CHAPTER 3

Gradient Descent

In the previous chapter, we showed how to describe an interesting objective function for machine learning, but we need a way to find the optimal $\Theta^* = \arg\min_\Theta J(\Theta)$, particularly when the objective function is not amenable to analytical optimization. For example, this can be the case when $J(\Theta)$ involves a more complex loss function, or more general forms of regularization. It can also be the case when there is simply too much data for it to be computationally feasible to analytically invert the required matrices.

There is an enormous and fascinating literature on the mathematical and algorithmic foundations of optimization, but for this class, we will consider one of the simplest methods, called *gradient descent*.

Which you should consider studying some day!

Intuitively, in one or two dimensions, we can easily think of $J(\Theta)$ as defining a surface over Θ; that same idea extends to higher dimensions. Now, our objective is to find the Θ value at the lowest point on that surface. One way to think about gradient descent is that you start at some arbitrary point on the surface, look to see in which direction the "hill" goes down most steeply, take a small step in that direction, determine the direction of steepest descent from where you are, take another small step, etc.

Below, we explicitly give gradient descent algorithms for one and multidimensional objective functions (Sections 3.1 and 3.2). We then illustrate the application of gradient descent to a loss function which is not merely mean squared loss (Section 3.3). And we present an important method known as *stochastic gradient descent* (Section 3.4), which is especially useful when datasets are too large for descent in a single batch, and has some important behaviors of its own.

3.1 Gradient descent in one dimension

We start by considering gradient descent in one dimension. Assume $\Theta \in \mathbb{R}$, and that we know both $J(\Theta)$ and its first derivative with respect to Θ, $J'(\Theta)$. Here is pseudo-code for gradient descent on an arbitrary function f. Along with f and its gradient f', we have to specify the initial value for parameter Θ, a *step-size* parameter η, and an *accuracy* parameter ϵ.

The parameter η is often called *learning rate* when gradient descent is applied in machine learning. Note also that η is a constant multiplier but the actual magnitude of the change to Θ is not constant, and changes depending on the magnitude of the gradient itself.

1D-GRADIENT-DESCENT($\Theta_{init}, \eta, f, f', \epsilon$)

```
Θ^(0) = Θ_init
t = 0
repeat
    t = t + 1
    Θ^(t) = Θ^(t−1) − η f′(Θ^(t−1))
until |f(Θ^(t)) − f(Θ^(t−1))| < ε
return Θ^(t)
```

Note that this algorithm terminates when the change in the function f is sufficiently small. There are many other reasonable ways to decide to terminate, including:

- Stop after a fixed number of iterations T, i.e., when $t = T$.
- Stop when the change in the value of the parameter Θ is sufficiently small, i.e., when $\left|\Theta^{(t)} - \Theta^{(t-1)}\right| < \epsilon$.
- Stop when the derivative f' at the latest value of Θ is sufficiently small, i.e., when $\left|f'(\Theta^{(t)})\right| < \epsilon$.

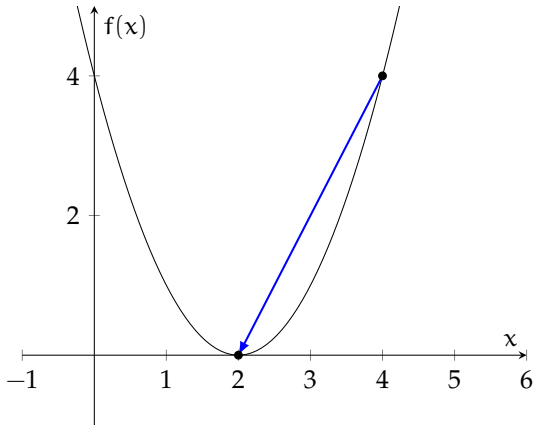
Study Question: Consider all of the potential stopping criteria for 1D-GRADIENT-DESCENT, both in the algorithm as it appears and listed separately later. Can you think of ways that any two of the criteria relate to each other?

Theorem 3.1.1. *Choose any small distance $\tilde{\epsilon} > 0$. If f is sufficiently "smooth" and convex, and if the step size η is sufficiently small, gradient descent will reach a point within $\tilde{\epsilon}$ of a global optimum point Θ.*

A function is convex if the line segment between any two points on the graph of the function lies above or on the graph.

