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

Daniil Merkulov

Optimization for ML. Faculty of Computer Science. HSE University

Direction of local steepest descent

$-\nabla f(x_k)$

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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.

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

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where $x_k \equiv x(t_k)$ and $\alpha = t_{k+1} - t_k$ - is the grid step.
From here we get the expression for x_{k+1}

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Open In Colab ♣

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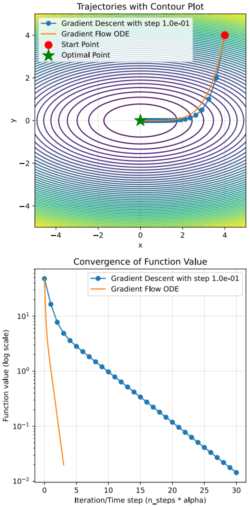
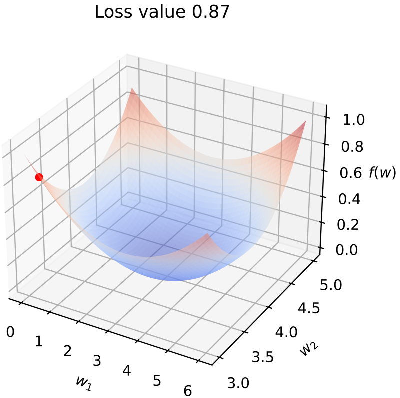
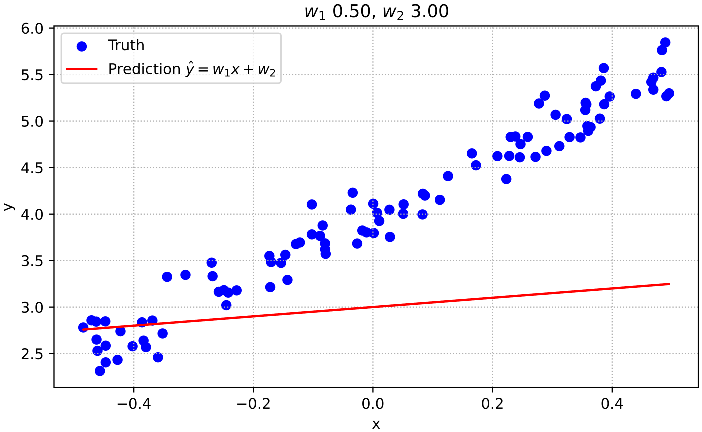


Figure 1: Gradient flow trajectory

Convergence of Gradient Descent algorithm

Heavily depends on the choice of the learning rate α:





Exact line search aka steepest descent

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

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:

$$
\boxed{\alpha_k = \text{arg}\min_{\alpha \in \mathbb{R}^+} \underbrace{f(x_k - \alpha \nabla f(x_k))}} = \varphi(\alpha) = f(x^{k+1})
$$

$$
: \mathbb{R} \to \mathbb{R}
$$

$$
\frac{\partial \varphi}{\partial \alpha} = \frac{\partial \varphi}{\partial x_{k+1}} \cdot \frac{\partial x_{k+1}}{\partial \alpha} = \nabla f(x^{k+1})^T \cdot \left(-\nabla f(x^k)\right) = 0
$$

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

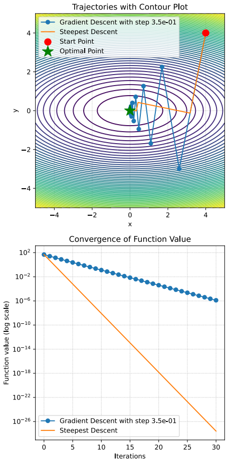

Figure 2: Steepest Descent

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Coordinate shift

Consider the following quadratic optimization problem:

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

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$\lambda_{min}(A) > 0 = \mu$

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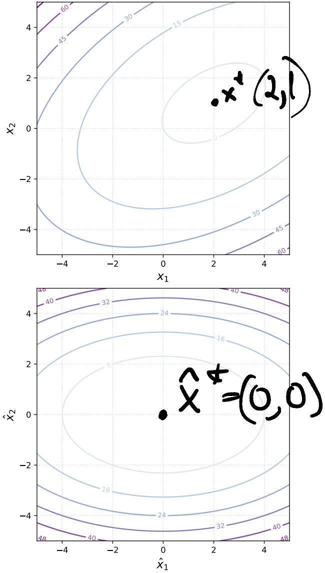
- Firstly, without loss of generality we can set $c = 0$, which will or affect optimization process.



