VI.4 | Gradient Descent Toward the Minimum

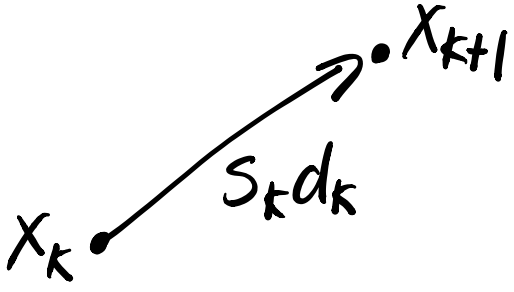
Algorithms for solving unconstrained optimization problems

$$\min_{x \in \mathbb{R}^n} f(x)$$

iterate

$$x_{k+1} = x_k + s_k d_k, \quad k = 0, 1, 2, \ldots,$$

where $s_k \in \mathbb{R}$ are the nonnegative step lengths and $d_k \in \mathbb{R}^n$ are the directions we move each iteration.



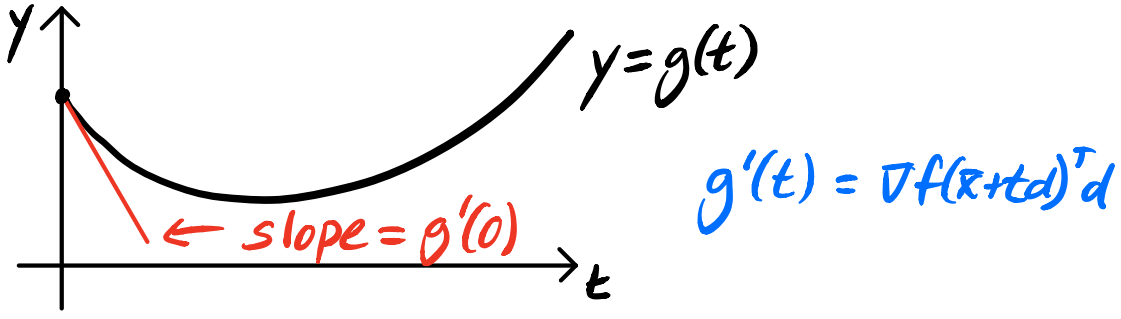
Line search methods choose d_k first and s_k second. Trust region methods choose s_k first and d_k second.

The direction of steepest descent

For which direction $d \in \mathbb{R}^n$ does the function $f: \mathbb{R}^n \to \mathbb{R}$ have the steepest negative slope at the point $\bar{x} \in \mathbb{R}^n$?

The value of the function f starting at $\bar{x}$ and moving in the direction d is given by:

$$g(t) = f(\bar{x} + td), \quad t \geq 0.$$



We want the $d \in \mathbb{R}^n$ such that $g'(0) = \nabla f(\bar{x})^T d$ is the most negative. We need to restrict ourselves to $\|d\|_2 = 1$ for this to make sense. Also, we need to assume that $\nabla f(\bar{x}) \neq 0$.

Thus, we want to solve

$$\boxed{\min \nabla f(\bar{x})^T d \quad \text{subject to} \quad \|d\|_2^2 = 1.}$$

The Lagrangian $\min_d \max_\lambda L(d,\lambda) \geq \max_\lambda \min_d L(d,\lambda)$

$$L(d,\lambda) = \nabla f(\bar{x})^T d + \lambda(1 - \|d\|_2^2)$$

has

$$\nabla_d L(d,\lambda) = \nabla f(\bar{x}) - 2\lambda d = 0$$

when $d = \frac{1}{2\lambda} \nabla f(\bar{x})$.

(Note that $\lambda \neq 0$ since $\nabla f(\bar{x}) \neq 0$.)

Now we use $\|d\|_2 = 1$ to find λ:

$$1 = \left\| \frac{1}{2\lambda} \nabla f(\bar{x}) \right\|_2 = \frac{1}{2|\lambda|} \|\nabla f(\bar{x})\|_2$$

$$\Rightarrow \quad \lambda = \pm \frac{1}{2} \|\nabla f(\bar{x})\|_2 .$$

The positive λ gives the <u>maximum</u> slope and the negative λ gives the <u>minimum</u>.

$\therefore \lambda = -\frac{1}{2}\|\nabla f(\bar{x})\|_2 \Rightarrow d = -\frac{\nabla f(\bar{x})}{\|\nabla f(\bar{x})\|_2}$

is the direction of steepest descent.

(Note: We also find that $d = \frac{\nabla f(\bar{x})}{\|\nabla f(\bar{x})\|_2}$ is the direction of steepest ascent.)