However, we must be careful when choosing the step size to prevent slow convergence, non-converging oscillation around the minimum, or divergence.

The following plot illustrates a convex function $f(x) = (x-2)^2$, starting gradient descent at $x_{\text{init}} = 4.0$ with a step-size of $1/2$. It is very well-behaved!



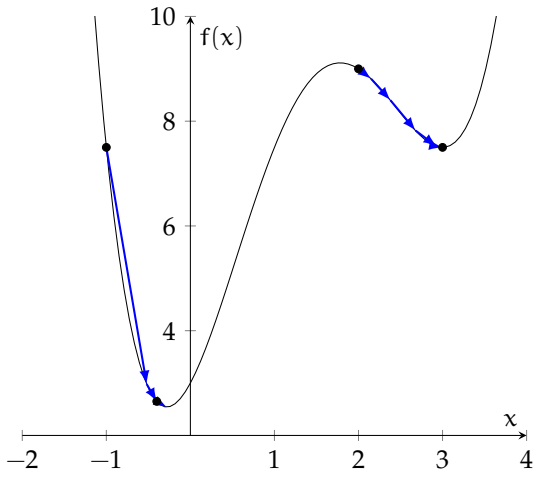
Study Question: What happens in this example with very small η? With very big η?

If f is non-convex, where gradient descent converges to depends on x_{init}. First, let's establish some definitions. Suppose we have analytically defined derivatives for f. Then we say that f has a *local minimum point* or *local optimum point* at x if $f'(x) = 0$ and $f''(x) > 0$, and we say that $f(x)$ is a *local minimum value* of f. More generally, x is a local minimum

point of f if $f(x)$ is at least as low as $f(x')$ for all points x' in some small area around x. We say that f has a *global minimum point* at x if $f(x)$ is at least as low as $f(x')$ for every other input x'. And then we call $f(x)$ a *global minimum value*. A global minimum point is also a local minimum point, but a local minimum point does not have to be a global minimum point.

If f is non-convex (and sufficiently smooth), gradient descent (run long enough with small enough step size) will get very close to a local minimum point, but we cannot guarantee that it will converge to a global minimum point.

The plot below shows two different x_{init}, and how gradient descent started from each point heads toward two different local optimum points.



3.2 Multiple dimensions

The extension to the case of multi-dimensional Θ is straightforward. Let's assume $\Theta \in \mathbb{R}^m$, so $f : \mathbb{R}^m \to \mathbb{R}$. The gradient of f with respect to Θ is

$$\nabla_\Theta f = \begin{bmatrix} \partial f/\partial \Theta_1 \\ \vdots \\ \partial f/\partial \Theta_m \end{bmatrix}$$

The algorithm remains the same, except that the update step in line 5 becomes

$$\Theta^{(t)} = \Theta^{(t-1)} - \eta \nabla_\Theta f(\Theta^{(t-1)})$$

and any termination criteria that depended on the dimensionality of Θ would have to change. The easiest thing is to keep the test in line 6 as $\left|f(\Theta^{(t)}) - f(\Theta^{(t-1)})\right| < \epsilon$, which is sensible no matter the dimensionality of Θ.

Study Question: Which termination criteria from the 1D case were defined in a way that assumes Θ is one dimensional?

3.3 Application to regression

Recall from the previous chapter that choosing a loss function is the first step in formulating a machine-learning problem as an optimization problem, and for regression we studied the

mean square loss, which captures loss as $(\text{guess} - \text{actual})^2$. This leads to the *ordinary least squares* objective

$$J(\theta) = \frac{1}{n}\sum_{i=1}^{n}\left(\theta^T x^{(i)} - y^{(i)}\right)^2 \quad . \tag{3.1}$$

