

Gradient Descent. Convergence rates

Daniil Merkulov

Optimization methods. MIPT

Previously

- Gradient Descent

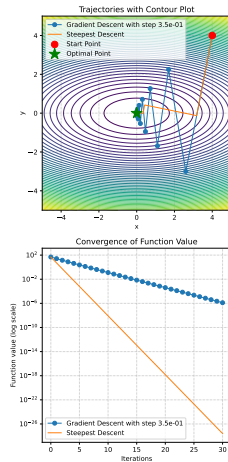



Figure 1: Steepest Descent

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- Gradient Descent
- Steepest descent

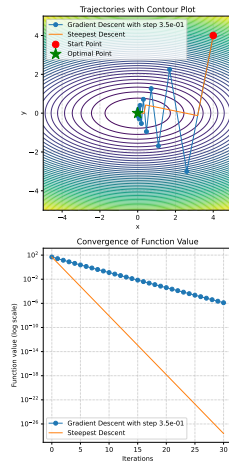



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- If $f : \mathbb{R}^d \rightarrow \mathbb{R}$ is L -smooth then for all $x, y \in \mathbb{R}^d$

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



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

- Let $f : \mathbb{R}^d \rightarrow \mathbb{R}$ be a twice differentiable L -smooth function. Then, for all $x \in \mathbb{R}^d$, for every eigenvalue λ of $\nabla^2 f(x)$, we have

$$|\lambda| \leq L.$$

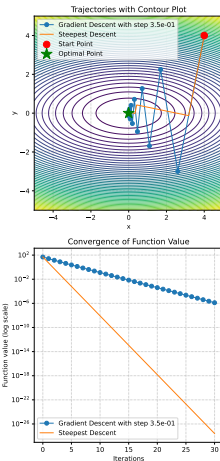


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Convergence rates

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

smooth	convex	smooth & convex	smooth & strongly convex (or PL)
$\ \nabla f(x_k)\ ^2 \approx \mathcal{O}\left(\frac{1}{k}\right)$	$f(x_k) - f^* \approx \mathcal{O}\left(\frac{1}{\sqrt{k}}\right)$	$f(x_k) - f^* \approx \mathcal{O}\left(\frac{1}{k}\right)$	$\ x_k - x^*\ ^2 \approx \mathcal{O}\left(\left(1 - \frac{\mu}{L}\right)^k\right)$

Coordinate shift for strongly convex quadratics

Consider the following quadratic optimization problem:

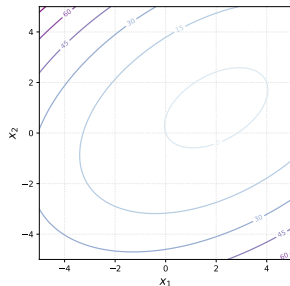
$$\min_{x \in \mathbb{R}^d} f(x) = \min_{x \in \mathbb{R}^d} \frac{1}{2} x^\top A x - b^\top x + c, \text{ where } A \in \mathbb{S}_{++}^d.$$

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- Secondly, we have a spectral decomposition of the matrix A :

$$A = Q\Lambda Q^\top$$



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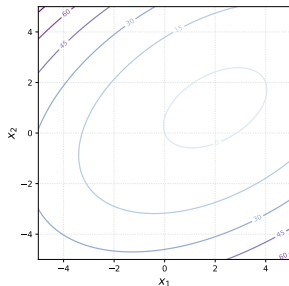
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- Let's show, that we can switch coordinates in order to make an analysis a little bit easier. Let $\hat{x} = Q^\top(x - x^*)$, where x^* is the minimum point of initial function, defined by $Ax^* = b$. At the same time $x = Q\hat{x} + x^*$.



