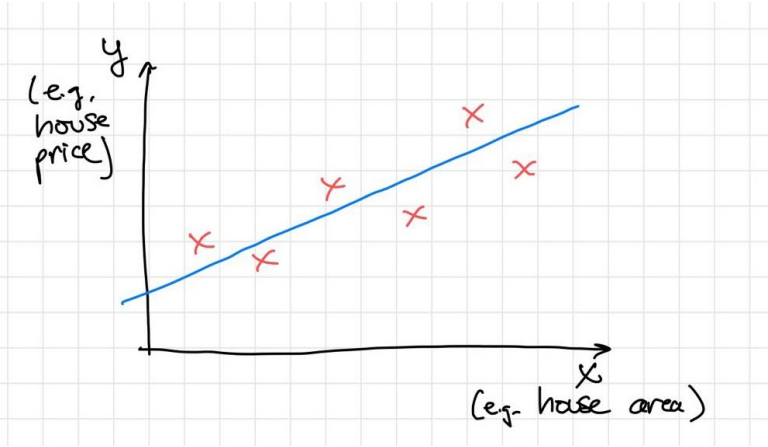


Figure 1.1: Linear regression in 1 dimension. Here we have six examples (in red), each of which is an (x, y) pair. We fit a line (in blue) which allows us to map any x to a predicted value for y.

1.1.1 Making predictions

Now we're ready to specify our linear regression model. Since we are modeling y as a linear function of the features x, our predictions are of the form:

$$f(x) \triangleq \left(\sum_{i=1}^{d} w_i \cdot x_i\right) + b = w^\top x + b, \tag{1.1}$$

where "weight vector" $w = [w_1, \ldots, w_d] \in \mathbb{R}^d$ and "bias term" $b \in \mathbb{R}$ are **parameters** of our model, i.e., the components that we will learn from data.[1]

What do these parameters mean? We can think of the bias as the baseline value (e.g., some baseline house price). Then, for each feature, there is an amount of increase/decrease per feature (e.g., for each bedroom, the price increases by 100k).

Throughout this class, we will use θ to denote all of the parameters of a model; for linear regression, $\theta = (w, b)$. We will write $f(x; \theta)$ or $f(x; w, b)$ in place of $f(x)$ to emphasize that f depends on θ.[2]

1.1.2 Learning

We have decided on the *form* or our predictions (i.e., a linear function of x); to complete the picture, we need to choose good values of w and b. The key idea in all of supervised learning is that the **training data** will help us determine which parameter values are good. Thus, we will assume access to a dataset D consisting of n training examples. Each training example is a pair $(x^{(i)}, y^{(i)})$, for $i = 1, \ldots, n$.[3]

How do we use D to choose θ? Our plan will be to write down a **loss function** $L(\theta)$ that describes how much our predictions $f(x; \theta)$ deviate from the true y's observed in D. We can then choose θ that minimize this loss. For linear regression, we will use the **squared loss** function—that is, we will measure the squared difference between our predictions $f(x; \theta)$ and true outputs y, averaged across the training examples.[4] Formally, we have

$$L(\theta) = \frac{1}{n}\sum_{i=1}^{n}\left(f(x^{(i)}; \theta) - y\right)^2 = \frac{1}{n}\sum_{i=1}^{n}\left(w^\top x^{(i)} + b - y\right)^2. \tag{1.2}$$

While other loss functions are possible, we will see later why squared loss is a natural choice. The best θ would have the smallest loss, so our goal now becomes to *minimize* $L(\theta)$ with respect to θ.

We have now defined all the core concepts in linear regression! We started with the goal of learning a linear function that maps features of inputs x to outputs y. We have now reduced this problem to the problem of finding values of w and b that minimize this loss function—that is, we have rewritten a *learning* problem as an *optimization* problem. It turns out that we now have several options for solving this optimization. In this class we will cover two: Gradient descent, a general-purpose optimization strategy that we will see many times in this course, and the Normal Equations, a closed-form solution that works specifically for linear regression.

[1] Technically, the presence of b makes this is an affine function, but it's common to call this linear.

[2] Note that this notation conveys something different than $f(x \mid \theta)$, which would signify "conditioning on" θ. This would be appropriate if θ were a random variable, but currently we are not viewing it as such. As we will discuss in a few classes, it is however possible to view things through a Bayesian lens, at which point we will think of θ as a random variable with some prior distribution.

[3] We use the notation $x^{(i)}$ to avoid confusion with x_i being the i-th component of the vector x.

[4] We could also use the sum instead of the average. The average has the slightly nicer property of being roughly the same magnitude regardless of how large the training dataset is.

1.1.3 Summary of Notation

To summarize the new notation, we have:

- x: An input vector. We often refer to each component of x as a different **feature** (e.g., area, number of bedrooms, etc.)
- y: An output/response (e.g., price) in $\mathbb{R}$
- w, b: "Weight" and "bias" **parameters** of the model, jointly denoted as θ.
- Given a new input x, our prediction is $f(x; w, b) \triangleq w^\top x + b$.
- D: A training dataset consisting of n training examples, denoted $\{(x^{(1)}, y^{(1)}), \ldots, (x^{(n)}, y^{(n)})\}$.
- $L(\theta)$: The **loss function** for linear regression, defined to be

$$\frac{1}{n} \sum_{i=1}^{n} \left(w^\top x^{(i)} + b - y^{(i)} \right)^2.$$

1.2 Gradient Descent

Gradient descent is a general algorithm for minimizing a differentiable function. In other words, given a differentiable **objective function** $F(x)$ that maps from $\mathbb{R}^d$ to $\mathbb{R}$, gradient descent tries to find a value x^* that minimizes $F(x)$. The intuition behind gradient descent is straightforward (and much more general than just gradient descent). We will start from some initial value for x, identify a direction to step in that will lower the value of $F(x)$, take a small step in that direction, and repeat many times.

This can be illustrated succinctly in pseudocode:

Algorithm 1 High-level description of gradient descent (and many other algorithms)

```
Choose initial guess x^(0)
for t = 1, ..., T do
    Choose x^(t) that slightly decreases F(x) relative to x^(t−1)
return x^(T)
```

1.2.1 Gradient Descent Intuition

Rough intuition: Thinking one coordinate at a time. Before we think about how to update x, let's just think about how to update one coordinate x_i. There are only two ways to slightly change a scalar—we can increase it slightly or decrease it slightly. Which one is better? This is exactly what the derivative tells us!

Recall that the derivative of a function is positive when it's increasing, and negative when it's decreasing. So, to decide whether to increase or decrease x_i at each step, we just need to look at the derivative with respect to x_i. To be slightly more precise, we care about the derivative with respect to x_i when all other components of x are held fixed; this is known as the *partial derivative* with respect to x_i, denoted $\frac{\partial F}{\partial x_i}$. You compute partial derivatives exactly the same way you compute normal single-variable derivatives; you just have to remember to differentiate with respect to x_i and treat everything else as a constant.

Once we compute the partial derivative with respect to x_i, we have three cases:

- If $\frac{\partial F}{\partial x_i} > 0$, then F is increasing in x_i, so to make F smaller we need to make x_i smaller.
- If $\frac{\partial F}{\partial x_i} < 0$, then F is decreasing in x_i, so to make F smaller we need to make x_i bigger.
- If $\frac{\partial F}{\partial x_i} = 0$, then we don't need to change x_i at all.

Thus, the takeaway is that we always want to update w_i in the *opposite* direction of its associated partial derivative.

Finally, let's define the **gradient**. The **gradient** $\nabla_x F(x)$ is simply defined to be the vector of all partial derivatives with respect to each x_i:

$$\nabla_x F(x) \triangleq \begin{pmatrix} \frac{\partial F}{\partial x_1} \\ \frac{\partial F}{\partial x_2} \\ \vdots \\ \frac{\partial F}{\partial x_d} \end{pmatrix}$$

Note that if $x \in \mathbb{R}^d$, then $\nabla_x F(x)$ is also a vector $\in \mathbb{R}^d$.

Let's think about what this gradient vector represents. We know that for every $i = 1, \ldots, d$, we want to nudge x in the opposite direction of the gradient. In other words, given our previous guess $x^{(t-1)}$, we can generate a better new for x by *subtracting* a small multiple of the gradient from $x^{(t-1)}$.

We can formalize this intuition to arrive at the **gradient descent algorithm**:

Algorithm 2 Gradient descent

1: $x^{(0)} \leftarrow \mathbf{0} \in \mathbb{R}^d$
2: **for** $t = 1, \ldots, T$ **do**
3: $\quad x^{(t)} \leftarrow x^{(t-1)} - \eta \nabla_x F(x^{(t-1)})$
return $x^{(T)}$

We have initialized $x^{(0)}$ to simply be the zero vector—for problems like linear regression, it turns out the initialization does not matter very much, for reasons we will discuss in the next class. η is the **learning rate**, a small number (e.g., 0.01) that determines how small of a step we want to take at each iteration. Note the negative sign, which ensures that we are always stepping in the direction that *minimizes* F; if that were a plus sign, this algorithm would instead maximize F. Finally, note that we are using both the sign and the magnitude of the derivative—we take a larger step if the derivative is larger in absolute value.

As written, this algorithm runs for some fixed number of steps T. Usually, you would try to choose T to be large enough that you get close to a stationary point (i.e., where the gradient is 0). There are also other possible criteria to use when deciding when to stop gradient descent, which we will discuss later in the course.

More precise intuition: Gradient as steepest ascent direction. The above argument doesn't precisely identify the gradient as the best direction to step in. Here, we more precisely show why the gradient is the most natural and efficient choice.

If you have taken multivariable calculus, you may have been taught that the gradient $\nabla_x F(x^{(t)})$ is the direction of steepest ascent—taking a step in that direction is the fastest way to increase the value of $F(x^{(t)})$. Since we want to minimize F, we will step in the exact opposite direction, i.e. $-\nabla_x F(x)$, the direction of steepest *descent*.

Why is the gradient the steepest ascent direction? One way to convince yourself of this is to think about the first-order Taylor expansion of F centered around $x^{(t)}$:

$$F(x) \approx F(x^{(t)}) + \left(\nabla_x F(x^{(t)})\right)^\top (x - x^{(t)}).$$

Re-arranging this, we have

$$F(x) - F(x^{(t)}) \approx \left(\nabla_x F(x^{(t)}\right)^\top (x - x^{(t)}). = \|\nabla_x F(x^{(t)})\| \cdot \|x - x^{(t)}\| \cdot \cos(\alpha)$$

where α is the angle between the vectors $\nabla_x F(x^{(t)})$ and $x - x^{(t)}$. The left hand side is just the amount by which F increases when we step from $x^{(t)}$ to x. If we want to take a step of a fixed size (i.e., fixed $\|x - x^{(t)}\|$), the way to have the biggest positive effect on F is thus to make $\cos(\alpha) = 1$, i.e., to make $x - x^{(t)}$ point in the same direction as $\nabla_x F(x^{(t)})$. Similarly, to have the biggest negative effect on F, we want to make $\cos(\alpha) = -1$, so $x - x^{(t)}$ should point in the exact opposite direction as the gradient.

1.2.2 Gradient Descent for Linear Regression

To apply gradient descent to linear regression, all that we need to do is derive the gradient for $L(\theta)$.

First, let's make one small change so we can stop thinking of w and b as different—they're actually essentially the same thing. I'm going to modify my dataset by adding an additional feature whose value is just always 1. The associated weight for this feature always just gets added to the final prediction, so it operates the exact same way that the bias does. This trick lets me omit the bias term—it's unnecessary now—so we can just use $w^\top x$ as the model's output.

Now let's remind ourselves of the loss function we want to optimize:

$$L(w) = \frac{1}{n} \sum_{i=1}^{n} \left(w^\top x^{(i)} - y^{(i)}\right)^2.$$

All we need to do is take the gradient with respect to w. We can do this by applying the chain rule—it works just as well for the gradient as for the normal derivative, since the gradient is just a bunch of derivatives.

$$\nabla_w L(w) = \frac{1}{n} \sum_{i=1}^{n} 2 \cdot \left(w^\top x^{(i)} - y^{(i)}\right) \cdot x^{(i)}. \tag{1.3}$$

Here we have used the fact that

$$\nabla_w w^\top x^{(i)} = x^{(i)}.$$

You can convince yourself of this by taking the partial derivative with respect to each component w_j, and show that it indeed equals $x_j^{(i)}$.

Now, all we have to do is plug these gradient formulas into the gradient descent update rule to get our full algorithm.

Algorithm 3 Gradient descent for linear regression

1: $w^{(0)} \leftarrow \mathbf{0} \in \mathbb{R}^d$
2: **for** $t = 1, \ldots, T$ **do**
3: $\quad w^{(t)} \leftarrow w^{(t-1)} - \eta \cdot \frac{2}{n} \sum_{i=1}^{n} (w^{(t-1)\top} x^{(i)} - y^{(i)}) \cdot x^{(i)}$
return $w^{(T)}$

Understanding the gradient formula. Let's try to understand why this gradient formula makes sense. First, note that each term in the sum is simply a scalar multiplied by the vector $x^{(i)}$. So the update corresponding to the i-the example either adds or subtracts some multiple of $x^{(i)}$ to w. The sign of this update is determined by the quantity $w^\top x^{(i)} - y^{(i)}$. If this quantity is positive, that means our model has overestimated $y^{(i)}$. Thus, the gradient contains a positive multiple of $x^{(i)}$, so when we do gradient descent we subtract off a multiple of $x^{(i)}$. This makes intuitive sense: we should want to decrease the dot product between w and $x^{(i)}$, so we should be subtracting off multiples of $x^{(i)}$. Conversely, if $w^\top x^{(i)} - y^{(i)} < 0$, that means our model has underestimated $y^{(i)}$, so the gradient descent update will add a multiple of $x^{(i)}$ to w.

1.3 Better Featurization

So far, we've talked about learning functions that were linear in the input x. What if we want to learn more complex functions? It turns out we can actually do this rather easily, if we just change what x is!

Polynomial features Suppose we have a dataset that looks like this:

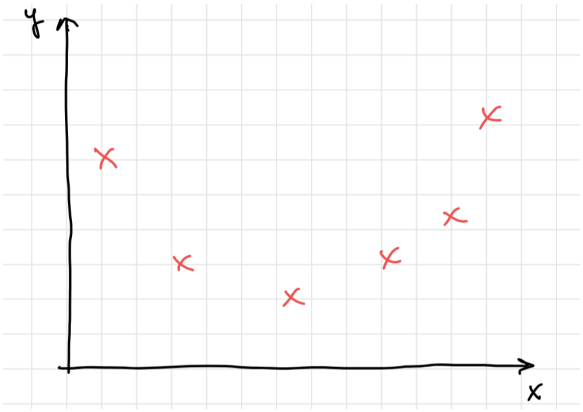


Figure 1.2: A regression dataset that cannot be fit with a straight line.

Clearly we cannot fit this data well with a straight line. But there's actually a simple solution! I can first modify x from a scalar to a vector with entries $[x, x^2]$, and run linear regression with these vectors as my inputs. Now that I have two features, I will have a separate parameter w_1 corresponding to x and w_2 corresponding to x^2, so I will be fitting a function of the form $w_1 x + w_2 x^2 + b$, i.e., a quadratic function. In general, I can apply any transformation to x I want, and then run linear regression on top of this transformed x.

