Gradient Descent (and Beyond)

Cornell CS 4/5780 — Spring 2022

Goal: We want to minimize a convex, continuous and differentiable loss function $\ell(w)$. In this section we discuss two of the most popular "hill-climbing" algorithms, gradient descent and Newton's method.

General form for the algorithm:

- Initialize $w_0 \in \mathbb{R}^d$, pick tolerance $\delta > 0$,
- Repeat until converge:
  - Let $s_t \in \mathbb{R}^d$ be some direction in which we believe the function decreases
  - $w_{t+1} = w_t + s_t$
  - If $\|w_{t+1} - w_t\|_2 \leq \delta$, converged!

Trick: Taylor Expansion

How can you minimize a function ℓ if you don't know much about it? The trick is to assume it is much simpler than it really is. This can be done with Taylor's approximation.

Taylor's Theorem (Lagrange form). Let $k \geq 1$ be a natural number, $x \in \mathbb{R}$, and $f : \mathbb{R} \to \mathbb{R}$ be a function that is $(k+1)$-times continuously differentiable on $[0, x]$. Then there exists some $\zeta \in [0, x]$ such that

$$f(x) = f(0) + xf'(0) + \frac{x^2}{2}f''(0) + \cdots + \frac{x^k}{k!}f^{(k)}(0) + \frac{x^{k+1}}{(k+1)!}f^{(k+1)}(\zeta).$$

As direct consequence of Taylor's theorem, we have the following result for multidimensional functions. If $\ell : \mathbb{R}^d \to \mathbb{R}$ is continuously twice differentiable, then for any $w \in \mathbb{R}^d$ and any $s \in \mathbb{R}^d$, there exists a $\zeta \in [0, 1]$ such that

$$\ell(w + s) = \ell(w) + s^T \nabla \ell(w) + \frac{1}{2} s^T \nabla^2 \ell(w + \zeta s) s = \ell(w) + s^T \nabla \ell(w) + \mathcal{O}(\|s\|^2),$$

where $\nabla \ell(w) \in \mathbb{R}^d$ is the gradient of ℓ and $\nabla^2 \ell(w) \in \mathbb{R}^{d \times d}$ is its second-derivative matrix, a.k.a. its Hessian matrix. Similarly, if $\ell : \mathbb{R}^d \to \mathbb{R}$ is continuously thrice differentiable, then

$$\ell(w + s) = \ell(w) + s^T \nabla \ell(w) + \frac{1}{2} s^T \nabla^2 \ell(w) s + \mathcal{O}(\|s\|^3).$$

So, provided that the norm $\|s\|_2$ is small (*i.e.* w + s is very close to w), we can approximate the function $\ell(w + s)$ by its first and second derivatives:

$$\ell(w + s) \approx \ell(w) + s^T \nabla \ell(w), \quad \text{and} \quad \ell(w + s) \approx \ell(w) + s^T \nabla \ell(w) + \frac{1}{2} s^T \nabla^2 \ell(w) s.$$

Both approximations are valid if $\|s\|_2$ is small, but the second one assumes that ℓ is twice differentiable (at least, and thrice differentiable if we want the error term to be $\mathcal{O}(\|s\|^3)$) and is more expensive to compute but also more accurate than only using gradient.

Gradient Descent: Use the first order approximation

In gradient descent we only use the gradient (first order). In gradient descent we simply set $s = -\alpha \nabla \ell(w)$, for some small scalar $\alpha > 0$ called the "step size" or "learning rate." It is straight-forward to prove that for sufficiently small α, $\ell(w + s) \leq \ell(w)$. For some $\zeta \in [0, 1]$, if the Hessian of ℓ is bounded everywhere, then

$$\begin{aligned}\ell(w - \alpha \nabla \ell(w)) &= \ell(w) + (-\alpha \nabla \ell(w))^T \nabla \ell(w) + \frac{1}{2}(-\alpha \nabla \ell(w))^T \nabla^2 \ell(w - \zeta \alpha \nabla \ell(w)) (-\alpha \nabla \ell(w)) \\ &= \ell(w) - \alpha \|\nabla \ell(w)\|^2 + \frac{\alpha^2}{2} \nabla \ell(w)^T \nabla^2 \ell(w - \zeta \alpha \nabla \ell(w)) \nabla \ell(w), = \ell(w) - \alpha \|\nabla \ell(w)\|^2 + \|\nabla \ell(w)\|^2 \mathcal{O}(\alpha^2).\end{aligned}$$

Of course $-\alpha + \mathcal{O}(\alpha^2)$ is guaranteed to be negative for sufficiently small step sizes α. In particular, there must be an α small enough that $\ell(w - \alpha \nabla \ell(w)) \leq \ell(w) - \frac{\alpha}{2} \|\nabla \ell(w)\|^2$.

