Optimization and Computational Linear Algebra for Data Science
Lecture 12: Gradient descent

Léo Miolane · leo.miolane@gmail.com

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Warning: *This material is not meant to be lecture notes. It only gathers the main concepts and results from the lecture, without any additional explanation, motivation, examples, figures...*

In these notes, f denotes a twice differentiable **convex** function from $\mathbb{R}^n$ to $\mathbb{R}$.

1 Gradient descent

Given an initial point $x_0 \in \mathbb{R}^n$, the gradient descent algorithm follows the updates:

$$x_{t+1} = x_t - \alpha_t \nabla f(x_t), \tag{1}$$

where the step-size α_t remains to be determined. The step (1) is a very natural strategy to minimize f, since $-\nabla f(x)$ is the direction of steepest descent at x. Since $f(x+h) = f(x) + \langle \nabla f(x), h\rangle + o(\|h\|)$ we have

$$\begin{aligned} f(x_{t+1}) &= f(x_t) - \alpha_t \|\nabla f(x_t)\|^2 + o(\alpha_t) \\ &< f(x_t) \end{aligned}$$

for α_t small enough (provided that $\nabla f(x_t) \neq 0$). Hence is the step-sizes α_t are chosen very small, the sequence $(f(x_t))_{t\geq 0}$ is decreasing! However, if α_t are too small, the algorithm may never converge.

1.1 Convergence analysis

Notation: Given a symmetric matrix M we will denote by $\lambda_{\min}(M)$ and $\lambda_{\max}(M)$ the smallest and largest eigenvalues of M.

Definition 1.1

For $L, \mu > 0$, we say that a twice-differentiable convex function $f : \mathbb{R}^n \to \mathbb{R}$ is

- *L-smooth if for all $x \in \mathbb{R}^n$, $\lambda_{\max}(H_f(x)) \leq L$.*
- *μ-strongly convex if for all $x \in \mathbb{R}^n$, $\lambda_{\min}(H_f(x)) \geq \mu$.*

Remark 1.1. *Smoothness and strong convexity are usually defined as follows. We say that f is*

- *L-smooth if f is differentiable and if its gradient is L-Lipschitz meaning that for all $x, y \in \mathbb{R}^n$, $\|\nabla f(x) - \nabla f(y)\| \leq L\|x - y\|$.*
- *μ-strongly convex if the function $x \mapsto f(x) - \frac{\mu}{2}\|x\|^2$ is convex.*

These definitions are more general since they do not require f to be twice differentiable (for smoothness) or differentiable (for strong convexity). However, one can check that they are equivalent to Definition 1.1 when f is twice differentiable. In these notes, we will prefer to use Definition 1.1 because it makes clear that these two assumptions are related to the eigenvalues of the Hessian of f.

Remark 1.2. *L-smooth and μ-strongly convex functions are very convenient since they can be "sandwiched" as follows (see homework 9 for a proof):*

$$f(x) + \langle h, \nabla f(x)\rangle + \frac{\mu}{2}\|h\|^2 \leq f(x+h) \leq f(x) + \langle h, \nabla f(x)\rangle + \frac{L}{2}\|h\|^2,$$

for all $x, h \in \mathbb{R}^n$.

Theorem 1.1

Assume that f is convex, L-smooth and that f admits a (global) minimizer $x^* \in \mathbb{R}^n$. Then the gradient descent iterates (1) with constant step-size $\alpha_t = 1/L$ verify

$$f(x_t) - f(x^*) \leq \frac{2L\|x_0 - x^*\|^2}{t+4}.$$

See Section 2.1.5 from [4] for a proof.

Why did we used step sizes of $1/L$? f is L-smooth, hence (see Remark 1.2) for all $x, h \in \mathbb{R}^n$:

$$f(x+h) \leq f(x) + \langle \nabla f(x), h\rangle + \frac{L}{2}\|h\|^2. \tag{2}$$

Then, one can check (exercise!) that when x is fixed, the minimum of the right-hand side is minimum for $h = -\frac{1}{L}\nabla f(x)$.

