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

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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

$$f(x^{(t+1)}) = f(x^{(t)}) - \alpha_t ||\nabla f(x^{(t)})||^2 + o(\alpha_t)$$

< $f(x^{(t)})$

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 $(f(x^{(t)}))_{k\geq 0}$ 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 $L, \gamma > 0$, we say that a twice-differentiable convex function $f: \mathbb{R}^n \to \mathbb{R}$ is

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

Theorem 1.1

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

$$f(x^{(t)}) - f(x^*) \le \frac{2L||x^{(0)} - x^*||^2}{t+4}.$$

Why did we used step sizes of 1/L? If f is L-smooth one can prove (see Homework 9) that for all $x, h \in \mathbb{R}^n$:

$$f(x+h) \le f(x) + \langle \nabla f(x), h \rangle + \frac{L}{2} ||h||^2.$$
 (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 γ -strongly convex. Then f admits a unique minimizer global x^* and the gradient descent iterates (1) with constant step-size $\alpha_k = 1/L$ verify

$$f(x^{(t)}) - f(x^*) \le \left(1 - \frac{\gamma}{L}\right)^t (f(x^{(0)}) - f(x^*)).$$

Remark 1.1. The γ -strong convexity of f implies that for all $x \in \mathbb{R}^n$,

$$\frac{\gamma}{2} ||x - x^*||^2 \le f(x) - f(x^*).$$

Combining this with Theorem 1.2 gives a bound of the distance to the minimizer x^* :

$$||x^{(t)} - x^*||^2 \le \frac{2}{\gamma} \left(1 - \frac{\gamma}{L}\right)^t (f(x^{(0)}) - f(x^*)).$$

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

$$f(x^{(t+1)}) \le f(x^{(t)}) - \frac{1}{L} \|\nabla f(x^{(t)})\|^2 + \frac{1}{2L} \|\nabla f(x^{(t)})\|^2 = f(x^{(t)}) - \frac{1}{2L} \|\nabla f(x^{(t)})\|^2.$$

Now, since f is γ -strongly convex, we have for all $x \in \mathbb{R}^n$

$$f(x) - f(x^*) \le 2\gamma \|\nabla f(x)\|^2$$
.

We get that $f(x^{(t+1)}) \le f(x^{(t)}) - \frac{\gamma}{L}(f(x^{(t)}) - f(x^*))$, hence

$$f(x^{(t+1)}) - f(x^*) \le (1 - \frac{\gamma}{L})(f(x^{(t)}) - f(x^*)),$$

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 $\alpha_t = \alpha$.

2 Newton's method

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

$$x^{(t+1)} = x^{(t)} - H_f(x^{(t)})^{-1} \nabla f(x^{(t)}).$$
(3)

The (important!) difference with gradient descent is that the step-size α_k is now replaced by the inverse¹ of the Hessian of f. The idea begin Newton's method is to minimize the second order approximation of f at $x^{(t)}$:

$$f(x^{(t)} + h) \simeq f(x^{(t)}) + \langle \nabla f(x^{(t)}), h \rangle + \frac{1}{2} h^{\mathsf{T}} H_f(x^{(t)}) h$$
 (4)

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 (4) is $h = -H_f(x^{(t)})^{-1}\nabla f(x^{(t)})$, leading to the recursion (5).

It can be shown (see for instance [1]) that for t large enough

$$||x^{(t)} - x^*||^2 \le Ce^{-\rho 2^t},\tag{5}$$

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 $C'e^{-\rho't}$.

The main drawback of Newton's method is its computational complexity. Each step of the method require to compute the inverse of the $n \times n$ Hessian matrix of f at $x^{(t)}$, which require $O(n^3)$ operations. This makes Newton's method unpractical for large scale applications.

Further reading



References

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

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