Just like we did for the perceptron, we can show that gradient descent converges: that is, that no matter what threshold δ we pick to stop at, our steps s_t will eventually have $\|s_t\| \leq \delta$. Here I'll outline a proof that if converges under the really simple assumptions that (1) ℓ is non-negative, i.e. $\ell(w) \geq 0$, and (2) we choose a fixed α small enough that $\ell(w - \alpha \nabla \ell(w)) \leq \ell(w) - \frac{\alpha}{2}\|\nabla \ell(w)\|^2$. (We can also prove gradient descent converges in a variety of other ways under different assumptions: there are whole courses on this sort of thing.)

Recall that $w_t \in \mathbb{R}^d$ denotes the state of gradient descent after t iterations. By our assumption that the step size is sufficiently small, we'll have that

$$\ell(w_{t+1}) \leq \ell(w_t) - \frac{\alpha}{2}\|\nabla \ell(w_t)\|^2 = \ell(w_t) - \frac{1}{2\alpha}\|s_t\|^2,$$

since $s_t = -\alpha \nabla \ell(w_t)$. Now, if we have not converged at step t, then ipso facto $\|s_t\| > \delta$ and so

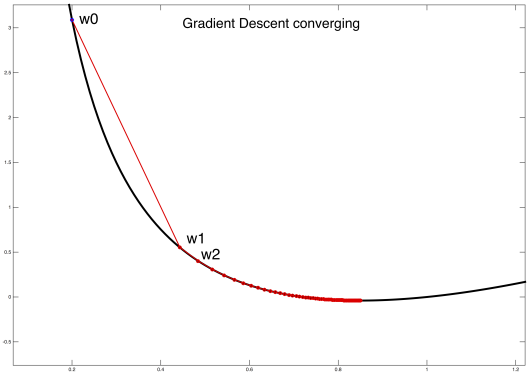
$$\ell(w_{t+1}) \leq \ell(w_t) - \frac{\delta^2}{2\alpha}.$$

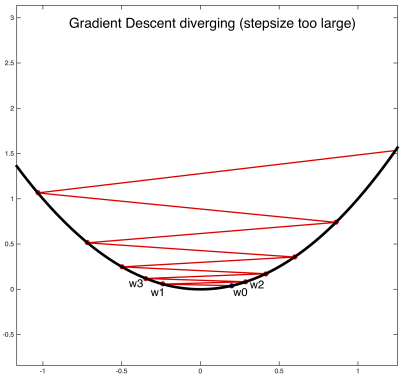
That is, at each step the loss must decrease by at least $\delta^2/2\alpha$. But this can't continue indefinitely! Applying this inductively over T total steps, and using our assumption that ℓ is non-negative,

$$0 \leq \ell(w_T) \leq \ell(w_0) - \frac{\delta^2 T}{2\alpha}, \;\; \Rightarrow \;\; T \leq \frac{2\alpha \ell(w_0)}{\delta^2}.$$

This shows that gradient descent must terminate eventually!

Setting the learning rate $\alpha > 0$ is a dark art. Only if it is sufficiently small will gradient descent converge (see the first figure below). If it is too large the algorithm can easily *diverge* out of control (see the second figure below). But on the other hand, if it's too small, then GD may make a small step (and so decide to stop since $\|s\| \leq \delta$) while still far from the optimum, and generally with smaller step sizes GD takes longer to converge to the same value of the loss. A safe (but sometimes slow) choice is to use a *diminishing step size scheme* $\alpha_t = \frac{\alpha_0}{t+1}$, which guarantees that it will eventually become small enough to converge (for any initial value $\alpha_0 \geq 0$.





Adagrad

One option is to set the step-size adaptively for *every feature*. Adagrad keeps a running average of the squared gradient magnitude and sets a small learning rate for features that have large gradients, and a large learning rate for features with small gradients. Setting different learning rates for different features is particularly important if they are of different scale or vary in frequency. For example, word counts can differ a lot across common words and rare words.