Theorem 1.2

Assume that f is L-smooth and μ-strongly convex. Then f admits a unique minimizer global x^* and the gradient descent iterates (1) with constant step-size $\alpha_t = 1/L$ verify

$$f(x_t) - f(x^*) \leq \left(1 - \frac{\mu}{L}\right)^t (f(x_0) - f(x^*)).$$

Remark 1.3. *Theorems 1.1-1.2 show that gradient descent is adaptive to strong convexity of f.*

Remark 1.4. *The ratio $\kappa = \frac{L}{\mu} \geq 1$ is called the condition number. The smaller the condition number, the faster the convergence.*

Proof. Let $t \geq 0$. Applying (2) for $x = x_t$ and $h = -L^{-1}\nabla f(x_t)$, we get

$$f(x_{t+1}) \leq f(x_t) - \frac{1}{L}\|\nabla f(x_t)\|^2 + \frac{1}{2L}\|\nabla f(x_t)\|^2 = f(x_t) - \frac{1}{2L}\|\nabla f(x_t)\|^2.$$

Now, since f is μ-strongly convex, we have (exercise!) for all $x \in \mathbb{R}^n$

$$f(x) - f(x^*) \leq \frac{1}{2\mu}\|\nabla f(x)\|^2. \tag{3}$$

We get that $f(x_{t+1}) \leq f(x_t) - \frac{\mu}{L}(f(x_t) - f(x^*))$, hence

$$f(x_{t+1}) - f(x^*) \leq \left(1 - \frac{\mu}{L}\right)(f(x_t) - f(x^*)),$$

from which the theorem follows. □

1.2 Choosing the step size in practice

In practice, one may not have access to L and need hence to choose the step size α_t. A popular method is the so-called "backtracking line search" a goes as follows. Fix a parameter $\beta \in (0,1)$. Start with $\alpha = 1$ and while

$$f(x_t - \alpha \nabla f(x_t)) > f(x_t) - \frac{\alpha}{2}\|\nabla f(x_t)\|^2,$$

update $\alpha = \beta\alpha$. Then choose $\alpha_t = \alpha$.

1.3 Accelerated gradient method

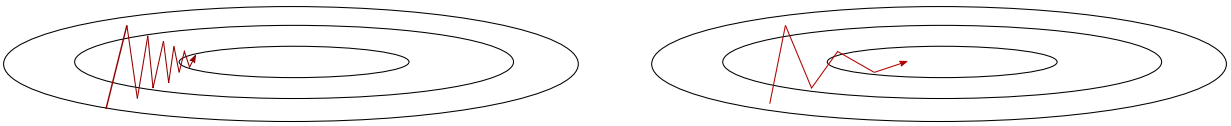


Figure 1: *Left*: gradient descent may oscillate in narrow valleys. *Right*: gradient descent with momentum accumulate momentum in the horizontal direction, while damping the oscillations on the vertical axis.

Gradient descent with momentum. Also known as "heavy ball" method, this scheme was introduced by Polyak in 1964. This is a way to prevent zigzagging trajectories when doing gradient descent by adding a momentum term:

$$x_{t+1} = x_t + v_t \quad \text{where} \quad v_t = -\alpha_t \nabla f(x_t) + \beta_t v_{t-1},$$

for some α_t, β_t. The idea is to keep momentum from past iterations in order to avoid zigzagging. It is possible to show that adding the momentum term leads to a better rate when f is twice differentiable, L-smooth and μ-strongly convex:

$$\|x_t - x^*\| \leq \left(\frac{\sqrt{L} - \sqrt{\mu}}{\sqrt{L} + \sqrt{\mu}}\right)^t \|x_0 - x^*\|,$$

when α_t and β_t are appropriately chosen.

Nesterov's accelerated gradient descent. Nesterov's accelerated gradient descent uses the idea of momentum, but evaluate the gradient at a different point that x_t:

$$x_{t+1} = x_t + v_t \quad \text{where} \quad v_t = \alpha_t v_{t-1} - \beta_t \nabla f(x_t + \alpha_t v_{t-1})$$

When α_t, β_t are properly chosen, it improves on the convergence rates of gradient descent (given by Theorems 1.1-1.2). Namely:

- if f is L-smooth and if its minimum is attained at some x^*, then for $\alpha_t = \frac{t-1}{t+2}$ and $\beta_t = 1/L$ we have
$$f(x_t) - f(x^*) \leq \frac{2L\|x_0 - x^*\|^2}{(t+1)^2}.$$
- if f is L-smooth and μ-strongly convex, then for $\alpha_t = \frac{1-\sqrt{\mu/L}}{1+\sqrt{\mu/L}}$ and $\beta_t = 1/L$ we have
$$f(x_t) - f(x^*) \leq L\|x_0 - x^*\|^2 \left(1 - \sqrt{\mu/L}\right)^t.$$

See for instance [6] for proofs of these results.