Gradient Descent: $d_k = -\nabla f(x_k)$

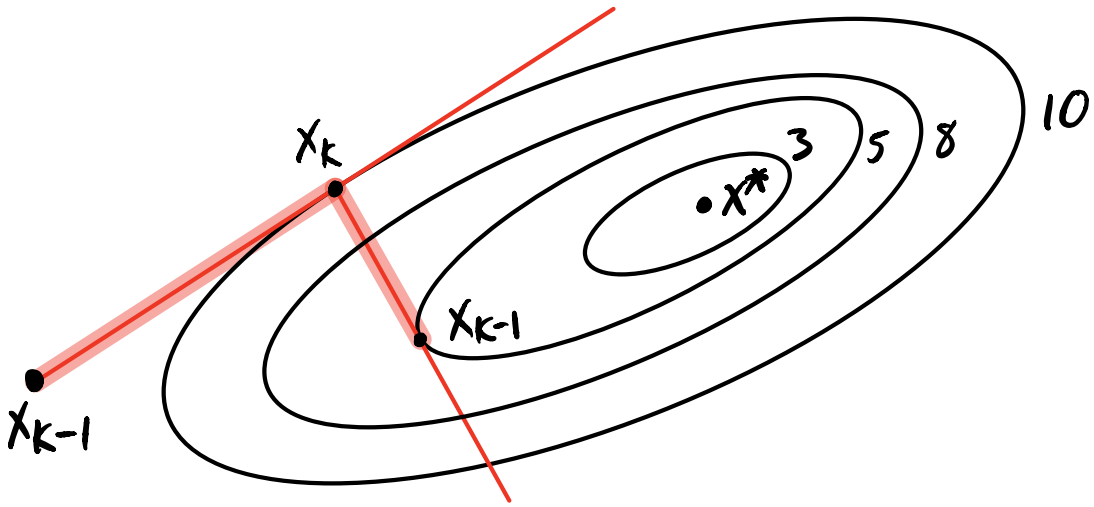
$$\boxed{x_{k+1} = x_k - s_k \nabla f(x_k)}$$

The step-size s_k can be found with an exact line search,

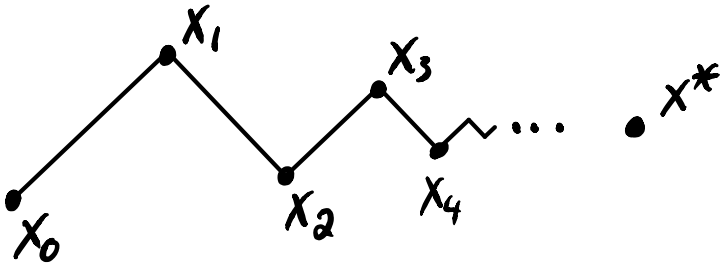
$$s_k = \underset{s \geq 0}{\operatorname{argmin}} \; f(x_k - s\nabla f(x_k))$$

or a backtracking line search that guarantees sufficient decrease.

Using the exact line search, our step directions will be orthogonal since $d_k = -\nabla f(x_k)$ is <u>orthogonal</u> to the current level curve $f(x) = f(x_k)$ and <u>tangent</u> to the next level curve $f(x) = f(x_{k+1})$.



We <u>zig-zag</u> toward the sol'n x^*.



The rate of convergence can be very slow.

Suppose $f: \mathbb{R}^n \to \mathbb{R}$ is convex and the eigenvalues of its Hessian matrix are bounded below by $m > 0$ and above by $M \geq m$:

$$\left[m \leq \lambda \leq M \quad \text{for all eigenvalues } \lambda \text{ of } \nabla^2 f(x), \text{ for all } x. \right]$$

Then we will reduce the distance between the objective value and the optimal value by at least a factor of $\left(1 - \frac{m}{M}\right)$:

$$\boxed{f(x_{k+1}) - f(x^*) \leq \left(1 - \frac{m}{M}\right)\left(f(x_k) - f(x^*)\right).}$$

This is a <u>linear rate</u> of convergence:

$$f(x_k) - f(x^*) \leq \left(1 - \frac{m}{M}\right)^k \left(f(x_0) - f(x^*)\right).$$

If m/M is close to zero, it can take a huge number of iterations to achieve a 99% reduction in the distance.

$$\left(1-\frac{m}{M}\right)^k \leq 0.01$$

m/M	k
0.9	2
0.1	44
0.01	459

Backtracking line search also gives a linear convergence rate, but with a larger reduction factor.

Momentum and the Path of a Heavy Ball

$$x_{k+1} = x_k - s z_k$$
$$z_k = \nabla f(x_k) + \beta z_{k-1}$$

Add momentum to the gradient.

How to choose s and β?

Consider $f(x) = \frac{1}{2} x^T S x$ with S positive definite and let

λ_{min} = smallest eigenvalue of S,

λ_{max} = largest eigenvalue of S.