Adagrad Algorithm:

- Given step size parameter $\alpha > 0$, tolerance $\delta > 0$ and "small number" parameter $\epsilon > 0$
- Initialize $w = 0$ and $z = 0$ both in $\mathbb{R}^d$
- Repeat until converge:
  - $g = \nabla f(w)$ # Compute gradient
  - for all $i \in \{1, \ldots, d\}$, set $z_d \leftarrow z_d + g_d^2$
  - for all $i \in \{1, \ldots, d\}$, update $w_d \leftarrow w_d - \alpha \frac{g_d}{\sqrt{z_d + \epsilon}}$
  - If $\|w^{t+1} - w^t\|_2 \leq \delta$, converged!

Newton's Method: Use 2nd order Approximation

Newton's method assumes that the loss ℓ is twice differentiable and uses the approximation with Hessian (2nd order Taylor approximation). The **Hessian Matrix** $H(w) = \nabla^2 \ell(w)$ contains all second order partial derivatives and is defined such that for all $u \in \mathbb{R}^d$

$$\frac{\partial^2}{\partial \alpha^2} \ell(w + \alpha u) = u^T H(w) u.$$

$$H(\mathbf{w}) = \begin{pmatrix} \frac{\partial^2 \ell}{\partial w_1^2} & \frac{\partial^2 \ell}{\partial w_1 \partial w_2} & \cdots & \frac{\partial^2 \ell}{\partial w_1 \partial w_n} \\ \vdots & \cdots & \cdots & \vdots \\ \frac{\partial^2 \ell}{\partial w_n \partial w_1} & \cdots & \cdots & \frac{\partial^2 \ell}{\partial w_n^2} \end{pmatrix},$$

and, because the convexity of ℓ, it is always a symmetric square matrix and is always positive semi-definite.

Note: A symmetric matrix $M \in \mathbb{R}^{d \times d}$ is positive semi-definite if it has only non-negative eigenvalues or, equivalently, for any vector $x \in \mathbb{R}^d$ we must have $x^T M x \geq 0$.

It follows that the approximation

$$\ell(w + s) \approx \ell(w) + s^T \nabla \ell(w) + \frac{1}{2} s^T H(w) s$$

describes a convex parabola, and we can find its minimum by solving the following optimization problem:

$$\arg\min_{s \in \mathbb{R}^d} \ \ell(w) + s^T \nabla \ell(w) + \frac{1}{2} s^T H(w) s.$$

To find the minimum of the objective, we take its first derivative with respect to s, equate it with zero, and solve for s:

$$\begin{aligned} g(w) + H(w)s &= 0 \\ \Rightarrow s &= -(H(w))^{-1} g(w). \end{aligned}$$

