

Gradient Descent. Convergence for quadratics; smooth convex case; PL case. Lower bounds.

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Optimization for ML. Faculty of Computer Science. HSE University



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The result of this method is

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

Gradient flow ODE

Let's consider the following ODE, which is referred to as the Gradient Flow equation.

$$\frac{dx}{dt} = -f'(x(t)) \quad (\text{GF})$$

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From here we get the expression for x_{k+1}

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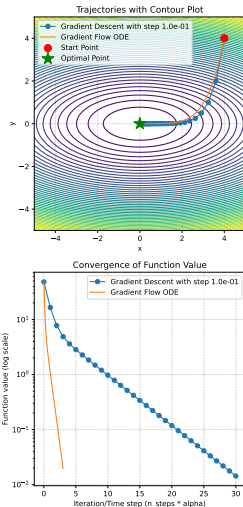


Figure 1: Gradient flow trajectory

Convergence of Gradient Descent algorithm

Heavily depends on the choice of the learning rate α :



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. An interesting theoretical property of this method is that each following iteration is orthogonal to the previous one:

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

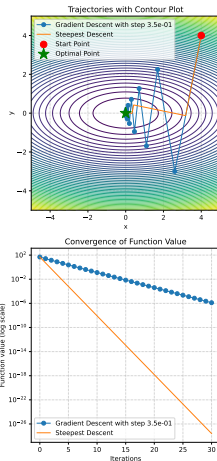



Figure 2: Steepest Descent

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Coordinate shift

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$$\min_{x \in \mathbb{R}^d} f(x) = \min_{x \in \mathbb{R}^d} \frac{1}{2} x^\top A x - b^\top x + c, \text{ where } A \in \mathbb{S}_{++}^d.$$

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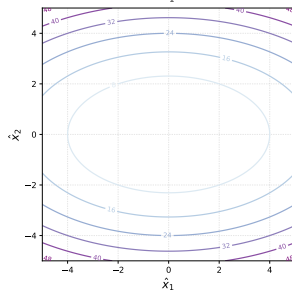
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$$\begin{aligned} f(\hat{x}) &= \frac{1}{2} (Q\hat{x} + x^*)^\top A (Q\hat{x} + x^*) - b^\top (Q\hat{x} + x^*) \\ &= \frac{1}{2} \hat{x}^\top Q^\top A Q \hat{x} + (x^*)^\top A Q \hat{x} + \frac{1}{2} (x^*)^\top A (x^*) - b^\top Q \hat{x} - b^\top x^* \end{aligned}$$



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Convergence analysis

Now we can work with the function $f(x) = \frac{1}{2}x^T \Lambda x$ with $x^* = 0$ without loss of generality (drop the hat from the \hat{x})

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$$\rho(\alpha) = \max_i |1 - \alpha \lambda_{(i)}| < 1$$

Remember, that $\lambda_{\min} = \mu > 0$, $\lambda_{\max} = L \geq \mu$.

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Now we would like to tune α to choose the best (lowest) convergence rate

$$\rho^* = \min_{\alpha} \rho(\alpha)$$

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$$\begin{aligned}x^{k+1} &= x^k - \alpha^k \nabla f(x^k) = x^k - \alpha^k \Lambda x^k \\&= (I - \alpha^k \Lambda)x^k\end{aligned}$$

$$x_{(i)}^{k+1} = (1 - \alpha^k \lambda_{(i)})x_{(i)}^k \quad \text{For } i\text{-th coordinate}$$

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Now we would like to tune α to choose the best (lowest) convergence rate

$$\rho^* = \min_{\alpha} \rho(\alpha) = \min_{\alpha} \max_i |1 - \alpha \lambda_{(i)}|$$

Let's use constant stepsize $\alpha^k = \alpha$. Convergence condition:

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$$\alpha^* = \frac{2}{\mu + L} \quad \rho^* = \frac{L - \mu}{L + \mu}$$

$$x^{k+1} = \left(\frac{L - \mu}{L + \mu}\right)^k x^0 \quad f(x^{k+1}) = \left(\frac{L - \mu}{L + \mu}\right)^{2k} f(x^0)$$

Convergence analysis

So, we have a linear convergence in the domain with rate $\frac{\kappa-1}{\kappa+1} = 1 - \frac{2}{\kappa+1}$, where $\kappa = \frac{L}{\mu}$ is sometimes called *condition number* of the quadratic problem.

