

Gradient Descent



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Also from Cauchy–Bunyakovsky–Schwarz inequality:

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

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

Thus, the direction of the antigradient

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

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

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

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

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

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

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

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

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where $x_k \equiv x(t_k)$ and $\alpha = t_{k+1} - t_k$ - is the grid step.

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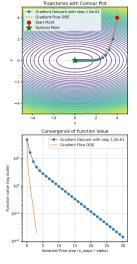
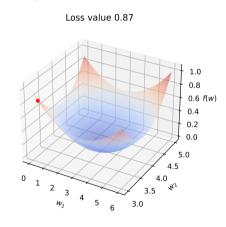
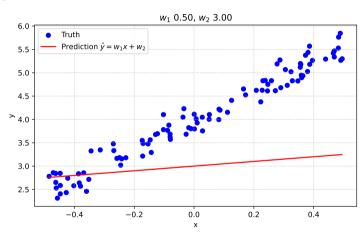


Figure 1: Gradient flow trajectory

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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Optimality conditions:

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

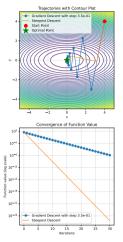


Figure 2: Steepest Descent

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Strongly convex quadratics



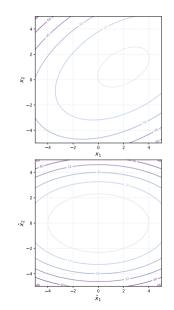
Consider the following quadratic optimization problem:

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

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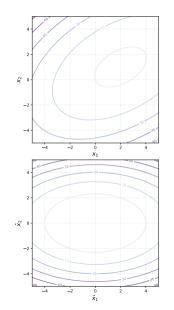


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$$A = Q\Lambda Q^T$$



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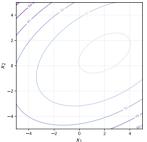
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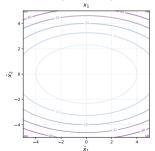
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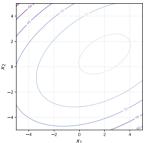
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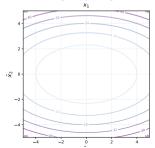
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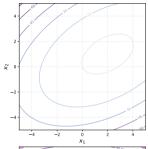
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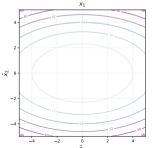
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$$f(\hat{x}) = \frac{1}{2} (Q\hat{x} + x^*)^{\top} A (Q\hat{x} + x^*) - b^{\top} (Q\hat{x} + x^*)$$
$$= \frac{1}{2} \hat{x}^T Q^T A Q \hat{x} + (x^*)^T A Q \hat{x} + \frac{1}{2} (x^*)^T A (x^*)^T - b^T Q \hat{x} - b^T x^*$$





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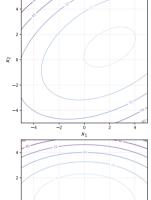
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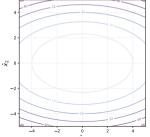
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$$= \frac{1}{2} \hat{x}^T Q^T A Q \hat{x} + (x^*)^T A Q \hat{x} + \frac{1}{2} (x^*)^T A (x^*)^T - b^T Q \hat{x} - b^T x^*$$

$$= \frac{1}{2} \hat{x}^T \Lambda \hat{x}$$





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 $\lambda_{\min} = \mu > 0, \lambda_{\max} = L \ge \mu$.

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$$x_{(i)}^{k+1}=(1-lpha^k\lambda_{(i)})x_{(i)}^k$$
 For i -th coordinate $x_{(i)}^{k+1}=(1-lpha^k\lambda_{(i)})^kx_{(i)}^0$

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

condition: $\rho(\alpha) = \max|1 - \alpha\lambda_{(i)}| < 1$

$$p(\alpha) = \min_{i} |1 - \alpha x_{(i)}| < 1$$

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

 $|1 - \alpha \mu| < 1 \qquad \qquad |1 - \alpha L| < 1$

$$\begin{array}{ll} -1<1-\alpha\mu<1 & -1<1-\alpha L<1 \\ \alpha<\frac{2}{\mu} & \alpha\mu>0 & \alpha<\frac{2}{L} & \alpha L>0 \\ \alpha<\frac{2}{T} \text{ is needed for convergence.} \end{array}$$

 $= (I - \alpha^k \Lambda) x^k$

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})

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

$$x_{(i)}^{k+1} = (1-\alpha^k\lambda_{(i)})^kx_{(i)}^0$$
 Let's use constant stepsize $\alpha^k = \alpha$. Convergence condition:
$$\rho(\alpha) = \max_i |1-\alpha\lambda_{(i)}| < 1$$