Indicator features. One common strategy for coming up with features is to create **indicator features**. These are binary features, meaning that they are always either 0 or 1. For any boolean expression over x, you can create an associated indicator function.

Indicator features are another way to help a linear regression model learn a non-linear function. For example, if we're trying to predict the sale price of a house, we might have a feature called "number of bedrooms," which is always an integer. If we were to directly use this feature in linear regression, the model could only learn a linear relationship between number of bedrooms and price. This is very limiting! Instead, we can create a group of indicator features, one for each possible

number of bedrooms. That is, we have a feature for "does it have 1 bedroom," "does it have 2 bedrooms," etc. Each of these features would be 1 if the answer is yes, and 0 otherwise. This lets you learn a custom change in price for every possible number of bedrooms, instead of forcing that the difference in price between 1 and 2 is the same as the difference between 2 and 3.

Note that it makes sense at some point to start grouping values together, say, considering everything with 10+ bedrooms to be the same feature. This is because your data will become very sparse. How many houses do you think you'll see with 27 bedrooms? Probably very few, so you can't estimate the weight of a feature for "is there exactly 27 bedrooms" very well. But it's reasonable to pool all these together under "at least 10 bedrooms" so that you can at least estimate the weight associated with having a large number of bedrooms.

Indicator features are also commonly used to handle **categorical** features, which are things that take on some fixed set of discrete values (e.g., "house type"—is it a condo, or town house, or single-family home?). These features are not even numerical by nature, so in order to use them in a linear regression, you have to convert them to something numerical.

Feature engineering. Indicator features can be whatever you want, which opens the door to a lot of possibilities. Let's take the example of zip code. There are $10^5 = 100,000$ possible five-digit zip codes. So you could create $100,000$ indicator features, one for each zip code. But is this the best thing to do? If your dataset isn't that big, there might be some zip codes for which you have very few training examples, or even zero training examples, but you still want to do something reasonable if they show up at test time. So, a better idea might be to group zip codes that are geographically close to each other. You can assume that the effect of zip code on price doesn't change that much if you move from one zip code to an adjacent one (e.g., any Los Angeles zip code will be very different from one in the middle of Illinois). There's no "right" or "wrong" answer here—depending on the task you're trying to solve and the data that's available, different choices of features may be preferable. The term **feature engineering** is commonly used to refer to the process of coming up with different ways to "featurize" your data to make your machine learning model more accurate.

So... is linear regression "linear"? The thing to remember is that linear regression learns a function that is **linear in your features**. However, you can choose features to be any function of the input, so the learned function can in fact be non-linear in your original input! You might be wondering if there is a compact way to automatically add a lot of complex features to a model. In fact the answer is yes, thanks to something called the kernel trick, which we will learn about in a few lectures.

1.4 Convexity: Why Gradient Descent Works

So far I haven't addressed a rather important question: How do we know that gradient descent will work? When we run gradient descent to minimize a function $f(x)$, will we actually find its global minimum?

Gradient descent is a very myopic algorithm—it just keeps taking steps to incrementally make our value a little better. Since it's so myopic, it can may converge to a *local* optimum that could be much worse than the *global* optimum. Luckily for us, there is a large class of objective functions for which all local optima are also global optima. When this property holds, we can guarantee that gradient descent converges to the global optimum. In particular, this holds if $f(x)$ is a **convex**

function, and many objective functions we care about are in fact convex. Thus, we will now take a slight detour into the world of *convex optimization*.

An informal definition. Pictorially, a function is convex if it "holds water," whereas a concave function (i.e., a function whose negative is convex) "spills water." This is illustrated in Figure 1.3.

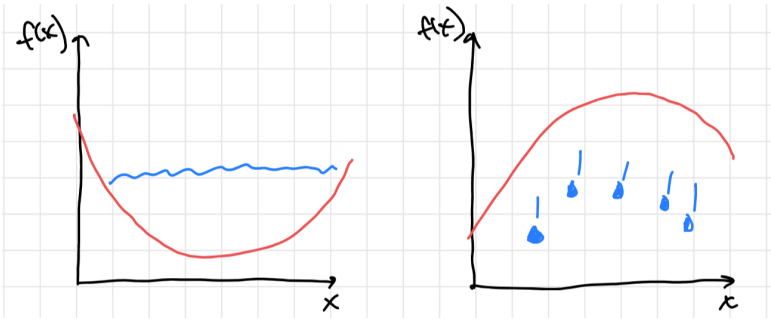


Figure 1.3: Left: A convex function "holds water." Right: A concave function "spills water." While this is not a precise definition, it can be a useful way to remember what a prototypical convex or concave function looks like.

This intuition is formalized in the following definition:

Definition 1.4.1. *A function $f : \mathbb{R}^d \to \mathbb{R}$ is **convex** if for all $x, x' \in \mathbb{R}^d$ and scalars $t \in [0, 1]$,*

$$f((1-t)x + tx') \leq (1-t)f(x) + tf(x'). \tag{1.4}$$

Geometrically, this definition says something very intuitive. Let's draw a function f and pick any two points x and x'. This inequality says that if you draw a line connecting these two points, the function has to stay below the line. The line is traced out by the right hand side of the inequality as t goes from 0 to 1, whereas the function itself is given by the left hand side.

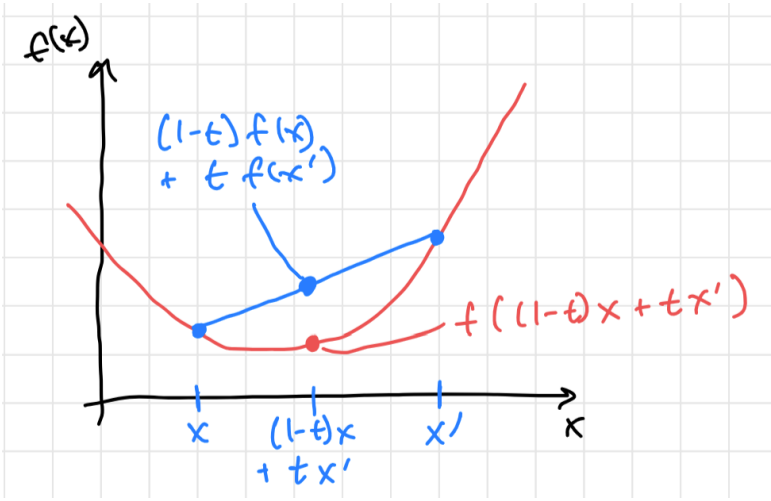


Figure 1.4: A function is convex if and only if every line segment you draw connecting two points on the function lies above the function itself.

All local minima of a convex function are global minima. With this definition, we can see geometrically that a convex function cannot have a local minimum that is not also a global minimum.[5] Figure 1.5 sketches out why this is the case.

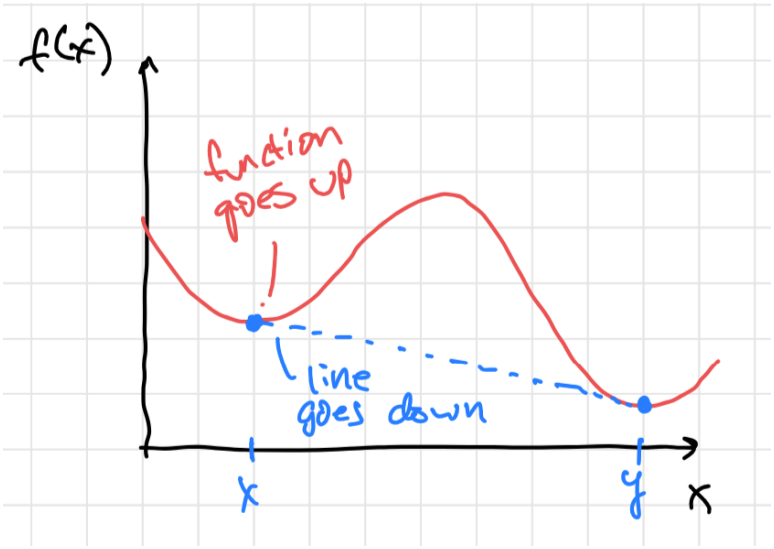


Figure 1.5: A sketch of why a convex function cannot have two distinct local minima (unless they are both equally good). If we draw a line connecting the worse local minimum (x) to the better one (y), that line must be going down, but the function around the worse local minimum must be going up. This is impossible if the function is convex.

Let's actually prove this. First, I need a formal definition of a local minimum:

Definition 1.4.2. *A point x is a **local minimum** of a function $f(x)$ if there exists $\epsilon > 0$ for which every $x' \in B_\epsilon(x)$ satisfies $f(x) \leq f(x')$. Note that $B_\epsilon(x)$ denotes the ball of radius ϵ centered around x, or equivalently, the set of points x' such that $\|x' - x\| < \epsilon$.*

Now let's suppose there are two points x and y that are both local minima of f, and $f(y) < f(x)$ (i.e., y is a "better" local minimum than x). We will show that if this is true, f cannot be convex. In other words, this situation is not possible when f is convex.

Since x is a local minimum, there is some ϵ for which every $x' \in B_\epsilon(x)$ satisfies $f(x) \leq f(x')$. Now, it is clear that we can choose some $t > 0$ such that $(1-t)x + ty = x + t(y-x) \in B_\epsilon(x)$. For example, we can choose $t = \frac{\epsilon}{2\|y-x\|}$, so that the distance from $x + t(y-x)$ to x is exactly $\epsilon/2$. By the definition of a local minimum, we know that

$$f((1-t)x + ty) \geq f(x).$$

Moreover, since $f(x) > f(y)$, we know

$$f((1-t)x + ty) > f(y).$$

Now let's multiply the top inequality by $(1-t)$ and the bottom equation by t. This gives us

$$f((1-t)x + ty) > (1-t)f(x) + tf(y).$$

[5] Note that a convex function *can* have multiple global minima—for instance, the constant function $f(x) = 0$ is convex.

Note that the left hand side is *strictly* greater than the right hand side because we knew $f(y) > f(x)$ and that $t > 0$. This is exactly the opposite of what the definition of convexity tells us, so f cannot be convex.

Showing that functions are convex. So far, I've shown you that convex functions have very nice properties. How do we know if a given function is convex? Luckily, there are rules we can use to prove a complex function is convex based on its building blocks. For our purposes right now, the following three rules will be sufficient:

1. **A univariate function $f : \mathbb{R} \to \mathbb{R}$ is convex if its second derivative is always ≥ 0.** Thus, for instance, the function $f(x) = x^2$ is convex because its second derivative $f''(x) = 2$.

   Proof: I'll provide a quick proof sketch here. The basic idea is to apply the mean value theorem multiple times. We can use a proof by contradiction: suppose that for some $x, y \in \mathbb{R}$, with $y > x$, and $t \in [0, 1]$, the value of f at $(1-t)x+ty$ lies above the line connecting $(x, f(x))$ and $(y, f(y))$. For ease of notation, define $z = (1-t)x + ty$, and let m be the slope of the line connecting $(x, f(x))$ and $(y, f(y))$. The line connecting $(x, f(x))$ and $(z, f(z))$ must have a slope larger than m, since it reaches a point above the line of slope m (see Figure 1.6 for an illustration). Similarly, the line connecting $(z, f(z))$ and $(y, f(y))$ must have a slope less than m. Call these two other slopes m_1 and m_2, respectively. By the mean value theorem, there must be some point $a \in [x, z]$ where $f'(a) = m_1$, and another point $b \in [z, y]$ where $f'(b) = m_2$. So this means that over the interval $[a, b]$, the first derivative f' must be going down. By the mean value theorem again, this means there is another point c where $f''(c) < 0$, since f'' is just the derivative of f'. This is a contradiction, so the function must have actually been convex.

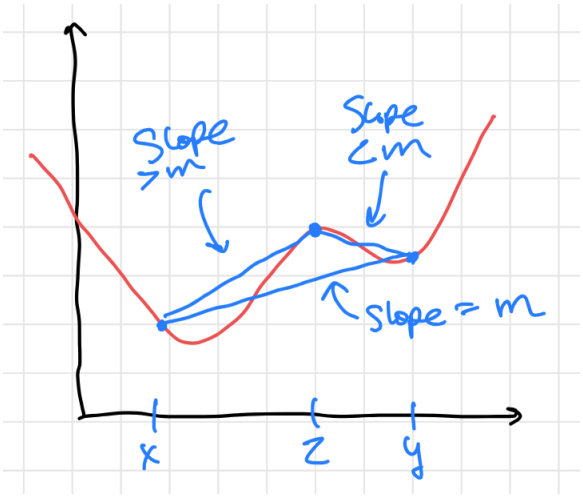


Figure 1.6: An illustration for the mean value theorem argument showing that a function with $f''(x) \geq 0$ everywhere must be convex.

2. **A convex function applied to an affine function is convex.** In other words, if $f(x)$ is convex, then so is $f(Ax + b)$ where A is a matrix/vector/scalar and b is a vector/scalar (depending on whether x is a vector or scalar, and whether f takes a vector or scalar as input). The intuition is clear in the univariate case: for any scalars a and b, $f(ax + b)$ just shifts the function along the x axis by $-b$ and scales it horizontally by a factor of a. This preserves the overall shape of the function, which is what determines convexity.

Proof: Let $g(x) = f(Ax + b)$. For all $x, y \in \mathbb{R}^d$ and all $t \in [0, 1]$, we have:

$$\begin{aligned} g((1-t)x + ty) &= f(A((1-t)x + ty) + b) && \text{By definition of } g \\ &= f((1-t)(Ax + b) + t(Ay + b)) && \text{Algebra} \\ &\leq (1-t)f(Ax + b) + tf(Ay + b) && \text{By convexity of } f \\ &= (1-t)g(x) + tg(y) && \text{By definition of } g \end{aligned}$$

3. **If $f(x)$ and $g(x)$ are convex, then so is $f(x) + g(x)$.** Again, in the univariate case this makes sense given rule 1. The second derivative of $f(x) + g(x)$ is simply $f''(x) + g''(x)$, and so if each one is individually ≥ 0 then so is the sum.

   Proof: Let $h(x) = f(x) + h(x)$. For all $x, y \in \mathbb{R}^d$ and all $t \in [0, 1]$, we have:

$$\begin{aligned} h((1-t)x + ty) &= f((1-t)x + ty) + g((1-t)x + ty) && \text{By definition of } h \\ &\leq (1-t)f(x) + tf(y) + (1-t)g(x) + tg(y) && \text{By convexity of } f \text{ and } g \\ &= (1-t)h(x) + th(y) && \text{By definition of } h \end{aligned}$$

4. **If $f(x)$ is convex and $c > 0$, then so is $cf(x)$.** Again this makes intuitive sense in 1-D, since scaling by a positive constant just stretches the function along the y-axis. The proof is straightforward and similar to the last two.

This is by no means an exhaustive set of rules, but these are the most common ones that come up. My goal in this lecture is not to give you a comprehensive tour of convex functions, but just to know some key rules of thumb so that you can look at a new loss function and quickly surmise whether it is convex. If it's convex, you can be confident that you will not run into bad local minima when optimizing it.