2 Newton's method

2.1 Newton's method

We assume here that f is μ-strongly convex and L-smooth. Newton's method performs updates according to

$$x_{t+1} = x_t - H_f(x_t)^{-1}\nabla f(x_t). \tag{4}$$

The (important!) difference with gradient descent is that the step-size α_t is now replaced by the inverse[1] of the Hessian of f. The idea begin Newton's method is to minimize the second order approximation of f at x_t :

$$f(x_t + h) \simeq f(x_t) + \langle \nabla f(x_t), h\rangle + \frac{1}{2}h^\intercal H_f(x_t)h \tag{5}$$

with respect to h and then choose $x_{t+1} = x_t + h$. It is an easy exercise to see that the minimizer of the right-hand side of (5) is $h = -H_f(x_t)^{-1}\nabla f(x_t)$, leading to the recursion (4).

It can be shown (see for instance [2]) that for t large enough

$$\|x_t - x^*\|^2 \leq Ce^{-\rho 2^t}, \tag{6}$$

where C, ρ are constants depending on f and x_0. We say that Newton's method converges *quadratically* to the minimizer x^*. Newton's method is much faster than gradient descent, whose speed (given by Theorem 1.2) is of order $C'e^{-\sqrt{\mu/L}\,t}$.

2.2 Quasi-Newton methods

The main drawback of Newton's method is its computational complexity. Each step of the method requires to compute the inverse of the $n \times n$ Hessian matrix of f at x_t, which requires $O(n^3)$ operations. This makes Newton's method unpractical for large scale applications.

Quasi-Newton methods have been developed to face these limitations. The idea behind quasi-Newton methods is to try to mimic the inverse Hessian $H_f(x_t)^{-1}$ by a sequence of symmetric positive semidefinite matrices $(Q_t)_{t\geq 0}$ that are recursively computed in an efficient way. We refer to Chapter 6 of [5] for a detailed introduction to this topic.

3 Stochastic gradient descent

3.1 Setting

A lot of machine learning problems fall in the following framework. Assume that there is a probability distribution P_0 on $\mathbb{R}^k \times \mathbb{R}^\ell$ and for $(X, Y) \sim P_0$ we would like to be able to estimate Y from X. To do so, we define a model depending on parameters $\theta \in \mathbb{R}^n$ that takes the form of a function

$$\varphi_\theta : \mathbb{R}^k \to \mathbb{R}^\ell.$$

Our estimate for Y will then be $\varphi_\theta(X)$. It remains then to find "good parameters" θ so that $\varphi_\theta(X) \simeq Y$. Hence we would like to find θ that minimize the risk

$$R(\theta) = \mathbb{E}\left[L(Y, \varphi_\theta(X))\right], \tag{7}$$

[1] The Hessian of f if indeed invertible at all x since its smallest eigenvalue is always greater than $\mu > 0$.

where $L : \mathbb{R}^\ell \times \mathbb{R}^\ell \to \mathbb{R}$ is some loss function, for instance $L(y, y') = \|y - y'\|^2$.

However we do not have access to the function R in general, because we do not know the distribution P_0. Instead, we usually have access to N samples $(X_i, Y_i) \overset{\text{i.i.d.}}{\sim} P_0$ and minimize then the *empirical risk*:

$$R_N(\theta) = \frac{1}{N} \sum_{i=1}^{N} L(Y_i, \varphi_\theta(X_i)) = \frac{1}{N} \sum_{i=1}^{N} f_i(\theta),$$

where we write $f_i(\theta) = L(Y_i, \varphi_\theta(X_i))$ for simplicity. In many cases, one minimizes $R_N(\theta)$ by gradient descent, following the opposite direction of the gradients:

$$\nabla R_N(\theta) = \frac{1}{N} \sum_{i=1}^{N} \nabla f_i(\theta).$$

However, when N (the number of training examples) and n (the number of parameters) are large, gradient descent becomes intractable since computing the gradient at a single point requires at least $N \times n$ computer operations.

3.2 Stochastic gradient descent

In order to face this issue, stochastic gradient descent (SGD) uses a single gradient $\nabla f_i(\theta)$ instead of the full-gradient $\nabla R_N(\theta) = \frac{1}{N} \sum_{i=1}^{N} \nabla f_i(\theta)$ to move:

$$\begin{aligned} &\text{Pick} \quad i \quad \text{uniformly at random in} \quad \{1, \dots, N\}, \\ &\text{Update} \quad \theta_{t+1} = \theta_t - \alpha_t \nabla f_i(\theta_t), \end{aligned}$$

where α_t is a step-size that has to be determined.