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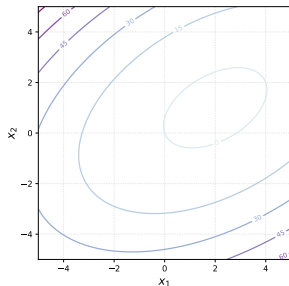
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$$f(\hat{x}) = \frac{1}{2} (Q\hat{x} + x^*)^\top A (Q\hat{x} + x^*) - b^\top (Q\hat{x} + x^*)$$



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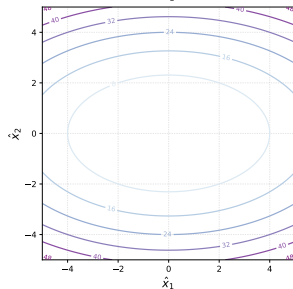
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$$\begin{aligned} f(\hat{x}) &= \frac{1}{2} (Q\hat{x} + x^*)^\top A (Q\hat{x} + x^*) - b^\top (Q\hat{x} + x^*) \\ &= \frac{1}{2} \hat{x}^\top Q^\top A Q \hat{x} + (x^*)^\top A Q \hat{x} + \frac{1}{2} (x^*)^\top A (x^*) - b^\top Q \hat{x} - b^\top x^*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



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Strongly convex quadratics

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

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

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

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

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

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$$\begin{aligned}\rho^* &= \min_{\alpha} \rho(\alpha) = \min_{\alpha} \max_i |1 - \alpha \lambda_{(i)}| \\&= \min_{\alpha} \{|1 - \alpha \mu|, |1 - \alpha L|\}\end{aligned}$$

$$\alpha^* : 1 - \alpha^* \mu = \alpha^* L - 1$$

Strongly convex quadratics

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})

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

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

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

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

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

Strongly convex quadratics

So, we have a linear convergence in 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 Gradient Descent algorithm has

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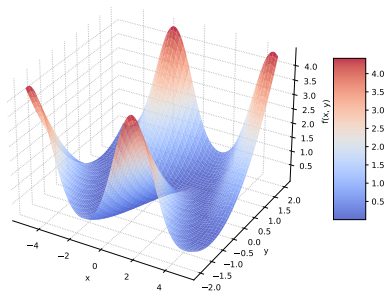
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$$f(x) = x^2 + 3\sin^2(x)$$



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

Non-convex PL function



Gradient Descent convergence. Polyak-Łojasiewicz case

Theorem

Consider the Problem

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

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

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

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

Gradient Descent convergence. Polyak-Lojasiewicz case

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

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

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:

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

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

Gradient Descent convergence. 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 $(x^t)_{t \in \mathbb{N}}$ 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 $t \in \mathbb{N}$ we have that

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

Gradient Descent convergence. Smooth convex case

Gradient Descent convergence. Smooth μ -strongly convex case

Theorem

Consider the Problem

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

and assume that f is μ -strongly convex and L -smooth, for some $L \geq \mu > 0$. Let $(x^t)_{t \in \mathbb{N}}$ 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 $x^* = \operatorname{argmin} f$ and for all $t \in \mathbb{N}$:

$$\|x^{t+1} - x^*\|^2 \leq (1 - \alpha\mu)^{t+1} \|x^0 - x^*\|^2.$$

Gradient Descent convergence. Smooth μ -strongly convex case

Gradient Descent for Linear Least Squares aka Linear Regression



Figure 4: Illustration

In a least-squares, or linear regression, problem, we have measurements $X \in \mathbb{R}^{m \times n}$ and $y \in \mathbb{R}^m$ and seek a vector $\theta \in \mathbb{R}^n$ such that $X\theta$ is close to y . Closeness is defined as the sum of the squared differences:

$$\sum_{i=1}^m (x_i^\top \theta - y_i)^2 = \|X\theta - y\|_2^2 \rightarrow \min_{\theta \in \mathbb{R}^n}$$

For example, we might have a dataset of m users, each represented by n features. Each row x_i^\top of X is the features for user i , while the corresponding entry y_i of y is the measurement we want to predict from x_i^\top , such as ad spending. The prediction is given by $x_i^\top \theta$.

Linear Least Squares aka Linear Regression ¹

1. Is this problem convex? Strongly convex?

Linear Least Squares aka Linear Regression ¹

1. Is this problem convex? Strongly convex?
2. What do you think about convergence of Gradient Descent for this problem?


¹Take a look at the  example of real-world data linear least squares problem

l_2 -regularized Linear Least Squares

In the underdetermined case, it is often desirable to restore strong convexity of the objective function by adding an l_2 -penalty, also known as Tikhonov regularization, l_2 -regularization, or weight decay.

$$\|X\theta - y\|_2^2 + \frac{\mu}{2}\|\theta\|_2^2 \rightarrow \min_{\theta \in \mathbb{R}^n}$$

Note: With this modification the objective is μ -strongly convex again.

Take a look at the code