Linear regression is convex. Let's apply what we learned to linear regression. Recall that our loss function was

$$L(w) = \frac{1}{n}\sum_{i=1}^{n}\left(f(x^{(i)}; w) - y^{(i)}\right)^2 = \frac{1}{n}\sum_{i=1}^{n}\left(w^\top x^{(i)} - y^{(i)}\right)^2. \tag{1.5}$$

We want to show that this is a convex function of w. Each term inside the sum is a convex function (i.e., the function $g(x) \to x^2$, which is convex by Rule 1) applied to an affine function of w. (Keep in mind that since this is a function of w, we just think of $x^{(i)}$ and $y^{(i)}$ as constants.) Thus, by Rule 2, each term of the sum is convex. Finally, by Rule 3, the sum of all these convex terms is also convex, and by Rule 4 we can safely multiply everything by $\frac{1}{n}$.

1.5 Maximum Likelihood Estimation

Finally, I want to come back to the question of why we use squared loss, and connect this to some much more general thoughts about how we can come up with machine learning algorithms. We will re-apply these principles in the next class on logistic regression, our first method for classification.

One general principle for designing machine learning algorithms is the framework of **Maximum Likelihood Estimation** (MLE). The idea is to view the observed data as being generated by some probabilistic process parameterized by our model parameters θ. The best θ is the one that best explains the data, i.e., the θ under which the data has the highest probability (hence, maximum likelihood).

1.5.1 MLE for coin flips

Let's warm up with a simple example. Suppose we have a coin that might be biased. Every time you flip it, it has some probability p of coming up heads (and thus probability $1-p$ of coming up tails).

Now suppose we flip it n times. Each time, we get an observation y_i that is either 1 (heads) or 0 (tails). Based on this observed data, we would like to infer what the value of p is. One principle by which we can make this inference is the principle of maximum likelihood estimation. Out of all possible p's (i.e., all possible numbers between 0 and 1), we want to figure out which one maximizes the probability of the observed data.

To do this, we need to do the following steps:

1. Write down the probability of the data as a function of our parameters (in this case, p).
2. Compute the value of p that maximizes this probability.

In Homework 0, you will carry out these two steps for this simple case of a weighted coin.

1.5.2 Deriving linear regression via MLE

Now we will derive linear regression by applying the principle of maximum likelihood estimation under a particular, natural probabilistic model. In particular, let's assume that each $y^{(i)}$ is drawn independently at random from a Gaussian distribution with variance σ^2 centered around $\theta^\top x^{(i)}$.[6] Why Gaussian? One can imagine that one reason we can't perfectly predict y is that there are many small, random effects that we are not modeling. By the Central Limit Theorem, the cumultative effective of many such small, independent, random effects will be normally distributed.

Remember that the Gaussian pdf for mean μ and variance σ^2 is given by

$$p(x;\mu,\sigma^2) = \frac{1}{\sigma\sqrt{2\pi}} \exp\left(-\frac{(x-\mu)^2}{2\sigma^2}\right)$$

The overall probability of the $y^{(i)}$'s given all the $x^{(i)}$'s is

$$\mathcal{L}(\theta) = \prod_{i=1}^{n} p(y^{(i)} \mid x^{(i)};\theta) \tag{1.6}$$

$$= \prod_{i=1}^{n} \frac{1}{\sigma\sqrt{2\pi}} \exp\left(-\frac{1}{2\sigma}(y^{(i)} - \theta^\top x^{(i)})^2\right) \tag{1.7}$$

We take the product because we assumed the $y^{(i)}$'s are sampled independently.[7]

In MLE, this is the objective function that we are trying to *maximize*. I now claim that this is exactly the same as minimizing our original linear regression objective. Let's start by taking the log of everything—since log is a monotonically increasing function, maximizing likelihood is the same as maximizing log-likelihood (which we denote $\mathcal{LL}(\theta)$). Taking the log often is useful because

[6] Note that we are only modeling the $y^{(i)}$'s here, and ignoring the probability of the $x^{(i)}$'s.

[7] A quick note on terminology: $\mathcal{L}(\theta)$ denotes the *likelihood* of θ, which is equal to the *probability* of the data under θ. Following convention, we will try to be consistent that likelihood refers to a function of θ, even though colloquially "likelihood" and "probability" can often refer to the same thing.

it converts products into sums, and sums are easy to differentiate. We have:

$$\mathcal{LL}(\theta) = \log\left(\prod_{i=1}^{n} \frac{1}{\sigma\sqrt{2\pi}} \exp\left(-\frac{1}{2\sigma}(y^{(i)} - \theta^\top x^{(i)})^2\right)\right) \tag{1.8}$$

$$= \sum_{i=1}^{n}\left(\log\left(\frac{1}{\sigma\sqrt{2\pi}}\right) - \frac{1}{2\sigma}(y^{(i)} - \theta^\top x^{(i)})^2\right) \tag{1.9}$$

$$= n\log\left(\frac{1}{\sigma\sqrt{2\pi}}\right) - \frac{1}{2\sigma}\sum_{i=1}^{n}(y^{(i)} - \theta^\top x^{(i)})^2. \tag{1.10}$$

The first term is a constant that does not depend on θ, so we can ignore it when optimizing with respect to θ. The latter term is exactly our familiar squared loss from before, multiplied by a negative constant. This means that *maximizing* $\mathcal{LL}$ is indeed equivalent to *minimizing* squared loss.

Chapter 2

Classification with Logistic Regression and Softmax Regression

2.1 Deriving Logistic Regression from MLE

Last class, we derived the equation for linear regression by applying the principle of Maximum Likelihood Estimation: We choose the parameters θ to maximize the log-likelihood of the data, i.e.

$$\log \mathcal{L}(\theta) = \sum_{i=1}^{n} \log p(y^{(i)} \mid x^{(i)}; \theta). \tag{2.1}$$

To come up with an algorithm for classification, let's use the same recipe but with a different probabilistic model. Logistic regression[1] starts with the following model:

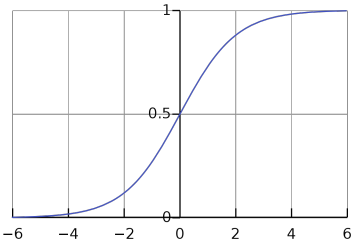
$$p(y = 1 \mid x; w) = \frac{1}{1 + \exp(-w^\top x)}, \tag{2.2}$$

where both our feature vector x and parameter vector w are in $\mathbb{R}^d$.[2] Note that $p(y = -1 \mid x; w) = 1 - p(y = 1 \mid x; w)$ by definition.

What's going on here? We can define the function $\sigma(z) = \frac{1}{1+\exp(-z)}$, called the "sigmoid" or "logistic" function, so we can now write:

$$p(y = 1 \mid x; w) = \sigma(w^\top x). \tag{2.3}$$

The function $\sigma(z)$ looks like the following:



[1] It is very unfortunate that this is called logistic *regression* because it is used for classification problems, not regression problems.

[2] Just as in linear regression, we can remove the need for a bias term by adding a feature whose value is 1 for every example.

The important things to note are:

- For large positive z, $\sigma(z)$ approaches 1.
- For small (very negative) z, $\sigma(z)$ approaches 0.
- When $z = 0$, $\sigma(z) = \frac{1}{2}$.
- $1 - \sigma(z) = \sigma(-z)$.

Now we see the point of $\sigma(z)$. We can view $w^\top x$ as a score of whether the example looks more like a positive example (if $w^\top x > 0$) or a negative example (if $w^\top x < 0$). σ transforms this raw score into a probability between 0 and 1.

Figure 2.1 below shows a geometric picture of what's going on. In two dimensions, the equation $w^\top x = 0$ defines a line (in d dimensions, it defines a $d-1$-dimensional hyperplane). This represents points where $p(y = 1 \mid x) = \frac{1}{2}$—that is, points that seem equally likely to be positive or negative. On one side of the line are points with positive dot product with w, which are more likely to be positive; on the other side, the points have negative dot product with w, and thus are more likely to be negative.

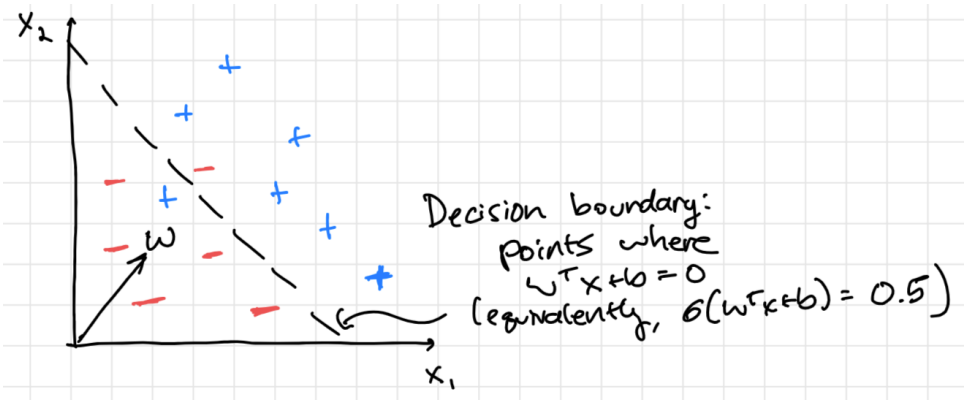


Figure 2.1: Illustration of logistic regression decision boundary. The decision boundary is the hyperplane defined by the equation $w^\top x + b = 0$. This hyperplane is always perpendicular to the weight vector w. Points on the decision boundary are predicted by the model to be equally likely to be positive or negative. Going further from the decision boundary, the model makes more confident predictions (i.e., the probabilities become closer to 1 or 0).

Since the decision boundary we learn is still a linear function of the features, logistic regression is another instance of a **linear model**, just like linear regression.[3]

Note that we can write $p(y = -1 \mid x; w) = 1 - p(y = 1 \mid x; w) = 1 - \sigma(w^\top x) = \sigma(-w^\top x)$. Thus, we can use this compact expression:

$$p(y \mid x; w) = \sigma(y \cdot w^\top x). \tag{2.4}$$

You can easily check that this is correct both when $y = 1$ and when $y = -1$.

[3]Note that just as in linear regression, we can define all sorts of complex features if we want to learn a complex decision boundary to separate the positive and negative examples.

Putting everything together, we arrive at this objective function:

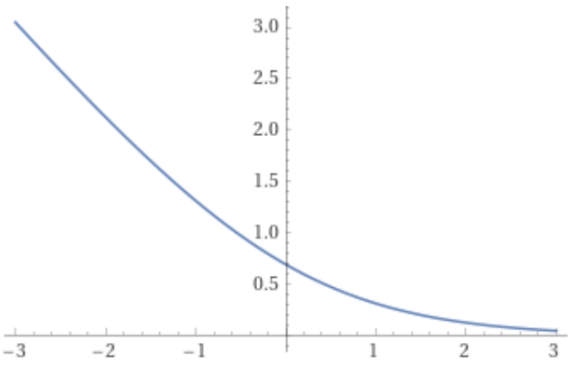
$$\log \mathcal{L}(w) = \sum_{i=1}^{n} \log p(y^{(i)} \mid x^{(i)}; w) \tag{2.5}$$

$$= \sum_{i=1}^{n} \log \sigma(y^{(i)} \cdot w^\top x^{(i)}). \tag{2.6}$$

Recall that we want to maximize (log-)likelihood. However, usually in machine learning convert problems into minimization problems. We can do this simply by adding a negative sign. I'll also multiply by $\frac{1}{n}$ just to make it easier to interpret this as an average across the dataset (this doesn't affect what w minimizes the loss):

$$L(w) = \frac{1}{n} \sum_{i=1}^{n} -\log \sigma(y^{(i)} \cdot w^\top x^{(i)}) \tag{2.7}$$

We can interpret the function $\ell(z) = -\log \sigma(z)$ as a **loss function** similar to squared loss from linear regression. If it is high, that means our model is doing a bad job, and if it is close to zero, it is doing a good job. Here's what this function looks like:



The expression $y \cdot w^\top x$ is called the **margin**, and is a quantity that we always want to be > 0, as that means y and $w^\top x$ have the same sign, and thus that we are classifying correctly. The loss function $\ell(z)$ is our way of saying exactly how unhappy we are with any particular value of the marign. You see that we are very unhappy when the margin is very negative, and then this amount of unhappiness decreases.

2.2 Gradient Descent for Logistic Regression

Let's keep going with the same recipe we used for linear regression. Remember that we first wrote down an objective function that we wanted to minimize, then used gradient descent to optimize the function with respect to w. We can do the exact same thing here. The only thing that changes is the gradient itself.

First, let's prove a useful fact about the σ function:

$$\begin{aligned}\frac{d}{dz}\log\sigma(z) &= \frac{1}{\sigma(z)}\cdot\frac{d}{dz}\sigma(z)\\ &= (1+\exp(-z))\cdot\left(-(1+\exp(-z))^{-2}\right)\cdot(-\exp(-z))\\ &= \frac{\exp(-z)}{1+\exp(-z)}\\ &= \sigma(-z).\end{aligned}$$

Now we just combine this fact with the chain rule to get the gradient of the objective L:

$$\nabla_w L(w) = \nabla_w \frac{1}{n}\sum_{i=1}^{n} -\log\sigma(y^{(i)}\cdot w^\top x^{(i)}) \tag{2.8}$$

$$= \frac{1}{n}\sum_{i=1}^{n} -\sigma(-y^{(i)}\cdot w^\top x^{(i)})\cdot y^{(i)}\cdot x^{(i)}. \tag{2.9}$$

Finally, recall that we want to decrease L, so we will be stepping in the *negative* direction of the gradient. This means that we will our update rule will look like:

$$w^{(t+1)} = w^{(t)} + \eta\frac{1}{n}\sum_{i=1}^{n}\sigma(-y^{(i)}\cdot w^\top x^{(i)})\cdot y^{(i)}\cdot x^{(i)} \tag{2.10}$$

where η is the learning rate, as before.

Let's try to understand why this expression makes sense. First, let's check that the signs of everything make sense. σ is always > 0 so let's put it aside for now. For a positive example, we will *add* some multiple of $x^{(i)}$ to w. This makes sense because we want positive examples to have high dot product with w. Conversely, we will *subtract* some multiple of $x^{(i)}$ to w for each negative example, since we want them to have low dot product with w. Finally let's look at the σ term. This is σ of the *negative margin*. That means that if the margin is very low (bad), then this number is close to 1. If the margin is very large (good), then the number is close to 0. This means that if we're doing very badly on a particular example, we do a large update to w. If we're doing well on a particular example, then we don't need to change w in a big way (as far as that example is concerned).

2.3 Multi-class Classification with Softmax Regression

Logistic regression works for binary classification. What if we have more than two classes? For example, what if we have an image and want to classify what species of animal it is? This is a **multi-class classification** problem. There is a natural way to extend logistic regression to multi-class settings, known as **softmax regression** or **multinomial logistic regression**.

Essentially, the idea is that if we have C classes, we will now have C parameter vectors of dimension d instead of a single vector. The j-th vector will score how well the input matches the j-th class. Formally, we have a set of parameters $W = \{w^{(1)}, \ldots, w^{(C)}\}$ where each $w^{(j)} \in \mathbb{R}^d$. Given an input x, the score for the j-th class is $w^{(j)\top}x$, where higher score corresponds to higher probability of x being from class j.

Now let's talk about how you get probabilities here. Intuitively, the model should predict whichever class j has the highest value of $w^{(j)\top}x$. But we can't directly use these dot product

scores as probabilities, since some might be negative. A natural thing to do is to first apply the exponential function, ensuring the score for every class is positive. Then we can simply normalize by the sum to get a probability distribution.

