Gradient Descent. Convergence rates

Seminar

Optimization for ML. Faculty of Computer Science. HSE University



Gradient Descent

Suppose, we have a problem of minimization of a smooth function $f(x): \mathbb{R}^n \to \mathbb{R}$:

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



Gradient Descent

Suppose, we have a problem of minimization of a smooth function $f(x): \mathbb{R}^n \to \mathbb{R}$:

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

One of the methods to solve this is gradient descent:

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



Gradient Descent

Suppose, we have a problem of minimization of a smooth function $f(x): \mathbb{R}^n \to \mathbb{R}$:

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

One of the methods to solve this is **gradient descent**:

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

The bottleneck (for almost all gradient methods) is choosing step-size, which can lead to the dramatic difference in method's behavior.



How to choose step sizes

• One of the theoretical suggestions: choosing stepsize inversly proportional to the gradient Lipschitz constant

$$\eta_k = \frac{1}{L}$$



How to choose step sizes

• One of the theoretical suggestions: choosing stepsize inversly proportional to the gradient Lipschitz constant

$$\eta_k = \frac{1}{L}$$

• Backtracking line search. Fix two parameters: $0 < \beta < 1$ and $0 < \alpha \leq 0.5$. At each iteration, start with t=1, and while

$$f(x_k - t\nabla f(x_k)) > f(x_k) - \alpha t \|\nabla f(x_k)\|_2^2,$$

shrink $t = \beta t$. Else perform Gradient Descent update $x_{k+1} = x_k - t \nabla f(x_k)$.



How to choose step sizes

• One of the theoretical suggestions: choosing stepsize inversly proportional to the gradient Lipschitz constant

$$\eta_k = \frac{1}{L}$$

• Backtracking line search. Fix two parameters: $0 < \beta < 1$ and $0 < \alpha \leq 0.5$. At each iteration, start with t=1, and while

$$f(x_k - t\nabla f(x_k)) > f(x_k) - \alpha t \|\nabla f(x_k)\|_2^2,$$

shrink $t = \beta t$. Else perform Gradient Descent update $x_{k+1} = x_k - t \nabla f(x_k)$.

Exact line search.

$$\eta_k = \operatorname*{arg\,min}_{\eta > 0} f(x_k - \eta \nabla f(x_k))$$

Let's consider a linear approximation of the differentiable function f along some direction $h, ||h||_2 = 1$:

Let's consider a linear approximation of the differentiable function f along some direction $h, \|h\|_2 = 1$:

$$f(x + \alpha h) = f(x) + \alpha \langle f'(x), h \rangle + o(\alpha)$$

Let's consider a linear approximation of the differentiable function f along some direction $h, \|h\|_2 = 1$:

$$f(x + \alpha h) = f(x) + \alpha \langle f'(x), h \rangle + o(\alpha)$$

We want h to be a decreasing direction:

$$f(x + \alpha h) < f(x)$$

$$f(x) + \alpha \langle f'(x), h \rangle + o(\alpha) < f(x)$$

Let's consider a linear approximation of the differentiable function f along some direction $h, ||h||_2 = 1$:

$$f(x + \alpha h) = f(x) + \alpha \langle f'(x), h \rangle + o(\alpha)$$

We want h to be a decreasing direction:

$$f(x + \alpha h) < f(x)$$

$$f(x) + \alpha \langle f'(x), h \rangle + o(\alpha) < f(x)$$

and going to the limit at $\alpha \to 0$:

$$\langle f'(x), h \rangle \leq 0$$

Let's consider a linear approximation of the differentiable function f along some direction $h, ||h||_2 = 1$:

$$f(x + \alpha h) = f(x) + \alpha \langle f'(x), h \rangle + o(\alpha)$$

We want h to be a decreasing direction:

$$f(x + \alpha h) < f(x)$$

$$f(x) + \alpha \langle f'(x), h \rangle + o(\alpha) < f(x)$$

and going to the limit at $\alpha \to 0$:

$$\langle f'(x), h \rangle \le 0$$

Also from Cauchy–Bunyakovsky–Schwarz inequality:

$$|\langle f'(x), h \rangle| \le ||f'(x)||_2 ||h||_2$$

 $\langle f'(x), h \rangle \ge -||f'(x)||_2 ||h||_2 = -||f'(x)||_2$

 $f \to \min_{x,y,z}$ Gradient Descent roots

Let's consider a linear approximation of the differentiable function f along some direction $h, ||h||_2 = 1$:

$$f(x + \alpha h) = f(x) + \alpha \langle f'(x), h \rangle + o(\alpha)$$

We want
$$h$$
 to be a decreasing direction:

We want h to be a decreasing direction:

$$f(x + \alpha h) < f(x)$$

$$f(x) + \alpha \langle f'(x), h \rangle + o(\alpha) < f(x)$$

and going to the limit at $\alpha \to 0$:

$$\langle f'(x), h \rangle \le 0$$

Also from Cauchy–Bunyakovsky–Schwarz inequality:

$$|\langle f'(x), h \rangle| \le ||f'(x)||_2 ||h||_2$$

 $\langle f'(x), h \rangle \ge -||f'(x)||_2 ||h||_2 = -||f'(x)||_2$

Thus, the direction of the antigradient

$$h = -\frac{f'(x)}{\|f'(x)\|_2}$$

gives the direction of the **steepest local** decreasing of the function f.