 $x^{k+1} = x^k - \alpha^k \nabla f(x^k) = x^k - \alpha^k \Lambda x^k$

 $\rho^* = \min \rho(\alpha)$

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

$$|1 - \alpha \mu| < 1$$
 $|1 - \alpha L| < 1$
- 1 < 1 - \alpha L < 1 - 1 < 1 - \alpha L < 1

$$\alpha<\frac{2}{\mu} \qquad \alpha\mu>0 \qquad \qquad \alpha<\frac{2}{L} \qquad \alpha L>0$$

$$\alpha<\frac{2}{L} \quad \text{ is needed for convergence}.$$

convergence rate

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

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

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})

$$\begin{split} x^{k+1} &= x^k - \alpha^k \nabla f(x^k) = x^k - \alpha^k \Lambda x^k \\ &= (I - \alpha^k \Lambda) x^k \\ x^{k+1}_{(i)} &= (1 - \alpha^k \lambda_{(i)}) x^k_{(i)} \text{ For } i\text{-th coordinate} \end{split}$$

 $x_{(i)}^{k+1} = (1 - \alpha^k \lambda_{(i)})^k x_{(i)}^0$

convergence rate

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

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

Let's use constant stepsize
$$\alpha^k=\alpha$$
. Convergence condition:
$$\rho(\alpha)=\max_i|1-\alpha\lambda_{(i)}|<1$$
 Remember, that $\lambda_{\min}=\mu>0, \lambda_{\max}=L>\mu.$

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

$$0. \lambda_{\text{max}} = L > \mu_{\text{s}}$$

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

$$|1 - \alpha \mu| < 1$$
 $|1 - \alpha L| < 1$
- 1 < 1 - \alpha L < 1 - 1 < 1 - \alpha L < 1

$$-1 < 1 - \alpha \mu < 1$$

$$\alpha < \frac{2}{\mu} \quad \alpha \mu > 0$$

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$$egin{aligned} x^{k+1} &= x^k - lpha^k
abla f(x^k) = x^k - lpha^k \Lambda x^k \ &= (I - lpha^k \Lambda) x^k \ x^{k+1}_{(i)} &= (1 - lpha^k \lambda_{(i)}) x^k_{(i)} & ext{For i-th coordinate} \end{aligned}$$

 $x_{(i)}^{k+1} = (1 - \alpha^k \lambda_{(i)})^k x_{(i)}^0$

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$$= \min_{\alpha} \left\{ |1 - \alpha \mu|, |1 - \alpha L| \right\}$$

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 $x_{(i)}^{k+1} = (1 - \alpha^k \lambda_{(i)})^k x_{(i)}^0$

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$$\alpha^k=\alpha$$
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Now we would like to tune α to choose the best (lowest) convergence rate

$$\rho^* = \min_{\alpha} \rho(\alpha) = \min_{\alpha} \max_{i} |1 - \alpha \lambda_{(i)}|$$
$$= \min_{\alpha} \{|1 - \alpha \mu|, |1 - \alpha L|\}$$
$$\alpha^* : 1 - \alpha^* \mu = \alpha^* L - 1$$

$$\alpha L - 1$$

condition:

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

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

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$$\alpha^k=\alpha.$$
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$$x^{k+1} = \left(\frac{L-\mu}{L+\mu}\right)^k x^0$$

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convergence rate

 $= \min\left\{|1 - \alpha \mu|, |1 - \alpha L|\right\}$ $\alpha^*: 1 - \alpha^* \mu = \alpha^* L - 1$

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

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

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

 $\alpha < \frac{2}{L}$ is needed for convergence. $f \to \min_{x,y,z}$ Strongly convex quadratics

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	ho	Iterations to decrease domain gap $10\ \mathrm{times}$	Iterations to decrease function gap $10\ \mathrm{times}$
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

Strongly convex quadratics

Polyak-Lojasiewicz smooth case



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

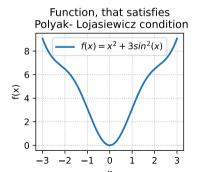
PL inequality holds if the following condition is satisfied for some $\mu > 0$,

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

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. **PL**ink to the code

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



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

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

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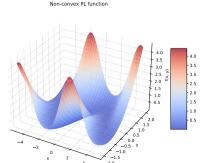
It is interesting, that the Gradient Descent algorithm might converge linearly even without convexity.