Translated into math, we get the following:

$$p(y = j \mid x; W) = \frac{\exp(w^{(j)\top} x)}{\sum_{k=1}^{C} \exp(w^{(j)\top} x)}. \tag{2.11}$$

This function—exponentiating everything and then normalizing—has a special name, called the **softmax** function. Let's try to understand what this function does. Suppose $K = 3$ and we have the following:

$$\begin{aligned} w^{(1)\top} x &= 2 \\ w^{(2)\top} x &= 1 \\ w^{(3)\top} x &= -3 \end{aligned}$$

These pre-softmax values are often referred to as the **logits**. (This term can also be used to refer to $w^\top x$ in logistic regression, i.e., what you get before the sigmoid function.)

After we exponentiate, we get:

$$\begin{aligned} \exp(w^{(1)\top} x) &\approx 7.4 \\ \exp(w^{(2)\top} x) &\approx 2.7 \\ \exp(w^{(3)\top} x) &\approx 0.1 \\ \sum_{k=1}^{3} \exp(w^{(k)\top} x) &\approx 7.4 + 2.7 + 0.1 = 10.2 \\ p(y = 1 \mid x; W) &\approx 7.4/10.2 \approx .72 \\ p(y = 2 \mid x; W) &\approx 2.7/10.2 \approx .27 \\ p(y = 3 \mid x; W) &\approx 0.1/10.2 \approx .01 \end{aligned}$$

What has happened? The softmax function found the index with the largest value (here, $k = 1$) and put most of the probability mass on this value. This is another one of those cases where the name of the function is misleading. You might think that softmax should be a "soft" version of the max function, but this is not the case. It is more similar to a soft arg max.

2.3.1 Objective and Cross Entropy

What do we do now? Once again we apply the principle of Maximum Likelihood Estimation: We search for the W that maximizes the (log-)probability of the data with gradient descent. By now, we know that we will want to maximize likelihood, which is the same as maximizing log-likelihood, which is the same as minimizing negative log-likelihood, which is the same as minimizing $\frac{1}{n}$ times the negative log-likelihood So I'm just going to skip straight to the last part:

$$\begin{aligned} L(W) &= -\frac{1}{n} \sum_{i=1}^{n} \log P(y^{(i)} \mid x^{(i)}; W) \\ &= -\frac{1}{n} \sum_{i=1}^{n} \left(w^{y^{(i)}\top} x - \log \sum_{k=1}^{C} \exp(w^{(k)\top} x^{(i)}) \right) \end{aligned}$$

This objective is also sometimes called the **cross-entropy loss**, because we can view it as the cross-entropy between the true label distribution and our predicted label distribution. For two distributions p and q over $\{1, \ldots, C\}$, the cross-entropy is defined as

$$H(p, q) = -\sum_{k=1}^{C} p_k \log q_k.$$

Cross-entropy is a measurement of how well q "covers" the distribution of p, where lower cross-entropy signifies that q is close to p. It is minimized when $q = p$, in which case it equals the entropy of p.

If we define $p_k^{(i)}$ to be 1 when $k = y^{(i)}$ and 0 otherwise, and $q_k^{(i)}$ to be our model's predicted distribution on example i, then our objective is simply minimizing cross-entropy:

$$L(W) = \frac{1}{n} \sum_{i=1}^{n} \sum_{k=1}^{C} -p_k^{(i)} \log q_k^{(i)}$$

2.3.2 Gradients

We take a gradient in much the same way. Let's focus on the gradient with respect to $w^{(c)}$, the weight vector for class c, i.e., $\nabla_{w^{(c)}} L(W)$.

The gradient for the first term is easy—it's either $x^{(i)}$ if $y^{(i)} = c$ or 0 otherwise.

The second log-sum-exp term is a bit more complex, but we can handle it with the chain rule:

$$\nabla_{w_c} \log \sum_{k=1}^{C} \exp(w^{(k)\top} x^{(i)}) = \frac{1}{\sum_{k=1}^{C} \exp(w^{(k)\top} x^{(i)})} \cdot \exp(w^{(c)\top} x^{(i)}) \cdot x^{(i)} \tag{2.12}$$

All we had to do is apply the chain rule twice, first to log and then to exp. Rewriting this, this is simply

$$q_c^{(i)} \cdot x^{(i)}.$$

Putting this all together, the full gradient expression is (folding in the negative signs):

$$\frac{1}{n} \sum_{i=1}^{n} (q_c^{(i)} - \mathbb{I}[y^{(i)} = c]) \cdot x^{(i)}.$$

This is kind of similar to logistic regression, in that again we have a scalar times $x^{(i)}$. There are two cases now. If $y^{(i)} \neq c$, then the scalar is positive, so we will subtract some multiple of $x^{(i)}$ to w_c. If $y^{(i)} = c$, then the scalar is negative (since q_c is a probability distribution), its entries are always ≤ 1, so when we do gradient descent we add. This makes intuitive sense in both cases.

2.3.3 Relationship to logistic regression

You might be wondering whether we can also use softmax regression when $K = 2$. It winds up essentially being the same as a reparameterized version of logistic regression.

Let w_0 and w_1 be the weight vectors for the two classes in binary classification. Then we have:

$$\begin{aligned} P(y = 1 \mid x; w) &= \frac{\exp(w_1^\top x)}{\exp(w_1^\top x) + \exp(w_0^\top x)} \\ &= \frac{1}{1 + \exp((w_0 - w_1)^\top x)}. \end{aligned}$$

This is just the same as logistic regression with parameter $w = w_1 - w_0$. Intuitively this makes sense—$w_1 - w_0$ is the key vector of interest because it captures what differentiates a positive example from a negative example.

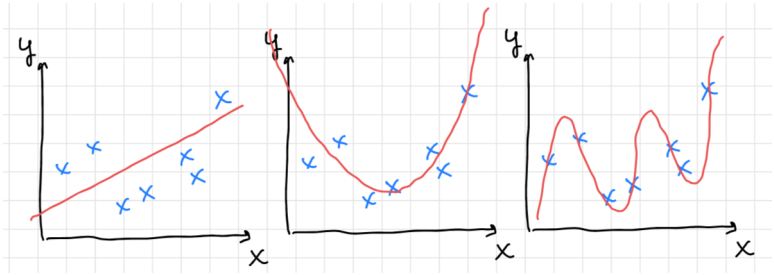
Chapter 3

Overfitting and Regularization

So far, we've talked a lot about training models—either regression or classification models. But just because we have run training correctly doesn't guarantee that the model is good or useful!

3.1 Overfitting

When we train a model, we find parameters that lead to low loss on the training data. Let's consider a simple example where we use linear regression with polynomial features to fit a dataset. We can use either linear features only, linear and quadratic features, or features up to degree 7. These three options might result in the following three predictors:

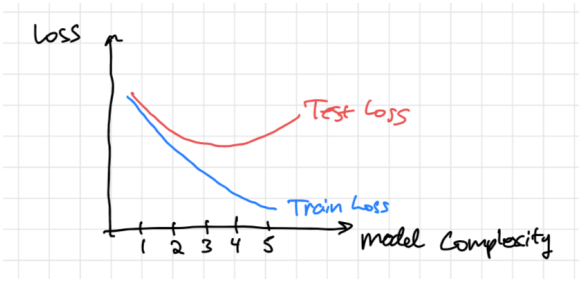


The first function seems to be too simple to fit the data well. We call this **Underfitting**. The second function seems to roughly capture the key trends. What about the last function? It perfectly fits all of the data, so it achieves zero training loss. But it seems like it has done so by fitting a lot of non-meaningful fluctuations. This is known as **Overfitting**. But by what principle do we avoid doing this? Based on training error, this is the best possible function.

3.2 Splitting your data

Okay, how do we detect that using a high-degree polynomial is a worse predictor, even though it fits the data better? The ultimate litmus test is whether our model makes good predictions on new, unseen examples. We use a **test dataset**, a separate dataset from the training dataset that's only used for evaluation. Accuracy on the test dataset is a proxy for how well the model predicts on a *new* example, which is actually what we care about. We don't actually care about how well we fit the training data—we already know the training labels!

Plotting train vs. test loss. A common way to visualize the difference between training loss and test loss is to plot the loss as a function of how complex your model is:



For a while, increasing the complexity of your model improves both training loss and test loss. But if you keep increasing it more, you improve training loss but hurt test loss! This is the regime where you are overfitting.

3.2.1 Development Sets

Okay, so we now understand why we might not want to throw all possible features into our model. But how do we decide exactly which features to use? The best way to do this is with a **development set**, also known as a validation set. The point is that you should actually always have three separate datasets. The training dataset is for training the model. The development set helps you choose **hyperparameters**, such as how many features to use. You can also use it to decide what is the best learning rate for gradient descent, or other settings of your training method that we'll talk about later. Once you do this, you evaluate on the test set to estimate how good your model is on unseen examples.

Hopefully it's clear why we can't choose hyperparameters on the training set (we'll always choose to have all the features). But why is separating the dev set and test set important? If you fit hyperparameters on the test set and then evaluate on that test set, you will have "cheated" in some way. We can draw an analogy to taking an exam:

- If you use the same dataset for training and evaluation, that's like cheating on an exam by getting a copy of it ahead of time and memorizing all the answers. It's very obvious here that your performance on the exam does not reflect your actual ability.
- If you use the same dataset for choosing hyperparameters and evaluation, that's like if you got to take the exam 100 times, where you get your memory wiped in between tries, but then you get to keep the best score out of those 100 tries. (Each "try" represents a different hyperparameter setting.) There's going to be some random fluctuation in how well you do on that exam, so at some point you're going to get lucky and do better than your average score. So this is still an overestimate of your true ability.

3.2.2 Splitting your dataset

In the real world, usually you're not given a dataset with pre-defined train, development, and test subsets. For example, if you're predicting house prices, you just have one big dataset of houses that have been sold and what their sale price was. So, before you do any machine learning, you first need to **split** your dataset into train, development, and test subsets (more commonly referred to as "splits"). The simplest way to do this is to randomly partition the dataset into three subsets. Usually you would reserve the most data for training, since that determines how well your model

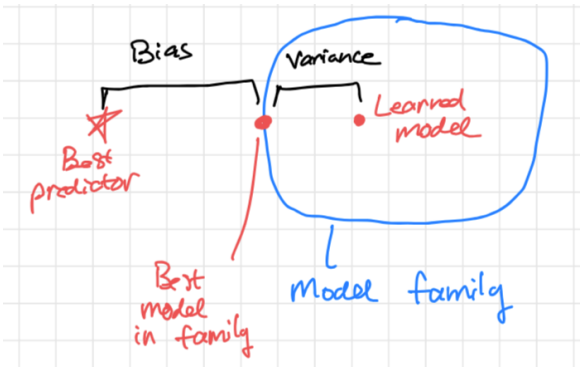


Figure 3.1: Illustration of the bias-variance trade-off. Bias describes the difference between the optimal predictor and the best predictor in the model family. Variance describes the difference between the best predictor in the model family and the predictor that we actually learn. Both together define how much worse our model is than the optimal function.

will work. Something like 70% train, 10% development, and 20% test is often reasonable, although you also want to make sure your development and test sets aren't too small (otherwise you won't be able to reliably estimate how well your model is doing).

3.3 Bias and Variance

One way to conceptualize the danger of overfitting is the **bias-variance tradeoff,** as illustrated in Figure 3.3. Any machine learning model will make mistakes for one of two reasons:

- **Bias.** Bias refers to errors that arise because assumptions of the model do not match the reality of the task. For example, maybe your model assumes that y is a linear function of your features. This is probably not literally true, which puts some upper bound on how well your model can fit the data. In general, whenever we use a machine learning algorithm, we are restricted to a particular **model family**—the set of possible functions we can learn. For linear regression, the model family is the set of linear functions of the features. Bias arises when our model family is too small to represent the actual function we're trying to model. When we have large bias, our models will underfit the training data.

- **Variance.** Variance is error from sensitivity to small fluctuations in the training set. Suppose we assume we need polynomial features of degree 20. There might be a "best" 20-degree polynomial, but given a finite training dataset you might learn one that is not as good. The difference between what you find and the best possible thing within your function class is variance. The larger your model family is, the larger your variance will be—when you have more candidates, it's harder to identify the best one. When we have high variance, our models are likely to overfit the training data.

Overall, our test accuracy is determined by both bias and variance. So, we must always be careful to achieve a good balance to avoid having either very high bias (underfitting) or very high variance (overfitting).

Note that some bias is always necessary in the real world. In the extreme, you can consider the function class of "all possible functions." This always has zero bias, but you also can never learn anything—no training dataset can tell you how to choose between the infinite possible functions

that perfectly fit your data but make different predictions on unseen data. The whole point of machine learning is that labels on seen examples must give you *some* information about labels on unseen examples. This is known as **inductive bias**, and is captured by the saying, "All models are wrong, but some are useful."

3.4 Regularization

How else can we prevent overfitting? The bias-variance diagram suggests that in order to do this, we should try to restrict the set of functions under consideration. Reducing the number of features is one way to do this. Another common idea is **regularization**. The idea of regularization is to impose a soft constraint to encourage "simpler" functions.

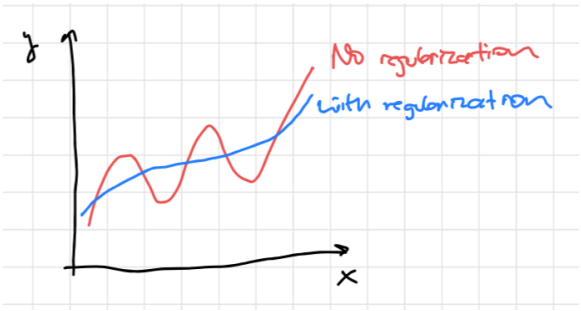
3.4.1 L_2 Regularization

Let's start with the most common version, called L_2 regularization. We simply add a term to the loss function that penalizes the L_2 norm of our parameters. For linear regression, this looks like:

$$L(w) = \left(\frac{1}{n} \sum_{i=1}^{n} (w^\top x^{(i)} - y^{(i)})^2 \right) + \lambda \|w\|^2.$$

Recall that $\|w\|^2 = \sum_{i=j}^{d} w_j^2$, just the sum of squared entries of w. The λ is a **hyperparameter** that determines how much we want to constrain w to have a small L_2 norm. $\lambda = 0$ corresponds to no regularization.

How does reducing the norm reduce the complexity of our function? In the linear regression case, this basically means we can only learn a polynomial whose coefficients aren't that large. This means it cannot have too many wiggles in it.



Note that L_2 regularization can be combined with any of the methods we've seen (logistic or softmax regression). Its overall effect is always the same—it encourages the w you learn to have smaller norm, which decreases the size of the model family and helps reduce overfitting.

Gradient for L_2 regularization. The L_2 regularization term just gets added to the original loss function, so its gradient also just gets added to the gradient for the original loss function. The gradient is simply:

$$\nabla_w \lambda \|w\|^2 = 2\lambda w.$$

Note that this is analogous to the derivative of x^2 in one dimension, since $\|w\|^2$ is just the sum of the squares of each element of w.

During gradient descent, we step in the direction of the negative gradient. Thus, the effect of L_2 regularization is that we always update w_j *towards* 0. If w_j is a large positive number, we will step in the negative direction; if it's a large negative number, we will step in the positive direction.