Let's consider a linear approximation of the differentiable function f along some direction $h, ||h||_2 = 1$:

$$f(x + \alpha h) = f(x) + \alpha \langle f'(x), h \rangle + o(\alpha)$$

We want
$$h$$
 to be a decreasing direction:

We want h to be a decreasing direction:

$$f(x + \alpha h) < f(x)$$

$$f(x) + \alpha \langle f'(x), h \rangle + o(\alpha) < f(x)$$

and going to the limit at $\alpha \to 0$:

$$\langle f'(x), h \rangle \le 0$$

Also from Cauchy-Bunyakovsky-Schwarz inequality:

$$|\langle f'(x), h \rangle| \le ||f'(x)||_2 ||h||_2$$

 $\langle f'(x), h \rangle \ge -||f'(x)||_2 ||h||_2 = -||f'(x)||_2$

Thus, the direction of the antigradient

$$h = -\frac{f'(x)}{\|f'(x)\|_2}$$

gives the direction of the **steepest local** decreasing of the function f. The result of this method is

$$x_{k+1} = x_k - \alpha f'(x_k)$$

Minimizer of Lipschitz parabola If a function $f:\mathbb{R}^n \to \mathbb{R}$ is continuously differentiable and its gradient satisfies Lipschitz conditions with constant L, then $\forall x, y \in \mathbb{R}^n$:

$$|f(y) - f(x) - \langle \nabla f(x), y - x \rangle| \le \frac{L}{2} ||y - x||^2,$$

If a function $f: \mathbb{R}^n \to \mathring{\mathbb{R}}$ is continuously differentiable and its gradient satisfies Lipschitz conditions with constant L, then $\forall x,y \in \mathbb{R}^n$:

$$|f(y) - f(x) - \langle \nabla f(x), y - x \rangle| \le \frac{L}{2} ||y - x||^2,$$

which geometrically means, that if we'll fix some point $x_0 \in \mathbb{R}^n$ and define two parabolas:

$$\phi_1(x) = f(x_0) + \langle \nabla f(x_0), x - x_0 \rangle - \frac{L}{2} ||x - x_0||^2,$$

$$\phi_2(x) = f(x_0) + \langle \nabla f(x_0), x - x_0 \rangle + \frac{L}{2} ||x - x_0||^2.$$

If a function $f: \mathbb{R}^n \to \mathbb{R}$ is continuously differentiable and its gradient satisfies Lipschitz conditions with constant L. then $\forall x, y \in \mathbb{R}^n$:

$$|f(y) - f(x) - \langle \nabla f(x), y - x \rangle| \le \frac{L}{2} ||y - x||^2,$$

which geometrically means, that if we'll fix some point $x_0 \in \mathbb{R}^n$ and define two parabolas:

$$\phi_1(x) = f(x_0) + \langle \nabla f(x_0), x - x_0 \rangle - \frac{L}{2} ||x - x_0||^2,$$

$$\phi_2(x) = f(x_0) + \langle \nabla f(x_0), x - x_0 \rangle + \frac{L}{2} ||x - x_0||^2.$$

Then

$$\phi_1(x) \le f(x) \le \phi_2(x) \quad \forall x \in \mathbb{R}^n.$$

 $f \to \min_{x,y,z}$ Gradient Descent roots

If a function $f: \mathbb{R}^n \to \mathring{\mathbb{R}}$ is continuously differentiable and its gradient satisfies Lipschitz conditions with constant L, then $\forall x,y \in \mathbb{R}^n$:

$$|f(y) - f(x) - \langle \nabla f(x), y - x \rangle| \le \frac{L}{2} ||y - x||^2,$$

which geometrically means, that if we'll fix some point $x_0 \in \mathbb{R}^n$ and define two parabolas:

$$\phi_1(x) = f(x_0) + \langle \nabla f(x_0), x - x_0 \rangle - \frac{L}{2} ||x - x_0||^2,$$

$$\phi_2(x) = f(x_0) + \langle \nabla f(x_0), x - x_0 \rangle + \frac{L}{2} ||x - x_0||^2.$$

Then

$$\phi_1(x) \le f(x) \le \phi_2(x) \quad \forall x \in \mathbb{R}^n.$$

Now, if we have global upper bound on the function, in a form of parabola, we can try to go directly to its minimum.