We use the gradient of the objective with respect to the parameters,

$$\nabla_\theta J = \frac{2}{n}\underbrace{\tilde{X}^T}_{d\times n}\underbrace{(\tilde{X}\theta - \tilde{Y})}_{n\times 1} \ , \tag{3.2}$$

to obtain an analytical solution to the linear regression problem. Gradient descent could also be applied to numerically compute a solution, using the update rule

$$\theta^{(t)} = \theta^{(t-1)} - \eta\frac{2}{n}\sum_{i=1}^{n}\left(\left[\theta^{(t-1)}\right]^T x^{(i)} - y^{(i)}\right)x^{(i)} . \tag{3.3}$$

Beware double superscripts! $[\theta]^T$ is the transpose of the vector θ

3.3.1 Ridge regression

Now, let's add in the regularization term, to get the ridge-regression objective:

$$J_{\text{ridge}}(\theta, \theta_0) = \frac{1}{n}\sum_{i=1}^{n}\left(\theta^T x^{(i)} + \theta_0 - y^{(i)}\right)^2 + \lambda\|\theta\|^2 \quad .$$

Recall that in ordinary least squares, we finessed handling θ_0 by adding an extra dimension of all 1's. In ridge regression, we really do need to separate the parameter vector θ from the offset θ_0, and so, from the perspective of our general-purpose gradient descent method, our whole parameter set Θ is defined to be $\Theta = (\theta, \theta_0)$. We will go ahead and find the gradients separately for each one:

Some passing familiarity with matrix derivatives is helpful here. A foolproof way of computing them is to compute partial derivative of J with respect to each component θ_i of θ. See Appendix A on matrix derivatives!

$$\nabla_\theta J_{\text{ridge}}(\theta, \theta_0) = \frac{2}{n}\sum_{i=1}^{n}\left(\theta^T x^{(i)} + \theta_0 - y^{(i)}\right)x^{(i)} + 2\lambda\theta$$

$$\frac{\partial J_{\text{ridge}}(\theta, \theta_0)}{\partial \theta_0} = \frac{2}{n}\sum_{i=1}^{n}\left(\theta^T x^{(i)} + \theta_0 - y^{(i)}\right) \quad .$$

Note that $\nabla_\theta J_{\text{ridge}}$ will be of shape $d \times 1$ and $\partial J_{\text{ridge}}/\partial\theta_0$ will be a scalar since we have separated θ_0 from θ here.

Study Question: Convince yourself that the dimensions of all these quantities are correct, under the assumption that θ is $d \times 1$. How does d relate to m as discussed for Θ in the previous section?

Study Question: Compute $\nabla_\theta \|\theta\|^2$ by finding the vector of partial derivatives $(\partial \|\theta\|^2/\partial\theta_1, \ldots, \partial \|\theta\|^2/\partial\theta_d)$. What is the shape of $\nabla_\theta \|\theta\|^2$?

Study Question: Compute $\nabla_\theta \mathcal{L}_{\text{ridge}}(\theta^T x + \theta_0, y)$ by finding the vector of partial derivatives $(\partial\mathcal{L}_{\text{ridge}}(\theta^T x + \theta_0, y)/\partial\theta_1, \ldots, \partial\mathcal{L}_{\text{ridge}}(\theta^T x + \theta_0, y)/\partial\theta_d)$.

Study Question: Use these last two results to verify our derivation above.

Putting everything together, our gradient descent algorithm for ridge regression becomes

RR-GRADIENT-DESCENT($\theta_{init}, \theta_{0init}, \eta, \epsilon$)

1 $\theta^{(0)} = \theta_{init}$
2 $\theta_0^{(0)} = \theta_{0init}$
3 $t = 0$
4 **repeat**
5 $\quad t = t + 1$
6 $\quad \theta^{(t)} = \theta^{(t-1)} - \eta \left(\frac{1}{n} \sum_{i=1}^{n} \left(\theta^{(t-1)^T} x^{(i)} + \theta_0^{(t-1)} - y^{(i)} \right) x^{(i)} + \lambda \theta^{(t-1)} \right)$
7 $\quad \theta_0^{(t)} = \theta_0^{(t-1)} - \eta \left(\frac{1}{n} \sum_{i=1}^{n} \left(\theta^{(t-1)^T} x^{(i)} + \theta_0^{(t-1)} - y^{(i)} \right) \right)$
8 **until** $\left| J_{\text{ridge}}(\theta^{(t)}, \theta_0^{(t)}) - J_{\text{ridge}}(\theta^{(t-1)}, \theta_0^{(t-1)}) \right| < \epsilon$
9 **return** $\theta^{(t)}, \theta_0^{(t)}$

Study Question: Is it okay that λ doesn't appear in line 7?