3.4.2 Maximum a Posteriori Estimation

There's yet another way to justify the use of regularization, and it relates to yet another probabilistic story. For this, we have to talk about Frequentism and Bayesianism.

So far, when we've done MLE, we've adopted a frequentist view of things: There's some true value of the parameters out there in nature, and our goal is to estimate that real value as close as possible.

An alternative is a Bayesian viewpoint: The parameters themselves are a random variable that are drawn from some distribution. In this view, we can view regularization as coming from a **prior distribution** on the parameter.

It's time to introduce the Bayesian version of MLE, called **Maximum a Posteriori Estimation** (MAP). In MAP, we imagine computing a posterior over the parameters conditioned on the data:

$$P(w \mid D) = \frac{P(w)P(D \mid w)}{P(D)}.$$

In MAP estimation, we find the w that maximizes $P(w \mid D)$—i.e., the most likely w according to the posterior distribution. The $P(D \mid w)$ term is the same thing we saw in MLE. The $P(w)$ term is the new thing, which is the prior. Finally, the denominator doesn't depend on w so it doesn't matter.

Where does L_2 regularization come from? Let's assume that $P(w)$ is a Gaussian, in particular that each component w_j is distributed as an independent Gaussian with variance σ^2 and mean 0. Then the $P(w)$ term is

$$\prod_{j=1}^{d} \frac{1}{\sigma\sqrt{2\pi}} \exp(-w_j^2/2\sigma^2).$$

Analogously to MLE, in MAP we want to find the w that is most likely under the posterior distribution $P(w \mid D)$; in other words, we want to maximize $P(w \mid D)$ with respect to w. As we know, this is equivalent to minimizing the negative log of $P(w \mid D)$. So we have

$$\begin{aligned}
-\log P(w \mid D) &= -\log P(w) - \log P(D \mid w) + \log P(D) \\
&= -\left(\sum_{j=1}^{d} -\log(\sigma\sqrt{2\pi}) - \frac{1}{2\sigma^2} w_j^2\right) - logP(D \mid w) + C_1 \\
&= \frac{1}{2\sigma^2} \sum_{j=1}^{d} w_j^2 + \log P(D \mid w) + C_2 \\
&= \frac{1}{2\sigma^2} \|w_j\|^2 + \log P(D \mid w) + C_2,
\end{aligned}$$

where C_1 and C_2 are constants that do not depend on w, so we can ignore them when trying to minimize this objective. Note that the second term is exactly the loss function for MLE (up to multiplication by a constant). THe first term is exactly L_2 regularization, where σ controls the strength of the regularization (i.e., $\lambda = \frac{1}{2\sigma^2}$). Smaller σ means a stronger prior towards small values, hence more regularization.

3.4.3 L_1 Regularization

Another common approach to regularization is to use L_1 regularization, which penalizes the 1-norm rather than the 2-norm. More formally, we add $\lambda\|w\|_1$ to the loss function, where

$$\|w\|_1 = \sum_{j=1}^{d} |w_j|.$$

Again, λ is a hyperparameter that controls how much regularization we want to add.

Gradient for L_1 regularization. To obtain the gradient, let's take the partial derivative of the L_1 regularization term with respect to w_j. We can show that

$$\frac{\partial}{\partial w_j}\lambda\|w\|_1 = \lambda \operatorname{sign}(w_j),$$

where the sign function is defined to be 1 if its input is positive, -1 if its input is negative, and 0 otherwise. So, overall we can write

$$\nabla_w \lambda\|w\|_1 = \lambda \operatorname{sign}(w)$$

where we understand $\operatorname{sign}(w)$ to denote element-wise application of sign to the vector w.

Comparison with L_2 regularization. Comparing the two gradient expressions helps us understand the difference between L_1 and L_2 regularization. In both cases, the gradient update rule always tells us to step towards 0. In L_2 regularization, we do a large gradient descent update if w_j is far from 0, and a small update when w_j is close to 0 (since the size of the step is just proportional to $|w_j|$). In L_1 regularization, we do a fixed size step no matter how big w_j is. Thus, L_1 has a **sparsifying effect**. It will keep pushing w_j to be smaller and smaller until it's at 0. But if w_j is already very large, it will not try to change it by a lot to get it closer to 0. In contrast, L_2 regularization prevents $|w_j|$ from getting too large by doing very large steps when that happens, but it does not really push it to be exactly 0.

In practice, L_2 regularization is often used by default unless there is a reason to want a sparse vector w (i.e., a w where many entries are exactly 0). Sparse vectors may be easier to understand, since we can just ignore certain features that correspond to a weight of 0. It is also possible to mix the two at the same time.

Chapter 4

Normal Equations for Linear Regression

So far, our recipe for coming up with machine learning problems has been the following:

1. Come up with a probabilistic story for how the data was generated.
2. Write down a loss function for which minimizing that function is equivalent to maximizing the likelihood of the data.
3. Optimize the loss function using gradient descent.

While gradient descent is undoubtedly the single most important and widely-used technique for optimizing loss functions in machine learning, it is not the only option. For linear regression, the optimal weight vector w actually has a closed-form solution given by the **Normal Equations**. In this chapter, we will sketch out how to derive this closed-form equation and what its implications are.

4.1 Deriving the Normal Equations

The basic strategy is something you may remember from your calculus class. We want to find the minimum of a convex function. We can do this by taking the gradient and setting it equal to zero. Recall the intuition for this: At the minimum of the function, there's no direction you can step in that would further decrease the value. That must mean that the derivative in every direction is zero, i.e., the gradient is zero.

So, let's start by writing down the gradient from the last lecture and setting it equal to zero.

$$\nabla_w L(w) = \frac{1}{n} \sum_{i=1}^{n} 2 \cdot \left(w^\top x^{(i)} - y^{(i)} \right) \cdot x^{(i)} = 0 \tag{4.1}$$

$$\sum_{i=1}^{n} w^\top x^{(i)} \cdot x^{(i)} = \sum_{i=1}^{n} y^{(i)} \cdot x^{(i)} \tag{4.2}$$

Keep in mind that both sides of this equation are vectors.

It turns out that both sides can be simplified quite a bit. To do this, I'm going to define the matrix $X \in \mathbb{R}^{n \times d}$ such that its i-th row is $x^{(i)}$. (Recall that n is the number of training examples and d is the number of features.) X is called the **design matrix**. Similarly, let's define the vector $y \in \mathbb{R}^n$ to be the vector of $y^{(i)}$'s.

Let's start by simplifying the right-hand side. This equation looks quite a bit like matrix multiplication—recall that one way to think about matrix multiplication is that you take a linear combination of *columns* of the matrix weighted by the entries of the vector. Since $x^{(i)}$'s are rows in X, but our expression is a linear combination of columns, we need to transpose X first. Thus, we can rewrite the right-hand side simply as $X^\top y$.

Now let's look at the left side. First I'm going to rearrange some pieces

$$\sum_{i=1}^{n} w^\top x^{(i)} \cdot x^{(i)} = \sum_{i=1}^{n} (x^{(i)\top} w) \cdot x^{(i)} \qquad \text{Dot product is symmetric} \tag{4.3}$$

$$= \sum_{i=1}^{n} x^{(i)} \cdot (x^{(i)\top} w) \qquad \text{Multiply scalar on right instead of left} \tag{4.4}$$

$$= \sum_{i=1}^{n} (x^{(i)} x^{(i)\top}) w \qquad \text{Matrix multiplication is associative} \tag{4.5}$$

$$= \left(\sum_{i=1}^{n} x^{(i)} x^{(i)\top} \right) w \qquad \text{Factor out } w \tag{4.6}$$

Essentially, we have carefully rearranged things so that we have a column vector (which can be thought of as a $d \times 1$ matrix) times a scalar (roughly speaking, a 1×1 matrix), so that we can safely multiply them as matrices and invoke the fact that matrix multiplication is associative.

Now, we just have to notice that

$$\sum_{i=1}^{n} x^{(i)} x^{(i)\top} = X^\top X. \tag{4.7}$$

I think the easiest way to convince yourself of this is simply to ask what the ij-th entry of each matrix is. In both cases, you'll find that it is equal to $\sum_{k=1}^{m} x_i^{(k)} x_j^{(k)}$. On the left side, $x_i^{(k)} x_j^{(k)}$ is the ij-th entry of each term in the sum. On the right side, the whole expression is the dot product of the i-th column of X (i.e., row of $X^\top$) with the j-th column of X.

Putting it all together. Okay, so what have we accomplished? Putting everything together, we have that setting the gradient equal to zero is equivalent to

$$(X^\top X)\theta = X^\top y. \tag{4.8}$$

Even if you don't remember this exact equation, you should remember the form—this is a linear equation with d equations and d unknowns.

How can we solve this? Well, we can invert the matrix $X^\top X$. This gives us the solution for w:

$$w = (X^\top X)^{-1} X^\top y. \tag{4.9}$$

4.2 Uniqueness and Non-invertibility

One thing that's immediately apparent from the Normal Equations formula is that we've implicitly assumed that $X^\top X$ is invertible. If that is true, then there is a unique w that minimzes the linear regression loss, and the Normal Equations find that w. But it's also possible for $X^\top X$ to not be invertible. Let's examine a few scenarios where that would happen.

More features than examples. One important cases is when there are more features than training examples. Recall that we use d to denote the number of features (i.e., the dimensionality of the data and of w) and n to denote the number of training examples. X is an $n \times d$ matrix. So, $X^\top X$ is a $d \times d$ matrix, but if $n < d$, then it can have rank at most n. This is because each column of $X^\top X$ is a linear combination of the columns of $X^\top$ (this is a basic property of matrix multiplication), and there are only n columns in $X^\top$ (it is a $d \times n$ matrix). Finally, recall that if a $d \times d$ matrix is not full-rank (i.e., its rank is $< d$), it is not invertible.

Dealing with non-invertibility To account for the fact that $X^\top X$ may not be invertible, the workaround is to use something called the pseudoinverse of $X^\top X$, denoted $(X^\top X)^+$. The pseudoinverse of a matrix M is equal to M^{-1} when M is invertible, and otherwise computes a generalization of the inverse. No matter whether $X^\top X$ is invertible or not, choosing

$$w = (X^\top X)^+ X^\top y$$

will always give **a** solution to the linear regression problem. If there are fewer examples than features, the resulting w will actually achieve 0 loss on the training set, which sounds good. Numpy has a special function (`numpy.linalg.pinv`) that will compute the pseudoinverse for you.

The problem from a machine learning is the issue of **generalization**. When $X^\top X$ is not invertible, there is not just a single w that minimizes the linear regression loss—there are many. Using the psuedo-inverse gives you one solution, but it's not the only one. We say that the training data **under-constrains** the choice of w: there is not enough information to choose between all these many w's that all look good based on training loss alone. But it's very likely that some of those w's have much better test loss than the other ones. In other words, when we have more features than examples, we will have **high variance**, following the bias-variance discussion from the previous chapter.

Redundant features. Another situation that can cause non-invertibility is the existence of redundant features. Suppose that the features at indices i and j that are identical—$x_i^{(k)} = x_j^{(k)}$ for all examples k. Then, $X^\top X$ would become non-invertible. To see this, note that this means that the i-th and j-th columns of X are identical. That means that the vector $v = e_i - e_j$, where e_i is the i-th basis vector, is in the null space, as Xv is just the i-th column minus the j-th column. A square matrix with non-trivial nullspace is not invertible.

The practical takeaway from this is that having redundant features can cause problems when solving for w. Essentially, when there are redundant features, there are many equally good values of w (e.g., you could learn a very positive weight for w_i and very negative weight for w_j, and they would cancel out). This makes things potentially unstable!

Even if you're solving linear regression with gradient descent, redundant features are annoying, since they mean that your algorithm isn't converging to a single unique solution, but an entire subspace of solutions. Think of it this way: suppose you have two features that are *almost* identical. The inclusion of a single example could make you decide to rely on one feature vs. another feature. So the problem becomes very *sensitive* to small changes in the input dataset, which can lead to unintuitive behavior.

Chapter 5

Generative Classifiers and Naive Bayes

Today, we will learn a different approach to classification called generative classifiers. We will look at one prototypical example of a generative classifier, Naive Bayes. As before, we'll assume there are C classes, where C may equal 2 or may be > 2.

We will focus first on a particular variant of Naive Bayes that is used for text classification tasks (i.e., x is a piece of text). After that, we will look at the more general Naive Bayes method that applies to any feature vector x.

5.1 Generative Classifiers Overview

So far, everything we've seen is a **discriminative** classifier. That means we're only modeling $p(y \mid x)$. All of our probabilistic stories were only about how y was created given x. But there is another way.

In a **Generative** classifier, we model the joint process of generating the x's and the y's. This allows us to use Bayes Rule to compute the final $p(y \mid x)$:

$$P(y = k \mid x) = \frac{P(y = k)P(x \mid y = k)}{P(x)} = \frac{P(y = k)P(x \mid y = k)}{\sum_{k'=1}^{C} P(y = k')P(x \mid y = k')}.$$

Let's remind ourselves about how expressions like this work. The numerator has two terms:

- The prior distribution over y. For classification, this can usually be easily estimated just by counting the frequency of each label.
- The conditional probability of x given y. If x is some complicated object, this may not be easy to do! However, there are some helpful modeling assumptions we can make that are false, but still useful in practice. Remember that "All models are wrong, but some are useful."
- The denominator is simply a normalizing constant. For classification, it's very easy because we just sum over the possible labels.

At test time, we are given a new x. If we have a learned way to compute $P(y)$ and $P(x \mid y)$ for all possible values of y, then we can compute $P(y \mid x)$. We can then predict the most likely y, i.e. the k for which $P(y = k \mid x)$ is largest.

Now, we will discuss Naive Bayes, which is one family of methods for estimating $P(y)$ and $P(x \mid y)$.

5.2 Naive Bayes for Text Classification

Now let's focus on a classic generative classifier called Naive Bayes. First, let us assume we are doing **text classification**, which just means that our inputs x are pieces of text (I will also refer to these as "documents"). We write that each input $x = (x_1, \ldots, x_d)$ where each x_j is a word belonging to a vocabulary V (i.e., a set of possible words).

The key to Naive Bayes is to make the following simplifying assumption when modeling $P(x \mid y)$:

$$\textbf{Naive Bayes Assumption:} \quad P(x \mid y) = \prod_{j=1}^{d} p(x_j \mid y).$$

This says that conditioned on the label y, each word of x is sampled *independently*.

We will also invoke a second assumption that is specific to text documents: we will also assume that for every j, the distribution $p(x_j \mid y)$ is identical. In other words, the first word, second word, third word, etc. all are drawn from the same distribution. Together, these two assumptions define a particular version of Naive Bayes known as **Multinomial Naive Bayes**.

Note that we don't really believe that either of these assumptions is true. In fact, they are both clearly false, given the complexities of real human language. Nonetheless, for many practical tasks, these assumptions are good enough to give us useful algorithms. In particular, if we mainly expect that the set of words used in different documents will change from one label to the next, then Naive Bayes can detect these sorts of changes. In a hypothetical situation where two labels were different only because of the order of words used, for instance, Naive Bayes would fail to distinguish them, but you can imagine that such situations may be rare.