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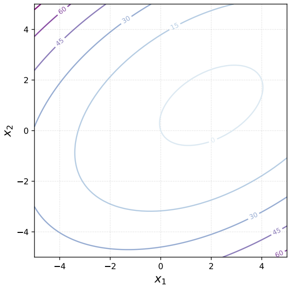
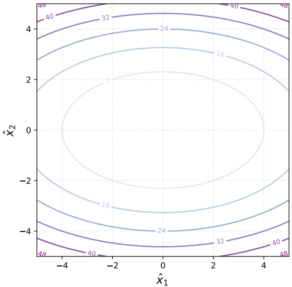
$$\boxed{A = Q \Lambda Q^T}$$





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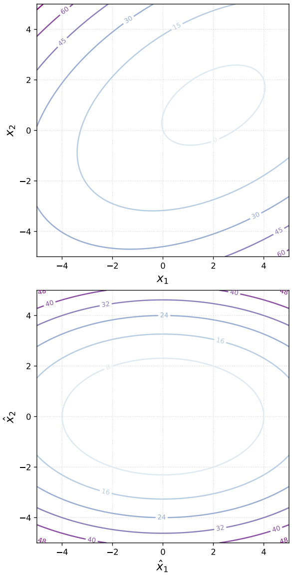

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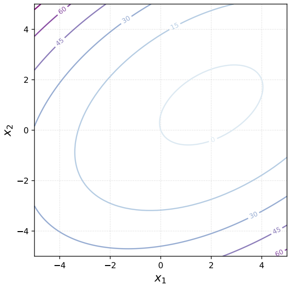

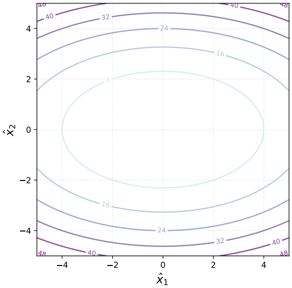

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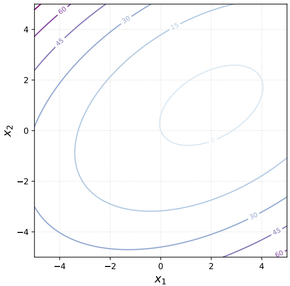

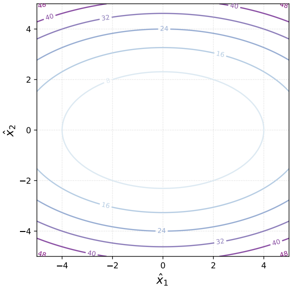

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$Q^T A Q = \Lambda$

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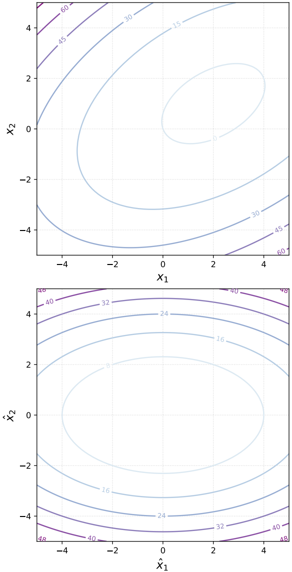

Convergence analysis

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

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

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$\nabla f = \Lambda x$

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&= (I - \alpha^k \Lambda) x^k
\end{aligned}
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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 $\hat{x}$)

$x \in \mathbb{R}^d$

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$$\boxed{x^{k+1}_{(i)} = (1 - \alpha^k \lambda_{(i)}) x^k_{(i)}}$$ For i-th coordinate

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$$

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

$\alpha^k = \alpha = \text{const}$

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\end{aligned}
$$

$\|\nabla f(x) - \nabla f(y)\|_2 \leq L\|x-y\|_2$

константа
липшиця
градієнта

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

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

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

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λ_{min}

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

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

$$
\begin{aligned}
|1 - \alpha\mu| &< 1 \\
-1 < 1 - \alpha\mu &< 1 \\
\alpha < \frac{2}{\mu} \quad & \quad \alpha\mu > 0
\end{aligned}
\qquad
\begin{aligned}
|1 - \alpha L| &< 1 \\
-1 < 1 - \alpha L &< 1
\end{aligned}
$$

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 $\hat{x}$)

$$\boxed{\alpha < \frac{2}{L}}$$

$$
\begin{aligned}
x^{k+1} &= x^k - \alpha^k \nabla f(x^k) = x^k - \alpha^k \Lambda x^k \\
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Now we would like to tune α to choose the best (lowest) convergence rate