κ	ρ	Iterations to decrease domain gap 10 times	Iterations to decrease function gap 10 times
1.1	0.05	1	1
2	0.33	3	2
5	0.67	6	3
10	0.82	12	6
50	0.96	58	29
100	0.98	116	58
500	0.996	576	288
1000	0.998	1152	576

Polyak-Lojasiewicz condition. Linear convergence of gradient descent without convexity

PL inequality holds if the following condition is satisfied for some $\mu > 0$,

$$\|\nabla f(x)\|^2 \geq 2\mu(f(x) - f^*) \quad \forall x$$

It is interesting, that the Gradient Descent algorithm might converge linearly even without convexity.

The following functions satisfy the PL condition but are not convex. [🔗Link to the code](#)

$$f(x) = x^2 + 3\sin^2(x)$$



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The following functions satisfy the PL condition but are not convex. [🔗Link to the code](#)

$$f(x) = x^2 + 3\sin^2(x)$$



$$f(x, y) = \frac{(y - \sin x)^2}{2}$$

Non-convex PL function



Convergence analysis

Theorem

Consider the Problem

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

and assume that f is μ -Polyak-Lojasiewicz and L -smooth, for some $L \geq \mu > 0$.

Consider $(x^k)_{k \in \mathbb{N}}$ a sequence generated by the gradient descent constant stepsize algorithm, with a stepsize satisfying $0 < \alpha \leq \frac{1}{L}$. Then:

$$f(x^k) - f^* \leq (1 - \alpha\mu)^k (f(x^0) - f^*).$$

Convergence analysis

We can use L -smoothness, together with the update rule of the algorithm, to write

$$f(x^{k+1}) \leq f(x^k) + \langle \nabla f(x^k), x^{k+1} - x^k \rangle + \frac{L}{2} \|x^{k+1} - x^k\|^2$$

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We can use L -smoothness, together with the update rule of the algorithm, to write

$$\begin{aligned} f(x^{k+1}) &\leq f(x^k) + \langle \nabla f(x^k), x^{k+1} - x^k \rangle + \frac{L}{2} \|x^{k+1} - x^k\|^2 \\ &= f(x^k) - \alpha \|\nabla f(x^k)\|^2 + \frac{L\alpha^2}{2} \|\nabla f(x^k)\|^2 \end{aligned}$$

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where in the last inequality we used our hypothesis on the stepsize that $\alpha L \leq 1$.

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where in the last inequality we used our hypothesis on the stepsize that $\alpha L \leq 1$.

We can now use the Polyak-Lojasiewicz property to write:

$$f(x^{k+1}) \leq f(x^k) - \alpha\mu(f(x^k) - f^*).$$

The conclusion follows after subtracting f^* on both sides of this inequality and using recursion.

Any μ -strongly convex differentiable function is a PL-function

Theorem

If a function $f(x)$ is differentiable and μ -strongly convex, then it is a PL function.

Proof

By first order strong convexity criterion:

$$f(y) \geq f(x) + \nabla f(x)^T (y - x) + \frac{\mu}{2} \|y - x\|_2^2$$

Putting $y = x^*$:

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$$\begin{aligned} \text{Let } a &= \frac{1}{\sqrt{\mu}} \nabla f(x) \text{ and} \\ b &= \sqrt{\mu}(x - x^*) - \frac{1}{\sqrt{\mu}} \nabla f(x) \end{aligned}$$

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Let $a = \frac{1}{\sqrt{\mu}} \nabla f(x)$ and

$$b = \sqrt{\mu} (x - x^*) - \frac{1}{\sqrt{\mu}} \nabla f(x)$$

Then $a + b = \sqrt{\mu} (x - x^*)$ and

$$a - b = \frac{2}{\sqrt{\mu}} \nabla f(x) - \sqrt{\mu} (x - x^*)$$

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$$f(x) - f(x^*) \leq \frac{1}{2} \left(\frac{1}{\mu} \|\nabla f(x)\|_2^2 - \left\| \sqrt{\mu}(x - x^*) - \frac{1}{\sqrt{\mu}} \nabla f(x) \right\|_2^2 \right)$$

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$$f(x) - f(x^*) \leq \frac{1}{2\mu} \|\nabla f(x)\|_2^2,$$

which is exactly the PL condition. It means, that we already have linear convergence proof for any strongly convex function.

Smooth convex case

Theorem

Consider the Problem

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

and assume that f is convex and L -smooth, for some $L > 0$.