We can think of Naive Bayes as positing yet another probabilistic story. This time, instead of just thinking about how the y's are generated, we will model how a piece of text x and its corresponding label y are *jointly* generated:

1. The label is first sampled from the prior distribution $P(y)$.
2. Each of the d words of x are then sampled *independently* from the conditional distribution $P(x_j \mid y)$.

5.2.1 Parameters

What are the parameters of our model? In general, parameters are whatever we are trying to learn from data, and they determine the predictions made by our method. For logistic regression, our parameters were weight vectors w that got dot-producted with the inputs. In the case of Naive Bayes, the parameters are just the probabilities associated with $P(y)$ and $P(x_j \mid y)$, which we will learn from our training data. So, the parameters are:

1. The prior term $p(y)$. If we have C classes, this is a distribution over the C classes, so the needed parameter vector is a vector $\pi \in \mathbb{R}^C$ where $P(y = k) = \pi_k$.
2. The posterior term $p(x \mid y)$. Given our Naive Bayes assumption, this boils down to knowing $p(x_j \mid y)$ for each possible value of y. This is a probability distribution over the vocabulary V, so it can be described by $|V|$ parameters, each of which denote the probability of a particular word $w \in V$ being generated conditioned on the label y. So, we have a total of $|V| \cdot C$ parameters. We can think of these as a $|V| \times C$ matrix called τ, where $\tau_{wk} = P(x_j = w \mid k)$.[1]

[1]Note that we're indexing into τ with actual words w rather than numerical indices. If this bothers you, you can equivalently imagine numbering all the words in the vocabulary from 1 to $|V|$ and using those numbers as indices.

5.2.2 Learning with MLE

Okay, so how do we estimate these parameters? Let's apply the principle of maximum likelihood yet again (or equivalently, minimizing the the negative log-likelihood). But this time, we will be modeling the probability of the x's and the y's in our dataset.

$$\begin{aligned} L(\pi, \tau) &= -\sum_{i=1}^{n} \log P(x^{(i)}, y^{(i)}) \\ &= -\sum_{i=1}^{n} \log P(y^{(i)}) + \log P(x^{(i)} \mid y^{(i)}). \end{aligned}$$

It's apparent that the first term depends only on π and the second one only depends on τ, so we can find the optimal π and τ by looking only at the first term and second term, respectively.

Learning π. Let's start with the first one. Summing up all the first terms, we have:

$$-\sum_{i=1}^{n} \log P(y^{(i)}) = -\sum_{k=1}^{C} \text{count}(k) \log \pi_k$$

where $\text{count}(k)$ is the amount of times that label k appears among the n training examples.

When $C = 2$, you can see that this is exactly your homework problem! You have a "coin" that is either $y = 1$ or $y = 2$. So as you recall, the solution is to make

$$\pi_1 = \frac{\text{count}(y = 1)}{n}, \pi_2 = \frac{\text{count}(y = 2)}{n}.$$

This is intuitive—you just compute the empirical distribution over the classes.

Now what if $C > 2$? You can think of this as observing a bunch of dice rolls, as opposed to a bunch of coin flips. But it turns out that the solution is basically the same. Let's just consider a particular choice of k in isolation and think about the optimal choice of π_k. Well, we can think of every example as either being from class k or not from class k, and the probability of the former is π_k. So, this is just like the coin flip example, and so the MLE estimate for π_k is just

$$\boxed{\pi_k = \frac{\text{count}(y = k)}{n}}.$$

Learning τ. Now let's think about the other term, which only includes τ but not π. I won't go through the algebra since it's a bit tedious; instead I will argue that conceptually this is basically the same as the case with π.

First, recall that we have a completely separate probability distribution $P(w_j \mid y)$ for each choice of y. So we can think of our dataset being split into C smaller datasets, each of which only contains examples where $y = k$ for some k. The log-likelihood of all the data is sum of the log-likelihoods of each subset, and within each smaller dataset the only parameters that affect the likelihood are τ_{wk} for one choice of k. So we can just consider each value of k in isolation.

Now, we have assumed that each word of each example with $y = k$ is generated independently from the same distribution, namely the one where $P(x_j = w \mid y = k) = \tau_{wk}$. This is kind of like we have a bunch of observations from a $|V|$-sided dice.

Let $\text{count}(w, y = k)$ be the number of times we see the word w in an example whose label is k. By the same logic we used earlier, the MLE choice for τ_{wk} is

$$\tau_{wk} = \frac{\text{count}(w, y = k)}{\sum_{w \in V} \text{count}(w, y = k)}.$$

Note that the denominator is the total number of observations we have for this particular $|V|$-sided dice, i.e., the total number of all words we've seen in examples that have the label $y = k$.

5.2.3 Laplace Smoothing

If you just use the above model naively, you are very likely to get poor results. Why? Suppose you get a pretty long document to classify. At least one of the words might be such that in the training dataset, it happened to only appear when $y = 1$. And another word might be such that in the training dataset, it happened to only appear when $y = 2$. Now what happens? Well, $P(x \mid y = 1)$ will be 0, as will $P(x \mid y = 2)$! In other words, your model just says that your input is impossible, and will not tell you anything useful.

The important lesson here is this: **Never assign probability zero to events that could plausibly happen!**

We can fix this problem with **pseudocounts**. Let's just pretend that we've actually seen every possible word-label combination λ times before. This adds λ to every $\text{count}(w, y = k)$. As a result of seeing each word λ times with $y = k$, our total number of observations seen with $y = k$ increases by $\lambda \cdot |V|$. So our new formula becomes:

$$\tau_{wk} = \frac{\text{count}(w, y = k) + \lambda}{\left(\sum_{w \in V} \text{count}(w, y = k)\right) + |V| \cdot \lambda}.$$

λ is a hyperparameter of the method. In practice, you normally choose a very small λ. Note that you are even allowed to choose λ that is not an integer, for example $\lambda = 0.1$.

5.2.4 Working in log space

At test time, we're given a document x and want to estimate $P(y \mid x)$. This involves computing $P(x \mid y) = \prod_{j=1}^{d} P(x_j \mid y)$ for all possible values of y. Note that each term in this product is a probability that is probably quite small. When you multiply many small numbers together on a computer, you will run into **numerical underflow**: the numbers will become too small to represent with normal floating-point numbers, and your computed value for $P(x \mid y)$ will just be 0.

To solve this, we often "work in log space." That means that instead of computing $P(x \mid y)$, we will actually compute

$$\log P(x \mid y) = \sum_{j=1}^{d} \log P(x_j \mid y).$$

This sum will not underflow anymore, since we're just adding up a bunch of not-that-negative numbers.

In the end, to make a prediction, we can compute $\log\left(P(x \mid y)P(y)\right) = \log P(x \mid y) + \log P(y)$ for each possible value of y. We know that the value of y that makes this largest also has the largest $P(y \mid x)$, so that becomes our prediction.

5.3 Naive Bayes for General Feature Vectors

Naive Bayes is applicable to much more than just text classification. Let's now consider the case where x is just some generic feature vector $\in \mathbb{R}^d$, as in linear/logistic/softmax regression.

The Naive Bayes assumption still holds exactly as before—we assume that

$$P(x \mid y) = \prod_{i=1}^{d} P(x_j \mid y).$$

Note that here, each x_j is a different feature, not a different word, since we're no longer assuming that x's are documents.

5.3.1 Parameters and Learning

In the general case, we no longer assume that all of the d features are sampled from the same distribution (just that they're independently sampled). So, to model $P(x \mid y)$, we have to model each feature individually, i.e., we will have separate parameters for each feature.

- **Binary features.** Some features are binary, i.e., they are either 1 or 0. For example, if we are classifying black-and-white images, each pixel could be one component of x_j, i.e. a 28×28 image would lead to $28^2 = 784$-dimensional vector ($d = 784$). If x_j is a binary feature, then for each possible $k \in \{1, \ldots, C\}$, $P(x_j \mid y = k)$ is completely described by a single parameter, which we can call p. To estimate p, we do the same thing we would do for estimating the probability of a coin landing heads:

  $$p = \frac{\text{count}(x_j = 1, y = k)}{\sum_{i=1}^{n} \mathbb{I}[y^{(i)} = k]}$$

  Note that here, for the denominator, we simply count the number of examples where $y = k$, as each feature shows up exactly once in each example; in contrast, for text, each example might contain a different number of words.

- **Categorical features.** Other features may take on more than two values. For example, suppose you are attempting to predict whether you will like a given song. You can frame this as binary classification—do you like the song or not? One relevant feature is the genre of the song, which can have M possible values (e.g., pop, country, classical, etc.). We can have one feature x_j whose value is the genre. Now, for each possible $k \in \{1, \ldots, C\}$, we would have a parameter vector $q \in \mathbb{R}^M$, where $q_m = P(x_j = m \mid y)$, the probability that x is of the m-th genre, conditioned on $y = k$. We would estimate this as:

  $$q_m = \frac{\text{count}(x_j = m, y = k)}{\sum_{i=1}^{n} \mathbb{I}[y^{(i)} = k]}$$

- **Numerical features.** Note that you can also incorporate real-valued features into Naive Bayes by assuming some probability distribution that they are sampled from. For instance, you could assume that $P(x_j \mid y)$ is a Gaussian distribution, and estimate its mean and variance based on the training data.

Finally, note that for a single x vector, you could have features of all these types. That is not a problem, since we're fitting a separate independent distribution $P(x_j \mid y)$ for each coordinate j.

5.3.2 Laplace Smoothing

Laplace smoothing for binary and categorical features works in much the same way as with text. For binary features, we assume we have seen both $x_j = 0$ and $x_j = 1$ λ times with each label. This adds 2λ to the denominator:

$$p = \frac{\text{count}(x_j = 1, y = k) + \lambda}{\left(\sum_{i=1}^{n} \mathbb{I}[y^{(i)} = k]\right) + 2\lambda}$$

Similarly, for a categorical variable with M possible values, we assume we see each possible value λ times with each label, which adds $M \cdot \lambda$ to the denominator:

$$q_m = \frac{\text{count}(x_j = m, y = k) + \lambda}{\left(\sum_{i=1}^{n} \mathbb{I}[y^{(i)} = k]\right) + M\lambda}$$

5.4 Generative vs. Discriminative classifiers

Overall, how do generative classification methods like Naive Bayes compare with the discriminative methods we saw earlier in class? Here are a few general advantages and disadvantages.

Advantages of discriminative classifiers:

- Usually have higher accuracy, especially when the dataset is large. $P(y \mid x)$ is simpler to model than $P(x \mid y)$, and is thus in some sense easier to learn.
- Arbitrary feature preprocessing is allowed. We don't have to worry if the input features are related, since we don't make any assumptions of conditional independence between features.

Advantages of generative classifiers:

- Learning is easier because you don't have to use an optimization method like gradient descent—you just count feature occurrences.
- It is easy to handle missing input features (just exclude them from the computation).
- Each class is modeled separately, so there's no need to retrain everything when you add a new class. In contrast, adding one new class for softmax regression would require completely retraining the model.

Chapter 6

Non-parametric Methods

So far, all the methods we've studied are **parametric** methods: our goal was to learn some set of parameters whose dimensionality (i.e., the number of parameters to learn) is fixed regardless of the training dataset size. For example, in logistic regression, our parameter was a single vector w of dimension d. In Naive Bayes, we learned some number of parameters proportional to the number of possible labels and the size of our vocabulary.[1] In all these cases, we use the training data to learn parameters, then use the parameters to predict on the test data. Once learning is finished, the training data is no longer needed to make predictions.

Today we will start discussing **non-parametric** methods: methods for which our model requires storing the training data in memory. The predictions that non-parametric methods make are dependent directly on the training examples. Why would we want to do this? We'll start with the simplest non-parametric method called k-Nearest Neighbors. Then we'll study a more sophisticated family of methods with a similar intuition, called kernel methods.

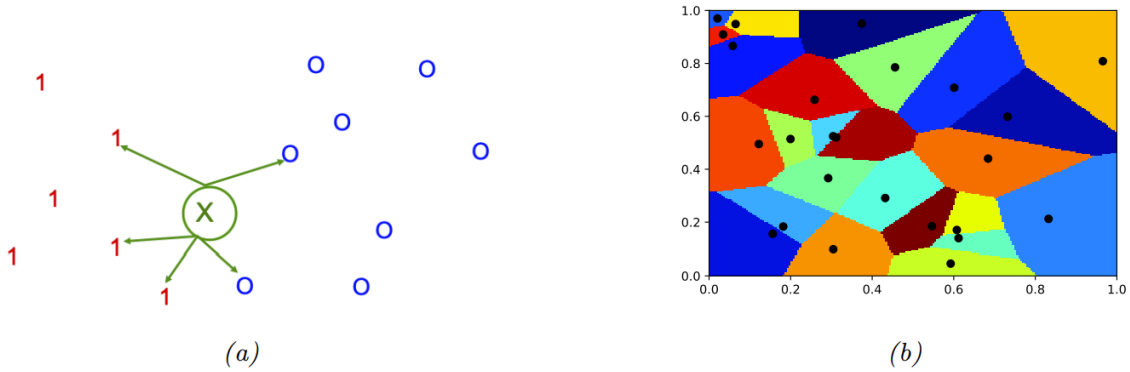
6.1 k-Nearest Neighbors

k-Nearest Neighbors (often abbreviated k-NN) is a classification algorithm motivated by a simple idea: similar examples are likely to have similar labels. Thus, when we get a new test input, we should predict the same label as the label for similar examples (i.e., "neighbors") from the training set.

Defining similarity. To define what examples are similar, we need to define some distance metric between examples. If our inputs x are vectors in $\mathbb{R}^d$, then one natural choice is to use the familiar Euclidean norm to define distance.

k-NN algorithm. The k-NN algorithm is very simple. The "training" step is simply to store the full training dataset in memory. At test time, we receive an input x that must be classified. We identify the k most similar points to x from the training dataset (i.e., the "nearest neighbors"), and return the most common label out of those nearest neighbors. Figure 6.1(a) shows an example with $k = 5$.

[1] Technically one could argue that the vocabulary increases in size as the training set grows. However, at some point your vocabulary will stop growing as you add new documents, since eventually you will have already seen all valid English words.



(a) *(b)*

Figure 6.1: (a) An illustration of k-NN for $k = 5$. Since 3/5 of the neighbors are of the $y = 1$ class, the overall prediction is $y = 1$. (b) An illustration of how 1-nearest neighbor classifies points. For each example (black dots), the surrounding colored region is the set of points for which that dot is its nearest neighbor. Thus, all points in each colored region would be given the same label as the corresponding black dot by 1-NN. Figure taken from Kevin Murphy's *Probabilistic Machine Learning* textbook.

Effect of k. k is a hyper-parameter that defines how many neighbors we care about. If we choose $k = 1$, then we would just find the single closest example and return its label. This is reasonable, but is in some sense "risky" because you're hoping that one example is correct. However, if that example is unusual or labeled incorrectly in your training data, you will get all of its neighbors wrong. The advantage of choosing a larger k is that you can average over a larger number of examples, thus reducing the impact of individual outliers or wrongly labeled datapoints.

Bias and variance. As illustrated in Figure 6.1(b), k-NN can learn highly expressive decision boundaries. Compared with logistic regression, which makes a strong assumption that the decision boundary is linear, k-NN has much lower bias, as it does not make any such assumption.