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

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Convergence analysis

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$$
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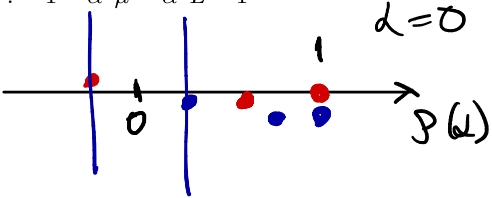
$$



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\alpha^* &: \quad 1 - \alpha^* \mu = \alpha^* L - 1
\end{aligned}
$$

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

Convergence analysis

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&= \min_\alpha \{|1 - \alpha\mu|, |1 - \alpha L|\} \\
\alpha^* &: \quad 1 - \alpha^*\mu = \alpha^* L - 1 \\
\alpha^* &= \frac{2}{\mu + L} \qquad \rho^* = \frac{L - \mu}{L + \mu}
\end{aligned}
$$

Convergence analysis

$\varkappa$

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^* &: \quad 1 - \alpha^* \mu = \alpha^* L - 1 \\
\alpha^* &= \frac{2}{\mu + L} \quad \rho^* = \frac{L - \mu}{L + \mu} = \frac{\varkappa - 1}{\varkappa + 1} \\
x^{k+1} &= \left(\frac{L - \mu}{L + \mu} \right)^k x^0
\end{aligned}
$$

$\varkappa = \frac{L}{\mu}$

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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\end{aligned}
$$

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

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

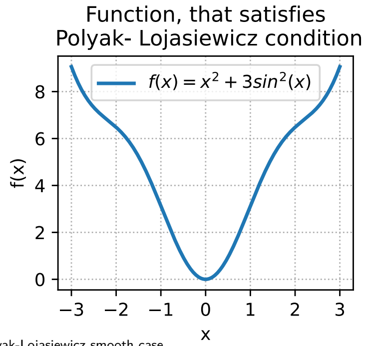
PL inequality holds if the following condition is satisfied for some $\mu > 0$,

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

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

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



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

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\|\nabla f(x)\|^2 \geq 2\mu(f(x) - f^*) \quad \forall x
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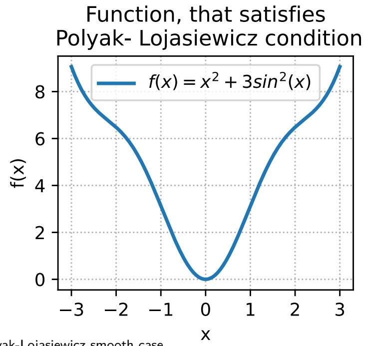
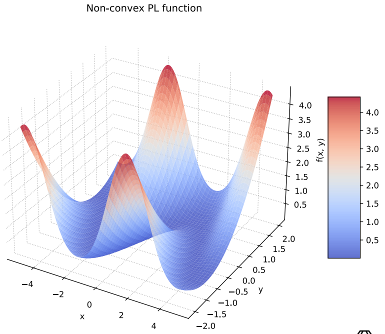
The following functions satisfy the PL condition but are not convex. Link to the code

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

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





Convergence analysis

Theorem

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

Consider the Problem

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

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

Липшицева парабола.

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

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

Convergence analysis

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

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

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

Convergence analysis

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

$$
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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}\left(2 - L\alpha\right)\|\nabla f(x^k)\|^2
\end{aligned}
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Convergence analysis

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

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

≤ -1

$\alpha L \leq 1$

$-\alpha L \geq -1$

$2 - \alpha L \geq 1$

$-(2 - \alpha L) \leq -1$

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

Convergence analysis

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

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

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

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

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

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

$-f^*$ $\quad$ $-f^*$

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

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.

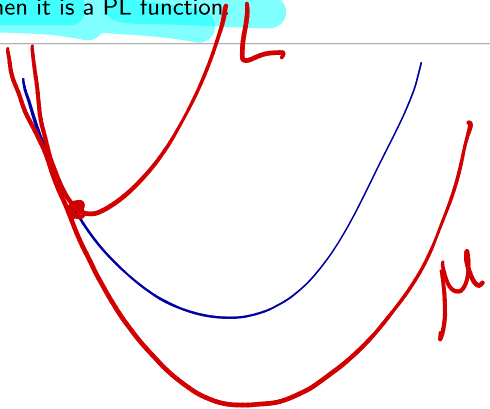
Proof

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 $y = x^*$:

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



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Let $a = \frac{1}{\sqrt{\mu}}\nabla f(x)$ and
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Any μ-strongly convex differentiable function is a PL-function

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

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

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

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

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

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

Convergence analysis

$\|\nabla f(x)-\nabla f(y)\| \le L\|x-y\| \qquad \lambda_{max}(\nabla^2 f) \le L$