The following functions satisfy the PL condition but are not convex. Link to the code

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

Function, that satisfies Polyak- Lojasiewicz condition $f(x) = x^2 + 3\sin^2(x)$ 8 6 **€** 4 2

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





i Theorem

Consider the Problem

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

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

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

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



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

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

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

$$= f(x^k) - \alpha \|\nabla f(x^k)\|^2 + \frac{L\alpha^2}{2} \|\nabla f(x^k)\|^2$$

$$= f(x^k) - \frac{\alpha}{2} (2 - L\alpha) \|\nabla f(x^k)\|^2$$

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

$$= f(x^k) - \alpha \|\nabla f(x^k)\|^2 + \frac{L\alpha^2}{2} \|\nabla f(x^k)\|^2$$

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$$\le f(x^k) - \frac{\alpha}{2} \|\nabla f(x^k)\|^2,$$

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$$\le f(x^k) - \frac{\alpha}{2} \|\nabla f(x^k)\|^2,$$

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

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

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



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$$\leq f(x^k) - \frac{\alpha}{2} \|\nabla f(x^k)\|^2,$$

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

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

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

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

i 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:

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

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

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Polyak-Loiasiewicz smooth case

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$$f(x) - f(x^*) \le \nabla f(x)^T (x - x^*) - \frac{\mu}{2} ||x^* - x||_2^2 =$$

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$$=\left(\nabla f(x)^{T} - \frac{\mu}{2}(x^{*} - x)\right)^{T}(x - x^{*}) =$$

$$= \frac{1}{2} \left(\frac{2}{\sqrt{\mu}} \nabla f(x)^T - \sqrt{\mu} (x^* - x) \right)^T \sqrt{\mu} (x - x^*) =$$

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

$$f(x^*) \ge f(x) + \nabla f(x)^T (x^* - x) + \frac{\mu}{2} ||x^* - x||_2^2$$
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$$= \left(\nabla f(x)^{T} - \frac{\mu}{2}(x^{*} - x)\right)^{T}(x - x^{*}) =$$

$$= \frac{1}{2} \left(\frac{2}{\sqrt{\mu}} \nabla f(x)^{T} - \sqrt{\mu} (x^{*} - x) \right)^{T} \sqrt{\mu} (x - x^{*}) =$$

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Putting $y = x^*$:

$$f(x^*) \ge f(x) + \nabla f(x)^T (x^* - x) + \frac{\mu}{2} ||x^* - x||_2^2$$
$$f(x) - f(x^*) \le \nabla f(x)^T (x - x^*) - \frac{\mu}{2} ||x^* - x||_2^2 =$$

$$= \left(\nabla f(x)^{T} - \frac{\mu}{2}(x^{*} - x)\right)^{T} (x - x^{*}) = \frac{1}{2} \left(\frac{2}{2} - \frac{\mu}{2}(x^{*} - x)\right)^{T} = \frac{1}{2} \left(\frac{2}{2} - \frac{\mu}{2}\right)^{T} = \frac{1}{2} \left(\frac{2}{2} - \frac{$$

$$= \frac{1}{2} \left(\frac{2}{\sqrt{\mu}} \nabla f(x)^{T} - \sqrt{\mu} (x^{*} - x) \right)^{T} \sqrt{\mu} (x - x^{*}) =$$

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

$$u = 0 - \sqrt{\mu} \sqrt{f(x)} - \sqrt{\mu(x - x)}$$

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

$$f(x) - f(x^*) \le \frac{1}{2} \left(\frac{1}{\mu} \|\nabla f(x)\|_2^2 - \left\| \sqrt{\mu} (x - x^*) - \frac{1}{\sqrt{\mu}} \nabla f(x) \right\|_2^2 \right)$$
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which is exactly the PL condition. It means, that we already have linear convergence proof for any strongly convex function.

Smooth convex case





Smooth convex case

i Theorem

Consider the Problem

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

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

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



• As it was before, we first use smoothness:

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

$$= f(x^k) - \alpha \|\nabla f(x^k)\|^2 + \frac{L\alpha^2}{2} \|\nabla f(x^k)\|^2$$

$$= f(x^k) - \frac{\alpha}{2} (2 - L\alpha) \|\nabla f(x^k)\|^2$$

$$\leq f(x^k) - \frac{\alpha}{2} \|\nabla f(x^k)\|^2,$$

$$f(x^k) - f(x^{k+1}) \geq \frac{1}{2L} \|\nabla f(x^k)\|^2 \text{ if } \alpha \leq \frac{1}{L}$$

$$(1)$$

Typically, for the convergent gradient descent algorithm the higher the learning rate the faster the convergence.

That is why we often will use $\alpha = \frac{1}{4}$.

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$$f(x^k) - f^* \le \langle \nabla f(x^k), x^k - x^* \rangle$$
(2)

 $f \to \min_{x,y,z}$ Smooth convex case

• Now we put Equation 2 to Equation 1:



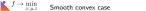


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$$f \to \min_{x,y,z}$$
 Smooth convex case

(3)

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$$f \to \min_{x,y,z}$$
 Smooth convex case

(3)

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convex case

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