On the other hand, k-NN can suffer from variance issues and may not always generalize well to test data. This is especially true in high-dimensional settings, i.e., if d is large, due to the "curse of dimensionality." The problem is that the amount of "space" grows exponentially with d, and thus in high dimensions the space of possible x's is very large. This means that the vast majority of possible test points x will be "far away" from all your training points (because the space is so vast). Essentially, this means that even your nearest neighbor is not that similar to you, so k-NN will struggle.

6.2 Kernel Methods

Now we will move on to a second type of non-parametric methods known as kernel methods. Kernel methods are widely used and often a good default choice when faced with a new classification problem. Pedagogically, kernel methods are also interesting because they combine ideas from linear classifiers (e.g., logistic regression) and k-Nearest Neighbors.

6.2.1 Motivation

We will continue with the same basic motivation we had with k-Nearest Neighbors: examples that are similar usually have the same labels. While this intuition is good, k-NN operationalizes this in quite a simplistic way. There are no parameters to tune, and very little way to add in regularization to control variance (besides changing k). So, we would like to combine the intuition of k-NN with the machinery we've established for methods like logistic regression, where we fit parameters from training data and can add regularization to manage the bias-variance trade-off.

6.2.2 Kernels and kernelized predictors

To achieve this goal, we will introduce the concept of a kernelized predictor. Given a training dataset $\{x^{(1)}, \ldots, x^{(n)}\}$ and test input x^{test}, a kernelized predictor makes a prediction by computing:

$$f(x) = \sum_{i=1}^{n} \alpha_i k(x^{(i)}, x^{\text{test}}).$$

Here, $k(x, z)$ is a **kernel function** that measures the similarity between point x and z. $k(x, z)$ should be large for points that are similar, and small for points that are dissimilar. $\alpha \in \mathbb{R}^n$ is a vector of learned parameters, one per training example. While kernelized predictors can be used for all sorts of tasks, we will focus on binary classification. We will predict the positive class if $f(x) > 0$ and the negative class otherwise. So, you can think of $f(x)$ as being analogous to the expression $w^\top x$ in logistic regression, since in logistic regression we classify positive if $w^\top x > 0$ and negative otherwise.

One of the most popular kernel functions is called the **radial basis function** (RBF) kernel. It is defined by the following equation:

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

where σ^2 is a hyperparameter, also referred to as the "bandwidth."

This expression should look familiar to you, as it is basically the Gaussian pdf formula! When $x = z$, this function reaches its maximum possible value of 1. If x and z are very far apart from each other (in terms of Euclidean distance), then this tends to 0. The bandwidth parameter controls how quickly you go to 0, or in other words, how close x and z have to be to be considered "pretty similar." A smaller bandwidth means the points have to be very close together to be similar; a larger bandwidth means the points can be further apart and still be similar.

Note that even though we can refer to α as parameters of the model, this model is still a non-parametric, since the predictions depend on both α and the training data, and also the number of parameters in α grows with the size of the training data. "Parametric" means that the model is entirely described by a set of fixed-size parameters, and anything that is not parametric is "non-parametric."

6.2.3 A Second Look at Logistic Regression

So far, we've decided what form we want our model to have, and it has some parameters (the α_i's) that have to be learned. How can we learn these?

It turns out that the logistic regression algorithm we've already learned can also learn a kernelized predictor! To demonstrate this, I will show that logistic regression is already, in some sense,

learning a kernelized predictor with a particular choice of kernel. By understanding exactly how this is true, we can figure out how to learn the kernelized predictor for any kernel function we want.

Let's focus on logistic regression with L_2 regularization. We can distill everything about this method into two important equations:

1. At training time, we repeatedly apply the gradient descent update rule:

$$w^{(t+1)} = w^{(t)} + \eta \sum_{i=1}^{m} \sigma(-y^{(i)} \cdot w^\top x^{(i)}) \cdot y^{(i)} \cdot x^{(i)} \tag{6.1}$$

   where λ is the hyperparameter that controls how much L_2 regularization we do.

2. At test time, when we get a new example x^{test}, we make a prediction based on $w^\top x^{\text{test}}$.

The key insight is that this algorithm, as well as many other typical linear classification algorithms, **only cares about the x's through their dot products with each other.** I'll make this more precise in a second. What this implies is that we can potentially run this same algorithm with a generalized notion of dot products, rather than the conventional one in which you add up the product of entries of two vectors. It turns out that the RBF kernel is one suitable replacement for the standard dot product, and this will give us a kernelized predictor.

But before we get ahead of ourselves, I want to show what I mean by only caring about dot products. Let's define another kernel, called the dot product kernel, whose value is simply $k(x, z) = x^\top z$. I claim that I can rewrite logistic regression as learning a kernelized predictor using this particular kernel.

The key step is to notice that w **is always a linear combination of $x^{(i)}$'s.** Here we are assuming that we initialize $w^{(0)}$ to the zero vector, which is routine. In every gradient update, we add some scalar times $x^{(i)}$ for each i. Thus, we can equivalently represent w with a vector $\alpha \in \mathbb{R}^n$, where n is the number of training examples, and we define $\theta = \sum_{i=1}^{n} \alpha_i x^{(i)}$.

What happens to our update rule now? We can directly update α instead of w:

$$\alpha_i^{(t+1)} = \alpha_i^{(t)} + \eta\sigma(-y^{(i)} \cdot w^\top x^{(i)}) \cdot y^{(i)}. \tag{6.2}$$

The rest is simply a matter of substituting in our new expression for w. In the training update, we get:

$$\alpha_i^{(t+1)} = \alpha_i^{(t)} + \eta\sigma\left(-y^{(i)} \cdot \sum_{j=1}^{n} \alpha_j x^{(j)\top} x^{(i)}\right) \cdot y^{(i)} \tag{6.3}$$

$$= \alpha_i^{(t)} + \eta\sigma\left(-y^{(i)} \cdot \sum_{j=1}^{n} \alpha_j k(x^{(j)}, x^{(i)})\right) \cdot y^{(i)}. \tag{6.4}$$

At test time, the output logit becomes:

$$w^\top x^{\text{test}} = \sum_{i=1}^{n} \alpha_i k(x^{(i)}, x^{\text{test}}). \tag{6.5}$$

To summarize:

1. We noticed that after every step of gradient descent, the current α is always a linear combination of the $x^{(i)}$'s.

2. Thus, we can represent α in terms of a vector of n numbers, one for each $x^{(i)}$ (we called this vector α).

3. We can then rewrite logistic regression so that we update α directly (which causes a corresponding update in w).

4. When we rewrite things in this way, we see that we don't actually need to know any of the $x^{(i)}$'s, as long as we know their dot product with every other $x^{(j)}$ as well as their dot product with any test example x^{test}.

Note that this is a different algorithm than standard logistic regression, since we maintain a vector $\alpha \in \mathbb{R}^n$ rather than $w \in \mathbb{R}^d$. This new version of logistic regression is called **kernel logistic regression**. When you use the dot product kernel, kernel logistic regression makes identical predictions to normal logistic regression. But, we don't have to use the dot product kernel only! We can choose a different kernel function, such as the RBF kernel, and run the exact same algorithm. This will learn α_i's that are suitable for this new kernel.

Why does this work? It turns out that the RBF kernel actually *does* compute a dot product between two vectors, just in a different feature space that is a transformation of the original feature space. This is why it is OK to simply replace every occurrence of dot product with the RBF kernel. Next time we will explain what this means, and use this observation to better understand why kernels are useful and come up with other useful kernels.

6.2.4 Kernels compute dot products in a different feature space

You're probably wondering what the point of this exercise was. Let's start with the following scenario. Recall from our linear regression discussion that we can apply any transformation to all of our x's to create a new, more complicated set of features. You can think of this transformation as a function ϕ that takes in an original x and outputs a larger vector with more features concatenated on. For example, you could try to add all *quadratic* features: for every pair of indices $i, j \in \{1, \ldots, d\}$, you could add the feature $x_i x_j$. This adds expressivity to the model because it previously could only represent linear functions like $ax_i + bx_j$.

But if you do this, then suddenly you will have $O(d^2)$ features. If you wanted to add cubic features, you would need $O(d^3)$ features. In general, if you wanted all polynomials up to degree q, you would need $O(d^q)$ features. This could get very large very quickly!

Now let's look back at our new version of logistic regression. It tells us that we never actually have to construct these enormous feature vectors, as long as we can figure out what the dot product between two of those feature vectors is. Okay, you might be saying, how can we compute the dot product of two vectors without actually writing down those vectors? It turns out that for polynomial features of degree q, there is a nice trick: we can just use $k(x, x') = (x^\top x' + 1)^q$!

The general, formal statement is that $(x^\top x' + 1)^q = \phi(x)^\top \phi(x')$ for some feature function $\phi(x)$ whose entries include a term proportional to every monomial of x of degree up to p.[2] On Homework 2, you will prove this for the special case of quadratic features (i.e., $q = 2$) and when the dimensionality of the original x is also 2 (i.e., $d = 2$).

This trick of using kernels as an efficient way to represent a large feature space is often called the **kernel trick**.

[2] A monomial is just a product of variables, so this says that it includes every way to multiply up to p coordinates of x together. E.g. $x_1^3 x_2 x_3^5$ is a monomial of degree $3 + 1 + 5 = 9$.

What about the RBF kernel? It turns out that the RBF kernel corresponds to an *infinite-dimensional* feature vector. In Homework 2, you will show this for the special case where $d = 1$. Without the kernel trick, it is literally impossible to actually implement logistic regression using these features, since you would have to instantiate an infinite-dimensional vector. However, the kernel trick makes using the RBF kernel possible.

Runtime analysis. It's worth taking a moment to compare the runtime of standard logistic regression with kernel logistic regression using polynomial features of degree q.

In normal logistic regression, the most expensive part is computing dot products of these massive $O(d^q)$-dimensional vectors. This takes time $O(d^q)$. Each gradient step is just a single loop over the data, so a training iteration takes time $O(nd^q)$. At test time, you just compute one dot product, so making a prediction takes $O(d^q)$.

In kernel logistic regression, each training iteration must update each of the n components of α. Each update involves n computations of the kernel $k(x^{(i)}, x^{(j)})$. Using the kernel trick, each kernel evaluation can just be done by taking the dot product between $x^{(i)}$ and $x^{(j)}$, then doing some arithmetic on top (i.e., adding 1 and raising to the q-th power), so this is $O(d)$ in total. So, overall each iteration takes $O(n^2 d)$ time. At test time, you have to compute the kernel between the test input and every training example, which takes $O(nd)$ time.

So, using the kernelized method gives us a much better dependence on d, at the cost of quadratic runtime in the number of training examples for training (instead of linear) and linear runtime in the number of training examples for testing (instead of constant). Thus, kernel methods can be effective when your dataset is not too big, but the $O(n^2)$ runtime becomes prohibitive with very large datasets.

6.3 Support Vector Machines

While I have focused on kernel logistic regression for pedagogical purposes, in practice you are much more likely to see a different (but highly related) linear classification method used with kernels called **Support Vector Machines** (SVM).

6.3.1 SVM without Kernels

There are many equivalent formulations of SVMs. In my opinion, the simplest one is to view SVM as a slight modification of logistic regression with L_2 regularization. In particular, SVMs without kernels are linear classifiers just like logistic regression, and they can be viewed as minimizing the following loss function:

$$L(w) = \left(\frac{1}{n} \sum_{i=1}^{n} [1 - y^{(i)} w^\top x^{(i)}]_+ \right) + \lambda \|w\|^2.$$

The notation $[z]_+$ denotes the "positive" part of the number z and is simply equal to z if $z > 0$ and 0 otherwise. You can also equivalently write $[z]_+ = \max(z, 0)$.

This should be quite reminiscent of logistic regression! In logistic regression, we applied the log-sigmoid function to the margin $yw^\top x$. For SVMs, we apply the **hinge loss** function, defined as $f(z) = [1 - z]_+$, to the margin. We can plot the hinge loss and log-sigmoid functions on the same plot to understand the difference, as shown in Figure 6.2.

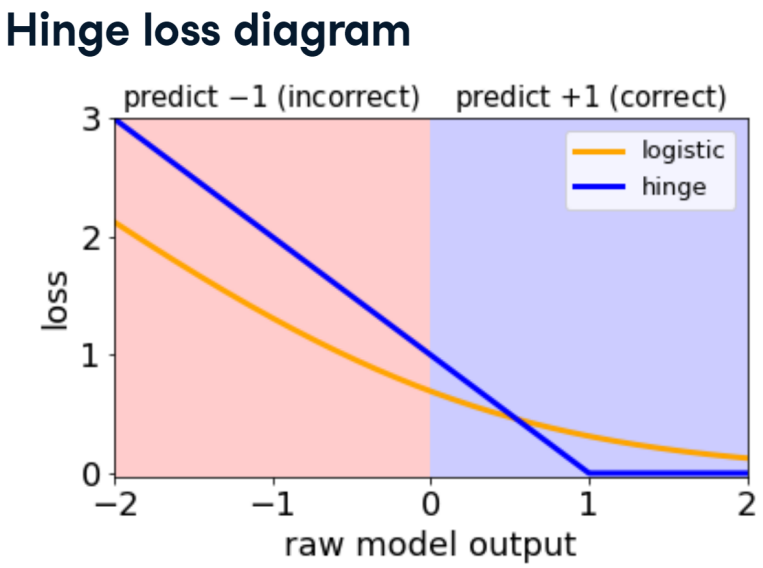


Figure 6.2: A comparison of hinge loss used in SVM and log-sigmoid loss used for logistic regression. (Note: what's called "raw model output" in this figure is what we've been calling the margin.)

Both log-sigmoid and hinge loss want to encourage the margin to be large, so the larger your margin, the smaller the loss. For log-sigmoid, you can never reach exactly 0 loss, so you're incentivized to always make the margin hire. On the other hand, for hinge loss, once your margin is ≥ 1, you get exactly 0 loss and there's no incentive to improve it further. Going the other direction, both functions are become linear in the margin as the margin tends towards negative infinity.

6.3.2 A kernelized loss function

Let's see how we can kernelize the SVM objective. While we can also try to kernelize the gradient descent step like we did with logistic regression, it turns out that with SVM's the best way to minimize the loss is actually not with normal gradient descent but with some more complicated optimization methods. I won't get into those here, so instead we'll just show how the *objective function* can be kernelized.

First, as before we can note that the optimal solution to w will be a linear combination of the $x^{(i)}$'s. One way to argue this is to again look at the gradient, as we did for logistic regression, and show that each gradient update always adds scalar multiples of the $x^{(i)}$'s and nothing more.[3]

Now that we know the optimal w will be a linear combination of $x^{(i)}$'s, we are justified in substituting

$$w = \sum_{i=1}^{n} \alpha_i x^{(i)}$$

for $\alpha \in \mathbb{R}^n$, and viewing the loss as a function of α rather than w.

[3]Gradient descent is still a valid way to minimize the SVM objective and will converge to the global minimum.