The optimal s and β are

$$s = \left(\frac{2}{\sqrt{\lambda_{max}} + \sqrt{\lambda_{min}}} \right)^2, \quad \beta = \left(\frac{\sqrt{\lambda_{max}} - \sqrt{\lambda_{min}}}{\sqrt{\lambda_{max}} + \sqrt{\lambda_{min}}} \right)^2.$$

Example:

$$f(x, y) = \frac{1}{2}(x^2 + by^2), \quad 0 < b \leq 1.$$

$$(x_0, y_0) = (b, 1), \quad (x^*, y^*) = (0, 0)$$

Gradient descent w/ exact line search:

$$f(x_k, y_k) = \left(\frac{1-b}{1+b} \right)^{2k} f(x_0, y_0).$$

Heavy ball:

$$f(x_k, y_k) = \left(\frac{1-\sqrt{b}}{1+\sqrt{b}} \right)^{2k} f(x_0, y_0).$$

If $b = 0.01$, then

$$\left(\frac{1-b}{1+b}\right)^2 = 0.96 \quad \text{and} \quad \left(\frac{1-\sqrt{b}}{1+\sqrt{b}}\right)^2 = 0.67.$$

Thus, <u>one</u> step of heavy ball is the same as <u>ten</u> steps of gradient descent.

Nesterov Acceleration

$$x_{k+1} = y_k - s\nabla f(y_k)$$
$$y_{k+1} = x_{k+1} + \beta(x_{k+1} - x_k)$$

Evaluate ∇f at a shifted point.

For $f(x) = \frac{1}{2}x^T S x$, with S pos. def., we use

$$s = \frac{1}{\lambda_{max}}, \quad \beta = \frac{\sqrt{\lambda_{max}} - \sqrt{\lambda_{min}}}{\sqrt{\lambda_{max}} + \sqrt{\lambda_{min}}}.$$

<u>Adaptive methods</u> (eg ADAM) use <u>all</u> earlier points $x_0, \ldots, x_k$ to compute x_{k+1}.

Summary:

All three methods can be written as:

$$x_{k+1} = x_k + \beta(x_k - x_{k-1}) - s\nabla f\left(x_k + \gamma(x_k - x_{k-1})\right)$$

Gradient descent: $s \neq 0,\ \beta = \gamma = 0$

Heavy ball: $s, \beta \neq 0,\ \gamma = 0$

Nesterov: $s, \beta, \gamma \neq 0$

Constraints and Proximal Methods

$$\min f(x) \text{ subject to } x \in K$$

Projection onto K:

$$\text{proj}_K(x) = \underset{z \in K}{\text{argmin}} \frac{1}{2}\|x - z\|_2^2$$

Projected gradient descent:

$$x_{k+1} = \text{proj}_K\left(x_k - s_k \nabla f(x_k)\right)$$

A generalization:

$$\min_x \; f(x) + g(x)$$

$f: \mathbb{R}^n \to \mathbb{R}$ convex and smooth

$g: \mathbb{R}^n \to \mathbb{R} \cup \{+\infty\}$ convex and nonsmooth

If $g(x) = \begin{cases} 0 & \text{if } x \in K \\ +\infty & \text{if } x \notin K \end{cases}$

Then $\min_x f(x) + g(x) = \min_{x \in K} f(x)$.

Another example is **LASSO regression**:

$$\min_x \; \frac{1}{2}\|b - Ax\|_2^2 + \lambda \|x\|_1.$$

Here $f(x) = \frac{1}{2}\|b - Ax\|_2^2$ and $g(x) = \lambda \|x\|_1$.

Proximal mapping:

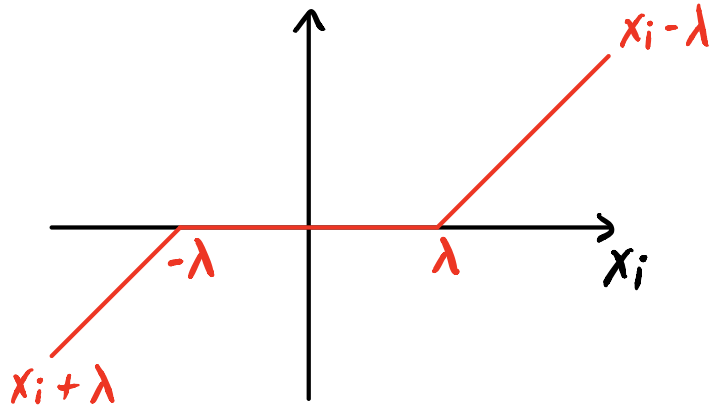
$$\text{prox}_g(x) = \underset{z \in \mathbb{R}^n}{\text{argmin}} \; \frac{1}{2}\|x - z\|_2^2 + g(z)$$

If $g(x) = \begin{cases} 0, & x \in K \\ +\infty, & x \notin K \end{cases}$

then $\text{prox}_g(x) = \text{proj}_K(x)$.

If $g(x) = \lambda \|x\|_1$, then

$$\text{prox}_g(x)_i = \text{sign}(x_i) \cdot \max(|x_i| - \lambda, 0).$$



"Soft thresholding"

Proximal gradient method:

$$x_{k+1} = \text{prox}_{s_k g}(x_k - s_k \nabla f(x_k))$$