- As it was before, we first use smoothness

$\frac{\|\nabla f(x)-\nabla f(y)\|}{\|x-y\|} \le L$

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

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

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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\begin{aligned}
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- After that we add convexity:

(2)

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f(y) \geq f(x) + \langle \nabla f(x), y - x \rangle \tag{2}
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$R^0 - \cancel{R^1} + \cancel{R^1} - \cancel{R^2} + \cancel{R^2} - R^3$

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$$
\begin{aligned}
f(x^{k+1}) &\leq f^* + \frac{1}{2\alpha}\left[\underbrace{\|x^k - x^*\|_2^2}_{a^2} - \underbrace{\|x^k - x^* - \alpha \nabla f(x^k)\|_2^2}_{b^2}\right] \\
&\leq f^* + \frac{1}{2\alpha}\left[\|x^k - x^*\|_2^2 - \|x^{k+1} - x^*\|_2^2\right] \\
2\alpha\left(f(x^{k+1}) - f^*\right) &\leq \|x^k - x^*\|_2^2 - \|x^{k+1} - x^*\|_2^2
\end{aligned}
$$

- Now suppose, that the last line is defined for some index i and we sum over $i \in [0, k-1]$. Almost all summands will vanish due to the telescopic nature of the sum:

$$ \tag{3} $$

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Let $a = x^k - x^*$ and $b = x^k - x^* - \alpha\nabla f(x^k)$. Then $a + b = \alpha \nabla f(x^k)$ and $a - b = 2\left(x^k - x^* - \frac{\alpha}{2}\nabla f(x^k)\right)$.

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\begin{aligned}
f(x^{k+1}) &\leq f^* + \frac{1}{2\alpha}\left[\|x^k - x^*\|_2^2 - \|x^k - x^* - \alpha \nabla f(x^k)\|_2^2\right] \\
&\leq f^* + \frac{1}{2\alpha}\left[\|x^k - x^*\|_2^2 - \|x^{k+1} - x^*\|_2^2\right] \\
2\alpha\left(f(x^{k+1}) - f^*\right) &\leq \|x^k - x^*\|_2^2 - \|x^{k+1} - x^*\|_2^2
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- Now suppose, that the last line is defined for some index i and we sum over $i \in [0, k-1]$. Almost all summands will vanish due to the telescopic nature of the sum:

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2\alpha \sum_{i=0}^{k-1}\left(f(x^{i+1}) - f^*\right) \leq \|x^0 - x^*\|_2^2 - \|x^k - x^*\|_2^2 \tag{3}
$$

Convergence analysis

- Now we put Equation 2 to Equation 1:

$$
\begin{aligned}
f(x^{k+1}) \leq f(x^k) - \frac{\alpha}{2}\|\nabla f(x^k)\|^2 &\leq f^* + \langle \nabla f(x^k), x^k - x^* \rangle - \frac{\alpha}{2}\|\nabla f(x^k)\|^2 \\
&= f^* + \langle \nabla f(x^k), x^k - x^* - \frac{\alpha}{2}\nabla f(x^k) \rangle \\
&= f^* + \frac{1}{2\alpha}\left\langle \alpha \nabla f(x^k), 2\left(x^k - x^* - \frac{\alpha}{2}\nabla f(x^k)\right)\right\rangle
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Convergence analysis

- Due to the monotonic decrease at each iteration $f(x^{i+1}) < f(x^i)$:

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kf(x^k) \leq \sum_{i=0}^{k-1} f(x^{i+1})
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$$
\boxed{f(x^k) - f^* \leq \frac{\|x^0 - x^*\|_2^2}{2\alpha k}} \leq \frac{L\|x^0 - x^*\|_2^2}{2k}
$$

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

- Is it somehow possible to understand, that the obtained convergence is the fastest possible with this class of problem and this class of algorithms?

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x^{k+1} &= x^k - \alpha^k \nabla f(x^k) \\
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\end{aligned}
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- Consider a family of first-order methods, where

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

Smooth convex case

$O\left(\frac{1}{k^2}\right)$

Theorem

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

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

Smooth convex case

выпуклые гладкие

сильно вып. гладкие

PL

GD

$O\left(\frac{1}{k}\right)$

$O\left(\left(\frac{\varkappa-1}{\varkappa+1}\right)^k\right)$

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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 $\mathcal{O}\left(\frac{1}{k^2}\right)$.

Негладкие функции

$O\left(\frac{1}{\sqrt{k}}\right)$

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

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$$
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$$

- And the objective value is

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