If a function $f: \mathbb{R}^n \to \mathbb{R}$ is continuously differentiable and its gradient satisfies Lipschitz conditions with constant L, then $\forall x,y \in \mathbb{R}^n$:

$$|f(y) - f(x) - \langle \nabla f(x), y - x \rangle| \le \frac{L}{2} ||y - x||^2,$$

which geometrically means, that if we'll fix some point $x_0 \in \mathbb{R}^n$ and define two parabolas:

$$\phi_1(x) = f(x_0) + \langle \nabla f(x_0), x - x_0 \rangle - \frac{L}{2} ||x - x_0||^2,$$

$$\phi_2(x) = f(x_0) + \langle \nabla f(x_0), x - x_0 \rangle + \frac{L}{2} ||x - x_0||^2.$$

Then

$$\phi_1(x) \le f(x) \le \phi_2(x) \quad \forall x \in \mathbb{R}^n.$$

Now, if we have global upper bound on the function, in a form of parabola, we can try to go directly to its minimum

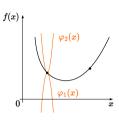


Figure 1: Illustration

If a function $f:\mathbb{R}^n \to \mathbb{R}$ is continuously differentiable and its gradient satisfies Lipschitz conditions with constant L, then $\forall x,y\in\mathbb{R}^n$:

$$|f(y) - f(x) - \langle \nabla f(x), y - x \rangle| \le \frac{L}{2} ||y - x||^2,$$

which geometrically means, that if we'll fix some point $x_0 \in \mathbb{R}^n$ and define two parabolas:

$$\phi_1(x) = f(x_0) + \langle \nabla f(x_0), x - x_0 \rangle - \frac{L}{2} ||x - x_0||^2,$$

$$\phi_2(x) = f(x_0) + \langle \nabla f(x_0), x - x_0 \rangle + \frac{L}{2} ||x - x_0||^2.$$

Then

minimum

$$\phi_1(x) < f(x) < \phi_2(x) \quad \forall x \in \mathbb{R}^n.$$

Now, if we have global upper bound on the function, in a form of parabola, we can try to go directly to its

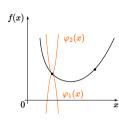


Figure 1: Illustration

$$\nabla \phi_2(x) = 0$$

$$\nabla f(x_0) + L(x^* - x_0) = 0$$

$$x^* = x_0 - \frac{1}{L} \nabla f(x_0)$$

$$x_{k+1} = x_k - \frac{1}{L} \nabla f(x_k)$$

This way leads to the $\frac{1}{L}$ stepsize choosing. However, often the L constant is not known.

PL-condition:

$$\|\nabla f(x)\|^2 \ge 2\mu(f(x) - f^*) \quad \forall x \in \mathbb{R}^n, \mu > 0,$$

where $f^* = f(x^*)$, $x^* = \arg\min f(x)$

PL-condition:

$$\|\nabla f(x)\|^2 \ge 2\mu(f(x) - f^*) \quad \forall x \in \mathbb{R}^n, \mu > 0,$$

where $f^* = f(x^*)$, $x^* = \arg\min f(x)$

if f(x) is differentiable and μ strongly convex then:

$$f(x^*) \ge f(x) + \nabla f(x)^T (x^* - x) + \frac{\mu}{2} ||x^* - x||^2$$

PL-condition:

$$\|\nabla f(x)\|^2 \ge 2\mu(f(x) - f^*) \quad \forall x \in \mathbb{R}^n, \mu > 0,$$

where $f^* = f(x^*)$, $x^* = \arg\min f(x)$

if f(x) is differentiable and μ strongly convex then:

$$f(x^*) \ge f(x) + \nabla f(x)^T (x^* - x) + \frac{\mu}{2} ||x^* - x||^2$$

$$f(x) - f(x^*) \le \nabla f(x)^T (x - x^*) - \frac{\mu}{2} ||x^* - x||^2 \le ||\nabla f(x)|| ||x - x^*|| - \frac{\mu}{2} ||x^* - x||^2$$

PL-condition:

$$\|\nabla f(x)\|^2 \ge 2\mu(f(x) - f^*) \quad \forall x \in \mathbb{R}^n, \mu > 0,$$

where $f^* = f(x^*)$, $x^* = \arg\min f(x)$

if f(x) is differentiable and μ strongly convex then:

$$f(x^*) \ge f(x) + \nabla f(x)^T (x^* - x) + \frac{\mu}{2} ||x^* - x||^2$$

$$f(x) - f(x^*) \le \nabla f(x)^T (x - x^*) - \frac{\mu}{2} ||x^* - x||^2 \le ||\nabla f(x)|| ||x - x^*|| - \frac{\mu}{2} ||x^* - x||^2$$

$$\leq [\mathsf{parabola's\ top}] \leq \frac{\|\nabla f(x)\|^2}{2\mu}$$

Thus, for a μ -strongly convex function, the PL-condition is satisfied

Exact line search aka steepest descent

$$\alpha_k = \arg\min_{\alpha \in \mathbb{R}^+} f(x_{k+1}) = \arg\min_{\alpha \in \mathbb{R}^+} f(x_k - \alpha \nabla f(x_k))$$