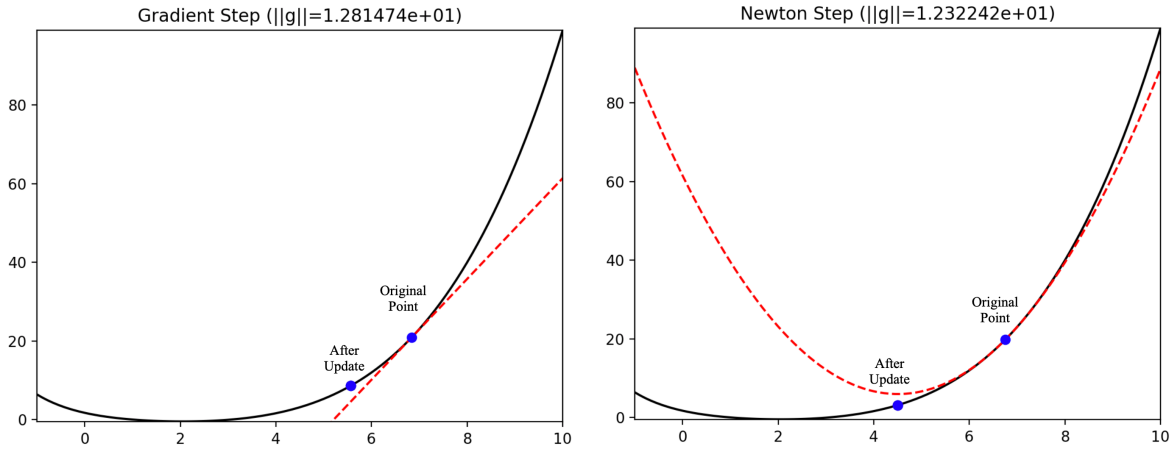
This results in the update step

$$w_{t+1} = w_t - (H(w_t))^{-1} g(w_t).$$

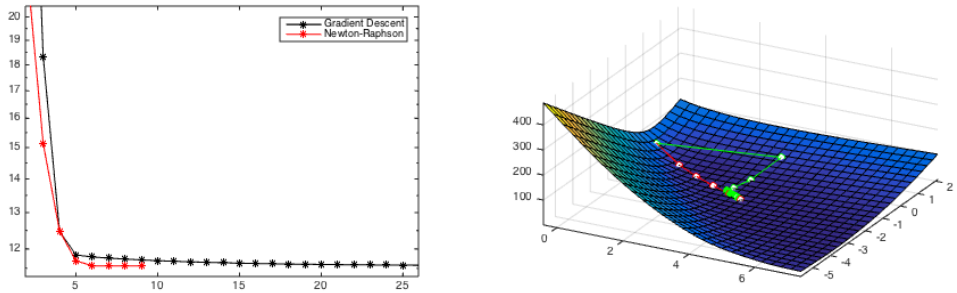
This choice of s converges extremely fast if the approximation is sufficiently accurate and the resulting step sufficiently small. Otherwise it can diverge. Divergence often happens if the function is flat or almost flat with respect to some dimension. In that case the second derivatives are close to zero, and their inverse becomes very large—resulting in gigantic steps. Different from gradient descent, here there is no step-size that guarantees that steps are all small and local. As the Taylor approximation is only accurate locally, large steps can move the current estimates far from regions where the Taylor approximation is accurate.

Best practices

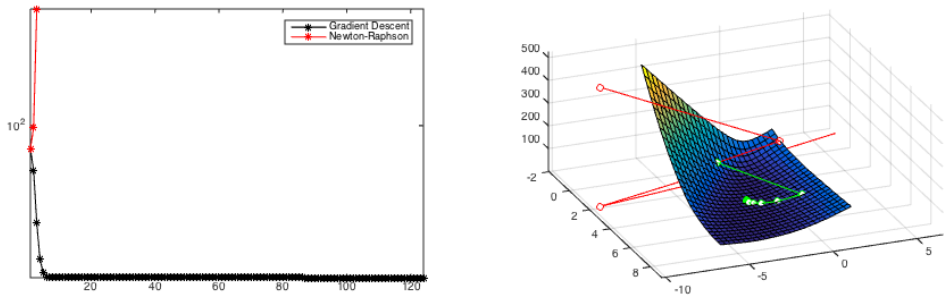
1. The matrix $H(w)$ scales $d \times d$ and is expensive to compute. A good approximation can be to only compute its diagonal entries and multiply the update with a small step-size. Essentially you are then doing a hybrid between Newton's method and gradient descent, where you weigh the step-size for each dimension by the inverse Hessian.
2. To avoid divergence of Newton's method, a good approach is to start with gradient descent (or even stochastic gradient descent) and then finish the optimization Newton's method. Typically, the second order approximation, used by Newton's Method, is more likely to be appropriate near the optimum.



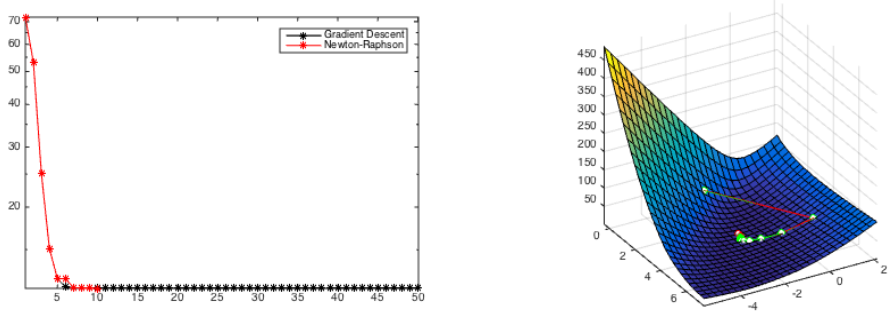
A gradient descent step (left) and a Newton step (right) on the same function. The loss function is depicted in black, the approximation as a dotted red line. The gradient step moves the point downwards along the linear approximation of the function. The Newton step moves the point to the minimum of the parabola, which is used to approximate the function.



(a) A starting point where Newton's Method converges in 8 iterations.



(b) A starting point where Newton's Method diverges.



(c) same starting point as in Figure 2, however Newton's method is only used after 6 gradient steps and converges in a few steps.

The three plots show a comparison of Newton's Method and Gradient Descent. Gradient Descent always converges after over 100 iterations from all initial starting points. If it converges (Figure 1), Newton's Method is much faster (convergence after 8 iterations) but it can diverge (Figure 2). Figure 3 shows the hybrid approach of taking 6 gradient descent steps and then switching to Newton's Method. It still converges in only 10 updates.