The direction of $\nabla f_i(\theta)$ is of course less accurate than the full gradient $\nabla R_N(\theta)$ and can hence be seen as a *noisy observation* of the full gradient. Hence, if we want SGD to converge we need that $\alpha_t \xrightarrow[t \to \infty]{} 0$. However, the step sizes should not decrease too fast, otherwise we may stay forever near the initial position θ_0 which will not perform well (because usually chosen at random). We have to make a trade-off:

- slowly decaying step-sizes: the gradient iterates θ_t moves fast, but keep a high variance.
- rapidly decaying step-sizes: the variance is reduced, but the iterates may move to slow to "forget" the initial condition θ_0.

In order to move in more accurate direction than ∇f_i, one often uses mini-batches of m gradients:

$$\begin{aligned} &\text{Pick} \quad i_1, \dots, i_m \quad \text{uniformly at random in} \quad \{1, \dots, N\}, \\ &\text{Update} \quad \theta_{t+1} = \theta_t - \frac{\alpha_t}{m} \sum_{k=1}^{m} \nabla f_{i_k}(\theta_t). \end{aligned}$$

Using mini-batches is computationally more expensive than using a single gradient, but leads to much accurate steps.

3.3 Convergence rate

A is usually recommended to take step-sizes α_t such that

$$\sum_{t=0}^{\infty} \alpha_t = +\infty.$$

If this condition is not met, SGD may remains to close from its initialization which will lead to bad performances. Classical results on stochastic gradient descent show that

- if the f_i are μ-strongly convex and smooth, then SGD with step sizes $\alpha_t = 1/(\mu t)$ achieves after t steps an error of $O(1/t)$.
- if the f_i convex and smooth, then SGD with step sizes $\alpha_t = 1/\sqrt{t}$ achieves after t steps an error of $O(1/\sqrt{t})$.

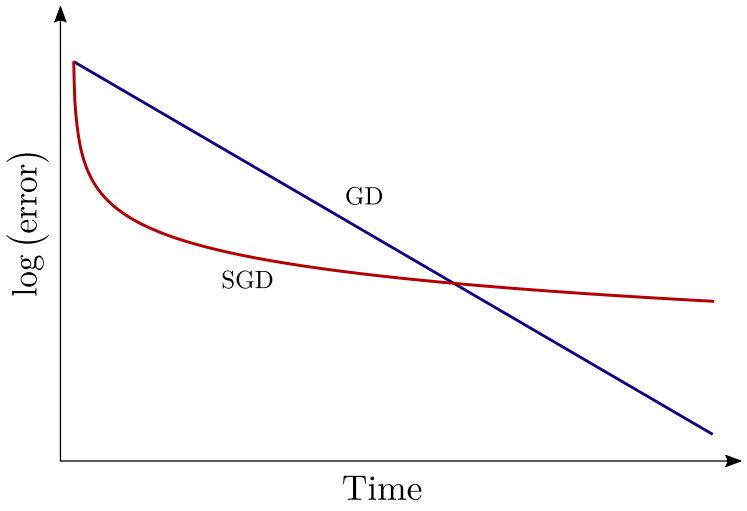
We give a proof in Appendix for the strongly convex case.

3.4 Concluding remarks

We summarize below the performances of gradient descent and stochastic gradient descent for optimizing R, when it is L-smooth and μ-strongly convex. Recall that N is the number of training examples and n is the number of parameters.

	Time per step	Error after t steps	log-error after τ time units
GD	Nn	$O(e^{-\rho t})$	$-\rho\tau/(Nn)$ + Cste
SGD	n	$O(1/t)$	$-\log(\tau/n)$ + Cste

We plot the log-error as a function of time below:



We see on the figure above that SGD obtains a decent solution reasonably fast. However, if one needs an high-accuracy solution, then standard gradient descent is more suitable.

In machine learning, objective functions are usually noisy because they depend on (noisy) data. That is, R_N is equal to the true risk R, plus some errors. Hence, there is no need to optimize R_N with an accuracy below the noise level, which makes SGD particularly suitable for large-scale machine learning problems.

Further reading

See chapter 9 of [2] for more background on gradient descent and Newton's method. See [1] for a more in-depth analysis of the tradeoffs discussed in Section 3.4. See chapter 8 of [3] for a discussion on the optimization of large neural nets.

References

[1] Léon Bottou and Olivier Bousquet. The tradeoffs of large scale learning. In *Advances in neural information processing systems*, pages 161–168, 2008.

[2] Stephen Boyd and Lieven Vandenberghe. *Convex optimization*. Cambridge university press, https://web.stanford.edu/~boyd/cvxbook/, 2004.