Let $(x^k)_{k \in \mathbb{N}}$ be the sequence of iterates generated by the gradient descent constant stepsize algorithm, with a stepsize satisfying $0 < \alpha \leq \frac{1}{L}$. Then, for all $x^* \in \operatorname{argmin} f$, for all $k \in \mathbb{N}$ we have that

$$f(x^k) - f^* \leq \frac{\|x^0 - x^*\|^2}{2\alpha k}.$$

Convergence analysis

- As it was before, we first use smoothness:

$$\begin{aligned} f(x^{k+1}) &\leq f(x^k) + \langle \nabla f(x^k), x^{k+1} - x^k \rangle + \frac{L}{2} \|x^{k+1} - x^k\|^2 \\ &= f(x^k) - \alpha \|\nabla f(x^k)\|^2 + \frac{L\alpha^2}{2} \|\nabla f(x^k)\|^2 \\ &= f(x^k) - \frac{\alpha}{2} (2 - L\alpha) \|\nabla f(x^k)\|^2 \\ &\leq f(x^k) - \frac{\alpha}{2} \|\nabla f(x^k)\|^2, \\ f(x^k) - f(x^{k+1}) &\geq \frac{1}{2L} \|\nabla f(x^k)\|^2 \text{ if } \alpha \leq \frac{1}{L} \end{aligned} \tag{1}$$

Typically, for the convergent gradient descent algorithm the higher the learning rate the faster the convergence. That is why we often will use $\alpha = \frac{1}{L}$.

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How optimal is $\mathcal{O}\left(\frac{1}{k}\right)$?

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- Consider a family of first-order methods, where

$$x^{k+1} \in x^0 + \text{span} \{ \nabla f(x^0), \nabla f(x^1), \dots, \nabla f(x^k) \} \quad (4)$$

Smooth convex case

Theorem

There exists a function f that is L -smooth and convex such that any method 4 satisfies

$$\min_{i \in [1, k]} f(x^i) - f^* \geq \frac{3L\|x^0 - x^*\|_2^2}{32(1+k)^2}$$

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- No matter what gradient method you provide, there is always a function f that, when you apply your gradient method on minimizing such f , the convergence rate is lower bounded as $\mathcal{O}\left(\frac{1}{k^2}\right)$.
- The key to the proof is to explicitly build a special function f .

Nesterov's worst function

- Let $d = 2k + 1$ and $A \in \mathbb{R}^{d \times d}$.

$$\begin{bmatrix} 2 & -1 & 0 & 0 & \cdots & 0 \\ -1 & 2 & -1 & 0 & \cdots & 0 \\ 0 & -1 & 2 & -1 & \cdots & 0 \\ 0 & 0 & -1 & 2 & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & 0 & \cdots & 2 \end{bmatrix}$$

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- Notice, that

$$x^T A x = x[1]^2 + x[d]^2 + \sum_{i=1}^{d-1} (x[i] - x[i+1])^2,$$

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- The optimal solution x^* satisfies $Ax^* = e_1$, and solving this system of equations gives

$$x^*[i] = 1 - \frac{i}{d+1},$$

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$$\begin{bmatrix} 2 & -1 & 0 & 0 & \cdots & 0 \\ -1 & 2 & -1 & 0 & \cdots & 0 \\ 0 & -1 & 2 & -1 & \cdots & 0 \\ 0 & 0 & -1 & 2 & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & 0 & \cdots & 2 \end{bmatrix}$$

- Notice, that

$$x^T A x = x[1]^2 + x[d]^2 + \sum_{i=1}^{d-1} (x[i] - x[i+1])^2,$$

and, from this expression, it's simple to check $0 \preceq A \preceq 4I$.

- Define the following L -smooth convex function

$$f(x) = \frac{L}{8} x^T A x - \frac{L}{4} \langle x, e_1 \rangle.$$

- The optimal solution x^* satisfies $Ax^* = e_1$, and solving this system of equations gives

$$x^*[i] = 1 - \frac{i}{d+1},$$

- And the objective value is

$$\begin{aligned} f(x^*) &= \frac{L}{8} x^{*T} A x^* - \frac{L}{4} \langle x^*, e_1 \rangle \\ &= -\frac{L}{8} \langle x^*, e_1 \rangle = -\frac{L}{8} \left(1 - \frac{1}{d+1} \right). \end{aligned}$$