More theoretical than practical approach. It also allows you to analyze the convergence, but often exact line search can be difficult if the function calculation takes too long or costs a lot. Interesting theoretical property of this method is that each following iteration is orthogonal to the previous one:

$$\alpha_k = \arg\min_{\alpha \in \mathbb{R}^+} f(x_k - \alpha \nabla f(x_k))$$

Optimality conditions:

$$\nabla f(x_{k+1})^{\top} \nabla f(x_k) = 0$$

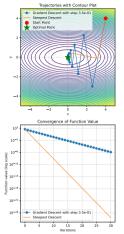


Figure 2: Steepest Descent

Open In Colab 🚓



Assume that f is convex, differentiable and Lipschitz gradient with constant L > 0.

Theorem

Gradient descent with fixed step size $t \leq 1/L$ satisfies

$$f(x^{(k)}) - f^* \le \frac{\|x^{(0)} - x^*\|_2^2}{2tk}$$

Assume that f is convex, differentiable and Lipschitz gradient with constant L > 0.

Theorem

Gradient descent with fixed step size $t \leq 1/L$ satisfies

$$f(x^{(k)}) - f^* \le \frac{\|x^{(0)} - x^*\|_2^2}{2tk}$$

Let's show that the convergence rate for the Backtracking line search is no worse than O(1/k)

Gradient Descent roots

Assume that f is convex, differentiable and Lipschitz gradient with constant L>0.

Theorem

Gradient descent with fixed step size $t \leq 1/L$ satisfies

$$f(x^{(k)}) - f^* \le \frac{\|x^{(0)} - x^*\|_2^2}{2tk}$$

Let's show that the convergence rate for the Backtracking line search is no worse than O(1/k)

Since ∇f is Lipschitz continuous with constant L>0, we have

$$f(y) \le f(x) + \nabla f(x)^{T} (y - x) + \frac{L}{2} ||y - x||_{2}^{2}, \forall x, y$$

 $f \to \min_{x,y,z}$ Gradient Descent roots

Assume that f is convex, differentiable and Lipschitz gradient with constant L>0.

Theorem

Gradient descent with fixed step size $t \leq 1/L$ satisfies

$$f(x^{(k)}) - f^* \le \frac{\|x^{(0)} - x^*\|_2^2}{2tk}$$

Let's show that the convergence rate for the Backtracking line search is no worse than O(1/k)

Since ∇f is Lipschitz continuous with constant L>0, we have

$$f(y) \le f(x) + \nabla f(x)^{T} (y - x) + \frac{L}{2} ||y - x||_{2}^{2}, \forall x, y$$

Let $y = x^+ = x - t\nabla f(x)$, then:

$$f(x^{+}) \le f(x) - \left(1 - \frac{Lt}{2}\right) t \|\nabla f(x)\|_{2}^{2} \le f(x) - \frac{1}{2L} \|\nabla f(x)\|_{2}^{2}$$

Assume that f is convex, differentiable and Lipschitz gradient with constant L > 0.

Theorem

Gradient descent with fixed step size $t \leq 1/L$ satisfies

$$f(x^{(k)}) - f^* \le \frac{\|x^{(0)} - x^*\|_2^2}{2tk}$$

Let's show that the convergence rate for the Backtracking line search is no worse than O(1/k)

Since
$$\nabla f$$
 is Lipschitz continuous with constant $L>0$, we have

$$f(y) \le f(x) + \nabla f(x)^{T} (y - x) + \frac{L}{2} ||y - x||_{2}^{2}, \forall x, y$$

Let $y = x^+ = x - t\nabla f(x)$, then:

$$f(x^{+}) \le f(x) - \left(1 - \frac{Lt}{2}\right) t \|\nabla f(x)\|_{2}^{2} \le f(x) - \frac{1}{2L} \|\nabla f(x)\|_{2}^{2}$$

This recalls us the stopping condition in Backtracking line search when $\alpha=0.5, t=\frac{1}{L}$. Hence, Backtracking line search with $\alpha=0.5$ plus condition of Lipschitz gradient will guarantee us the convergence rate of O(1/k).

Python Examples

Why convexity and strong convexity is important? Check the simple �code snippet.

Cool illustration of gradient descent 🕏

Lipschitz constant for linear regression 🕏



♥ ೧ ⊘