[3] Ian Goodfellow, Yoshua Bengio, and Aaron Courville. *Deep learning*. MIT press, 2016.

[4] Yurii Nesterov. *Lectures on convex optimization*, volume 137. Springer, 2018.

[5] Jorge Nocedal and Stephen Wright. *Numerical optimization*. Springer Science & Business Media, 2006.

[6] Mark Schmidt, Nicolas L Roux, and Francis R Bach. Convergence rates of inexact proximal-gradient methods for convex optimization. In *Advances in neural information processing systems*, pages 1458–1466, 2011.

Appendix: Analysis of SGD for strongly convex objective functions

In this section we assume N to be very large, and typically larger than the total number of steps of SGD that we are going to make. This allows us to never use at each time t a different gradient $\nabla f_{i_t}(\theta_t)$.

We start by rewriting SGD can be rewritten as

$$\theta_{t+1} = \theta_t - \alpha_t(\nabla R(\theta_t) + \varepsilon_t) \tag{8}$$

where $\varepsilon_t \stackrel{\text{def}}{=} \nabla f_{i_t}(\theta_t) - \nabla R(\theta_t)$. We use this notation to make clear that $\nabla f_{i_t}(\theta_t)$ is a noisy observation of $\nabla R(\theta_t)$, where ε_t denotes the error. Notice that $\mathbb{E}[\nabla f_{i_t}(\theta_t)|\theta_t] = \nabla R(\theta_t)$, thus $\mathbb{E}[\varepsilon_t|\theta_t] = 0$. We make the following additional assumptions:

- There exists $\sigma > 0$ such that $\mathbb{E}[\|\varepsilon_t\|^2|\theta_t] \leq \sigma^2$ for all $t \geq 0$.
- R is μ-strongly convex and L-smooth.
- $\min_{\theta\in\mathbb{R}^n} R(\theta) = 0$. (This can be easily verified by shifting R by a constant.)

Applying R on both sides of (8) and using the L-smoothness of L, we get

$$R(\theta_{t+1}) \leq R(\theta_t) - \alpha_t\langle\nabla R(\theta_t), \nabla R(\theta_t) + \varepsilon_t\rangle + \frac{L}{2}\alpha_t\|\nabla R(\theta_t) + \varepsilon_t\|^2.$$

Taking expectations on both sides gives:

$$\begin{aligned}\mathbb{E}R(\theta_{t+1}) &\leq \mathbb{E}R(\theta_t) - \alpha_t\mathbb{E}\|\nabla R(\theta_t)\|^2 + \frac{L}{2}\alpha_t^2\left(\mathbb{E}\|\nabla R(\theta_t)\|^2 + \sigma^2\right).\\ &\leq \mathbb{E}R(\theta_t) - \frac{\alpha_t}{2}\mathbb{E}\|\nabla R(\theta_t)\|^2 + \frac{L}{2}\alpha_t^2\sigma^2,\end{aligned}$$

assuming $\alpha_t \leq 1/L$. By strong convexity we have (as in (3)): $R(\theta) \leq 2\mu \|\nabla R(\theta)\|^2$. Hence:

$$\mathbb{E}R(\theta_{t+1}) \leq (1 - \mu\alpha_t)\,\mathbb{E}R(\theta_t) + \frac{L}{2}\alpha_t^2\sigma^2.$$

Using this inequalities, assuming that $(\alpha_t)_{t\geq 0}$ is non-increasing and less that $1/L$, one can prove that for all $0 \leq t \leq T$:

$$\mathbb{E}[R(\theta_T)] \leq \mathbb{E}[R(\theta_0)] \prod_{t=1}^{T}(1 - \mu\alpha_t) + \frac{L\sigma^2}{2} \exp\Big(-\mu \sum_{s=t+1}^{T} \alpha_t\Big) \sum_{t=1}^{T} \alpha_t^2 + \frac{L\sigma^2\alpha_t}{2\mu}.$$

Analysis of the first term. When $\alpha_t \to 0$,

$$\log \prod_{t=1}^{T}(1 - \mu\alpha_t) = \sum_{t=1}^{T} \log(1 - \mu\alpha_t) \sim -\mu \sum_{t=0}^{T} \alpha_t.$$

Hence, we need that $\sum_{t\geq 0} \alpha_t = +\infty$ in order to make the first term go to zero.

Conclusion. Taking $\alpha_t = 1/(\mu t)$, we get:

$$\mathbb{E}[R(\theta_T)] = O(1/T).$$