Applying that substitution everywhere leads to the following:

$$
\begin{aligned}
L(\alpha) &= \frac{1}{n}\sum_{i=1}^{n}\left[1 - y^{(i)}\left(\sum_{j=1}^{n}\alpha_j x^{(j)}\right)^\top x^{(i)}\right]_+ + \lambda\left\|\sum_{j=1}^{n}\alpha_j x^{(j)}\right\|^2 \\
&= \frac{1}{n}\sum_{i=1}^{n}\left[1 - y^{(i)}\sum_{j=1}^{n}\alpha_j x^{(j)\top} x^{(i)}\right]_+ + \lambda\left(\sum_{i=1}^{n}\alpha_i x^{(i)}\right)^\top\left(\sum_{j=1}^{n}\alpha_j x^{(j)}\right) \\
&= \frac{1}{n}\sum_{i=1}^{n}\left[1 - y^{(i)}\sum_{j=1}^{n}\alpha_j x^{(j)\top} x^{(i)}\right]_+ + \lambda\left(\sum_{i=1}^{n}\sum_{j=1}^{n}\alpha_i\alpha_j x^{(i)\top} x^{(j)}\right) \\
&= \frac{1}{n}\sum_{i=1}^{n}\left[1 - y^{(i)}\sum_{j=1}^{n}\alpha_j k(x^{(j)}, x^{(i)})\right]_+ + \lambda\left(\sum_{i=1}^{n}\sum_{j=1}^{n}\alpha_i\alpha_j k(x^{(i)}, x^{(j)})\right),
\end{aligned}
$$

where in the last line we have made the substitution $x^\top z = k(x, z)$. Now we can replace any generalized definition of dot product, such as one that involves the quadratic or RBF kernel, for the original dot products between examples. Note also that just as in kernelized logistic regression, we have $O(n^2)$ runtime in the number of training examples, as there are these double sums over the training dataset.

6.3.3 What are support vectors?

SVMs get their name from the concept of support vectors. Let's consider a simple, linearly separable classification dataset as shown in Figure 6.3.

Here, the SVM objective will encourage all the margins to be at least 1, but there's no reason to go beyond 1. The decision boundary, defined by $w^\top x = 0$, is parallel to other hyperplanes defined by $w^\top x = -1$ and $w^\top x = 1$, which correspond to the place where the margin becomes 1 for negative examples and positive examples, respectively. It turns out that the distance between two adjacent parallel hyperplanes in the diagram is just $1/\|w\|$. So, minimizing the L_2 regularization term is equivalent to maximizing this distance.

Finally, note that the only points that really matter are the ones highlighted in green, which have margin of ≤ 1. These are referred to as **support vectors**. The other points are classified correctly with margin > 1, and don't have any effect on the loss. For example, if you took one of those points and moved it around a little bit, the optimal decision boundary wouldn't change. It turns out that at the minimum of the SVM objective function, the learned w is a linear combination of *just the support vectors*. No other datapoints contribute to w.

If we now look at the kernelized form, this means that $\alpha_i = 0$ for all $(x^{(i)}, y^{(i)})$ that are not support vectors. Thus, predictions of the SVM only depend on the dot products with the support vectors. When we want to predict on a new test point, we just have to compute its kernel with all the support vectors, which can be much less than the number of training examples, n. This is the big reason why SVMs and kernels are a good match!

Let's contrast this with logistic regression. Since the log-sigmoid loss never reaches 0, even points that are very far on the correct side of the decision boundary still affect the overall loss a little bit. Since every datapoint influences the loss a little bit, the final w you learn is going to depend on all of the datapoints, so making a prediction will take the full $O(n)$ time.

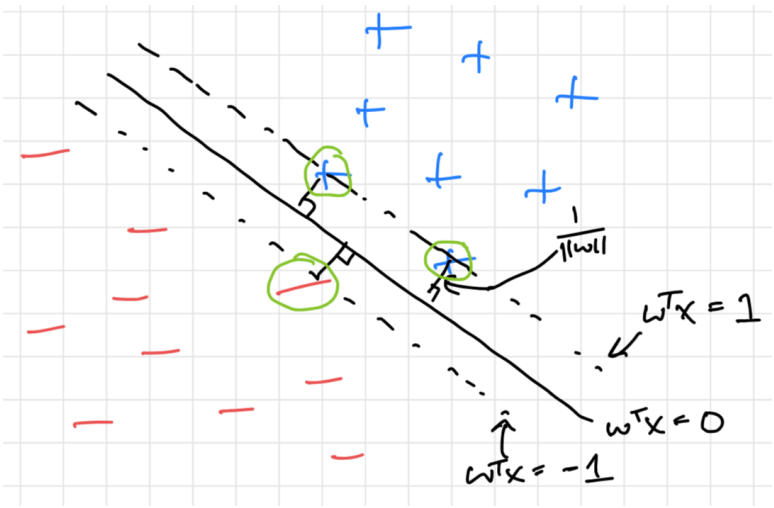


Figure 6.3: Illustration of a support vector machine. The decision boundary, defined by $w^\top x = 0$, is chosen to balance two considerations. The first is ensuring that all examples have margin of at least 1 (illustrated by the lines $w^\top x = 1$ and $w^\top x = -1$). The second is minimizing the L_2 norm of w, which corresponds to maximizing the distance (which is $1/\|w\|$) between the hyperplanes where the margin is 1 and the decision boundary. Thus, the SVM wants to classify all points correctly using a decision boundary along which the two classes are furthest apart. The resulting decision boundary is only dependent on the points with margin ≤ 1 (circled in green), which are known as the support vectors.

6.3.4 Optimization

It turns out the fact that the hinge loss is piecewise linear enables some more complex optimization techniques that we won't discuss here. But the important thing to know is that these optimization techniques also only care about dot products between examples, and thus we can use the same kernel trick to replace dot products with kernels.

Chapter 7

k-Means Clustering

7.1 Introduction to Unsupervised Learning

Let's take stock of where we are. In the first half of the class, we saw a variety of methods for doing supervised learning. In all of them, the basic recipe was the same. We obtained a training dataset that had examples of an input x paired with a correct output y, which we denoted $\{(x^{(1)}, y^{(1)}), \ldots, (x^{(n)}, y^{(n)})\}$. We then trained some model with this data such that it can take in a new input x_{test} and predict what the correct output y_{test} should be for that previously unseen input.

Today we will start learning about *unsupervised* learning. In unsupervised learning, we are no longer concerned with learning a mapping from inputs to outputs. In fact, we no longer have a "correct output" associated with each example. Our dataset is only x's—we write it simply as $\{x^{(1)}, \ldots, x^{(n)}\}$. What can we do with this data? In unsupervised learning, we hope to learn something about the **structure** of our data. We will cover three types of unsupervised learning:

- **Clustering**: Are my datapoints naturally grouped into multiple **subgroups**?
- **Dimensionality Reduction**: For data that is high-dimensional, is there a **low-dimensional subspace** that actually captures (almost) everything that's happening in the data?
- **Embeddings**: For data about objects that are not vectors, can we learn a vector for each object that captures the **similarity relationships** between objects?

7.2 Clustering

The first type of unsupervised learning problem we will study is called *clustering*. The idea of clustering is that we are trying to learn **subgroup structure** within the dataset. A clustering algorithm takes in a dataset D that consists solely of x's, i.e., $D = \{x^{(1)}, \ldots, x^{(n)}\}$. It then assigns each x to one of k possible **clusters**, or subsets of the data. Formally, we can write the output of the clustering algorithm as an **assignment** $z_1, \ldots, z_n$ where each $z_i \in \{1, 2, \ldots, k\}$ denotes the cluster assigned to datapoint $x^{(i)}$. We can say that the "j-th cluster" is just the set of all examples $x^{(i)}$ where $z_i = j$. For brevity, I will write $z_{1:n}$ to refer to the complete list of assignments $[z_1, \ldots, z_n]$.

Note that the maximum number of clusters k is a hyperparameter of the algorithm. In other words, before we run the clustering algorithm, we should already have a guess of how many total clusters there are in the data. If we don't know ahead of time, there are some heuristics we can use to choose a good value of k, just as we had ways of choosing hyperparameters in supervised learning. We'll discuss these after introducing our first clustering algorithm.

7.3 k-Means Clustering

Now we will dive into the most famous clustering and widely-used clustering algorithm, k-means clustering.

7.3.1 Setup

The main idea of k-means clustering is that we can represent each cluster of the dataset with a "cluster mean" or "cluster centroid," denoted μ_j for the j-th cluster. μ_j represents the center of all the points in cluster j. In order for something to be a good clustering, we should have all examples $x^{(i)}$ to be close to the corresponding cluster mean, μ_{z_i}.

To formalize this intuition, we can write down a loss function that we want to minimize in order to find the best cluster assignment (just like we did whenever we wanted to derive a new supervised learning algorithm). We want to minimize the sum of the distances between each point and its cluster centroid, which we can write as

$$L(z_{1:n}, \mu_{1:k}) = \sum_{i=1}^{n} \|x^{(i)} - \mu_{z_i}\|^2.$$

Let's unpack this equation. On the left hand side, note that our loss L is a function of both our assignment z_i for each $i = 1, 2, \ldots, n$, and our cluster centroid μ_j for each $j = 1, 2, \ldots, k$. When we run the k-means algorithm, we will want to find values of both $z_{1:n}$ and $\mu_{1:k}$ that minimize this loss. This accomplishes the main goal of a clustering algorithm—assigning each point to a cluster—but as a byproduct it also computes centroids for each cluster.

On the right hand side, we compute the squared Euclidean distance between each example $x^{(i)}$ and its assigned cluster centroid μ_{z_i}. This sort of loss function is sometimes referred to as the *reconstruction error*. The reason is that we can view clustering as a way of simplifying the dataset—instead of remembering the exact location of each datapoint, we can just remember the cluster centroids and what cluster each datapoint belongs to. If we did that, how well could we "reconstruct" the original dataset? Well, our best guess for the location of each datapoint is just that it's roughly located at its corresponding cluster centroid. So the error of this reconstruction is exactly how far away each original datapoint is from its corresponding cluster centroid.

7.3.2 Algorithm

Now that we have a loss function, we need to find an algorithmic way to minimize it. First, let's note that we cannot use gradient descent in this case. Why not? gradient descent requires us to compute the gradient of the loss with respect to all of our input variables. However, the z_i's are not continuous variables at all—they're a discrete choice of one of the k clusters. There's no way to slightly perturb these variables, so the concept of a derivative with respect to z_i doesn't make any sense.

Instead, we'll choose a different general strategy known as **alternating minimization**. You can think of alternating minimization as a high-level strategy rather than an algorithm itself. All it means is that if we have a loss function that depends on two variables, we can first minimize it with respect to the first variable while holding the second fixed, then minimize it with respect to the second variable while holding the first fixed, and repeat. This is often an effective strategy even if we just start from a random guess for both variables. In this way, philosophically there are some similarities between alternating minimization and gradient descent: in both cases, we start with a possibly bad guess, then go through many iterations of improvement.

In the case of k-means, alternating minimization will alternate between the following two steps until convergence (i.e., until the values stop changing):

1. Given our current guess for $\mu_{1:k}$, update our guess for $z_{1:n}$ to be the one that minimizes L.
2. Given our current guess for $z_{1:n}$, update our guess for $\mu_{1:k}$ to be the one that minimizes L.

The nice thing about k-means is that it turns out that both of these updates have very simple closed-form solutions. Let's see the full algorithm in detail. In addition to seeing how we do each update, we also need to know how to initialize our guess.

Choosing an initial guess for $\mu_{1:k}$. Note above that in the alternating minimization loop, we chose to start with updating $z_{1:n}$ given a guess for $\mu_{1:k}$. That means that to get everything started, we just need an initial guess of $\mu_{1:k}$ (and not $z_{1:n}$). There are several possible strategies here, but one simple one is simply to choose each μ_j to be a different random example from the dataset. This is reasonable because we start each cluster in a different place, even if it's not at the optimal position. The further steps of alternating minimization will refine this guess

Updating $z_{1:n}$. Given our current guess of the cluster centroids $\mu_{1:k}$, what is the best choice of z_i? Well, for each example, we should just assign it to the cluster centroid it is closest to. Formally, we can write

$$z_i = \arg\min_{j=1,\dots,k} \|x^{(i)} - \mu_j\|^2.$$

In other words, we compute the distance between $x^{(i)}$ and each μ_j, and choose whichever j gives the smallest distance as our new value of z_i.

Updating $\mu_{1:k}$. Now, given our current guess of the cluster assignments, what is the best choice of $\mu_{1:k}$? Intuitively, for each $j = 1, \dots, k$, there are a bunch of points that have been assigned to cluster j. To minimize the distance between all those points and μ_j, we should want μ_j in the middle of all those points, so it should be something like the average of all those points. In fact, it turns out we have cleverly chosen our loss function so that μ_j should exactly be the average of the points assigned to cluster j.

We can prove this mathematically. First, let's rewrite the loss function by grouping all of the examples in terms of which cluster they're assigned to:

$$\sum_{i=1}^{n} \|x^{(i)} - \mu_{z_i}\|^2. = \sum_{j=1}^{k} \sum_{i:z_i=j} \|x^{(i)} - \mu_j\|^2.$$

Now, for each j, μ_j appears in exactly one of these terms, so we can focus on one j at a time. In general, for a fixed choice of j, we need to minimize

$$\sum_{i:z_i=j} \|x^{(i)} - \mu_j\|^2.$$

Now we can take the gradient with respect to μ_j and set it equal to 0:

$$\nabla_{\mu_j} \sum_{i:z_i=j} \|x^{(i)} - \mu_j\|^2 = \sum_{i:z_i=j} \cancel{2}(x^{(i)} - \mu_j) \cdot \cancel{-1} = 0$$

$$\sum_{i:z_i=j} x^{(i)} = |\{i : z_i = 1\}| \cdot \mu_j$$

$$\mu_j = \frac{1}{|\{i : z_i = 1\}|} \sum_{i:z_i=j} x^{(i)}$$

This final expression is simply the average of all $x^{(i)}$'s assigned to cluster j.

Convergence. In the full k-means algorithm, we keep alternating between these two minimization steps until we reach a fixed point—a point where the updates to $z_{1:n}$ don't change anything, and so the updates to $\mu_{1:k}$ also don't change anything.

Are we guaranteed to have reached the global minimum of the k-means loss? Not necessarily. Each step of alternating minimization reduces the loss, but we can get stuck at a local optimum. In fact, with the same dataset and different random initializations of the cluster centroids, you can arrive at different clusterings. It is not uncommon to do multiple random restarts (i.e., just try multiple random initializations) and choose the best one as the final clustering.

7.3.3 Choosing k

Note that the entire k-means clustering assumes that we have chosen a good value for the hyperparameter k (the number of clusters) ahead of time. In some applications, we may simply want to divide the dataset up into a fixed number of subgroups, so this is fine. But if we actually want to understand the structure of the data, we also need to determine how many distinct clusters are actually present in the data.

Let's start by thinking about how we did this for supervised learning. To choose hyperparameters, we tried many different values and measured the loss on a development set. Whichever hyperparameter value led to the lowest loss was considered the best. Does this also work for k-means? Unfortunately, no. In general, the k-means loss function will always decrease if you add more clusters. This is just because if there are more cluster centroids, then the closest centroid is almost certainly closer than if there were fewer centroids.

Instead, an informal rule we can use is called the "elbow criterion." To apply the elbow criterion, you try running k-means with different values of k and make a plot with the k-means loss on the y-axis and k on the x-axis. This will create a curve that slopes downwards to the right. The point where the curve bends and starts becoming flat is called the "elbow," and is usually a reasonable choice for k, because it signifies a point where increasing k no longer decreases the loss by that much.

Elbow method