Study Question: Is it okay that the 2's from the gradient definitions don't appear in the algorithm?

3.4 Stochastic gradient descent

When the form of the gradient is a sum, rather than take one big(ish) step in the direction of the gradient, we can, instead, randomly select one term of the sum, and take a very small step in that direction. This seems sort of crazy, but remember that all the little steps would average out to the same direction as the big step if you were to stay in one place. Of course, you're not staying in that place, so you move, in expectation, in the direction of the gradient.

The word "stochastic" means probabilistic, or random; so does "aleatoric," which is a very cool word. Look up aleatoric music, sometime.

Most objective functions in machine learning can end up being written as a sum over data points, in which case, stochastic gradient descent (SGD) is implemented by picking a data point randomly out of the data set, computing the gradient as if there were only that one point in the data set, and taking a small step in the negative direction.

Let's assume our objective has the form

$$f(\Theta) = \sum_{i=1}^{n} f_i(\Theta) \ ,$$

where n is the number of data points used in the objective (and this may be different from the number of points available in the whole data set). Here is pseudocode for applying SGD to such an objective f; it assumes we know the form of $\nabla_\Theta f_i$ for all i in $1 \ldots n$:

STOCHASTIC-GRADIENT-DESCENT($\Theta_{init}, \eta, f, \nabla_\Theta f_1, \ldots, \nabla_\Theta f_n, T$)

1 $\Theta^{(0)} = \Theta_{init}$
2 **for** $t = 1$ **to** T
3 $\quad$ randomly select $i \in \{1, 2, \ldots, n\}$
4 $\quad \Theta^{(t)} = \Theta^{(t-1)} - \eta(t) \nabla_\Theta f_i(\Theta^{(t-1)})$
5 **return** $\Theta^{(t)}$

Note that now instead of a fixed value of η, η is indexed by the iteration of the algorithm, t. Choosing a good stopping criterion can be a little trickier for SGD than traditional gradient descent. Here we've just chosen to stop after a fixed number of iterations T.

For SGD to converge to a local optimum point as t increases, the step size has to decrease as a function of time. The next result shows one step size sequence that works.

Theorem 3.4.1. *If* f *is convex, and* $\eta(t)$ *is a sequence satisfying*

$$\sum_{t=1}^{\infty} \eta(t) = \infty \quad \textit{and} \quad \sum_{t=1}^{\infty} \eta(t)^2 < \infty \ ,$$

then SGD converges with probability one *to the optimal* Θ.

We have left out some gnarly conditions in this theorem. Also, you can learn more about the subtle difference between "with probability one" and "always" by taking an advanced probability course.

Why these two conditions? The intuition is that the first condition, on $\sum \eta(t)$, is needed to allow for the possibility of an unbounded potential range of exploration, while the second condition, on $\sum \eta(t)^2$, ensures that the step sizes get smaller and smaller as t increases.

One "legal" way of setting the step size is to make $\eta(t) = 1/t$ but people often use rules that decrease more slowly, and so don't strictly satisfy the criteria for convergence.

Study Question: If you start a long way from the optimum, would making $\eta(t)$ decrease more slowly tend to make you move more quickly or more slowly to the optimum?

There are multiple intuitions for why SGD might be a better choice algorithmically than regular GD (which is sometimes called *batch* GD (BGD)):

- BGD typically requires computing some quantity over every data point in a data set. SGD may perform well after visiting only some of the data. This behavior can be useful for very large data sets – in runtime and memory savings.
- If your f is actually non-convex, but has many shallow local optimum points that might trap BGD, then taking *samples* from the gradient at some point Θ might "bounce" you around the landscape and away from the local optimum points.
- Sometimes, optimizing f really well is not what we want to do, because it might overfit the training set; so, in fact, although SGD might not get lower training error than BGD, it might result in lower test error.