# Gradient descent and accelerated methods - heavy ball method. Nesterov's accelerated method. Features of nonsmooth optimization. Subgradient method. Proximal gradient method. Newton's method and quasi-Newton's methods

Daniil Merkulov

Applied Math for Data Science. Sberuniversity.

# Gradient Descent

# Exact line search aka steepest descent

Наискорейший спуск

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

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:

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

Optimality conditions:

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

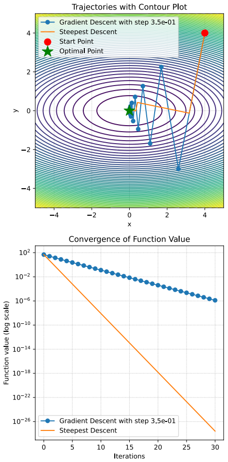



Figure 1: Steepest Descent

Open In Colab ♣

# Strongly convex quadratics

# Coordinate shift

Consider the following quadratic optimization problem:

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

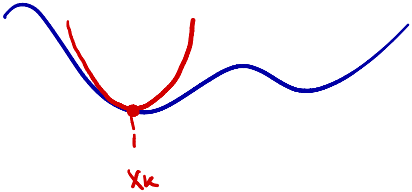
$\nabla^2 f = A$

пример:
Lin Reg

пример неквадр. задачи
LogReg, SVM, NN, LP

локально даже неквадр. $f(x)$:
(больше $x_k$)

$$f(x) \approx f^{II}_{x_k}(x)$$




$$f^{II}_{x_k}(x) = f(x_k) + \langle \nabla f(x_k), x - x_k \rangle + \frac{1}{2} \langle \nabla^2 f(x_k)(x - x_k), x - x_k \rangle$$

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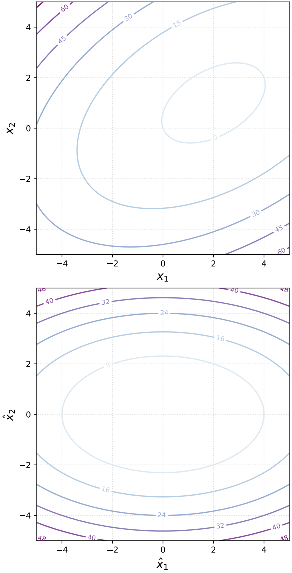
- Firstly, without loss of generality we can set $c = 0$, which will or affect optimization process.



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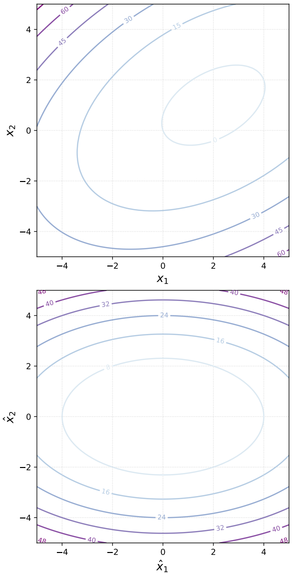
- Firstly, without loss of generality we can set $c = 0$, which will or affect optimization process.
- Secondly, we have a spectral decomposition of the matrix $A$:

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



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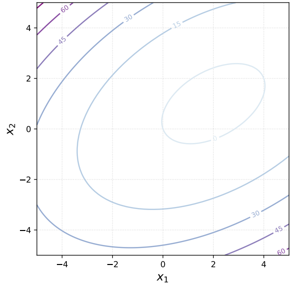
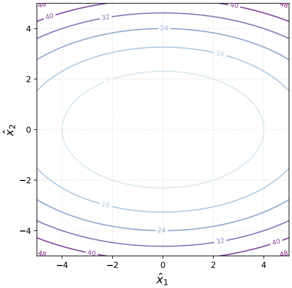
- Let's show, that we can switch coordinates to make an analysis a little bit easier. Let $\hat{x} = Q^T(x - x^*)$, where $x^*$ is the minimum point of initial function, defined by $Ax^* = b$. At the same time $x = Q\hat{x} + x^*$.



# Coordinate shift

Consider the following quadratic optimization problem:

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

сильно выпуклая

линии уровня f(x)

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

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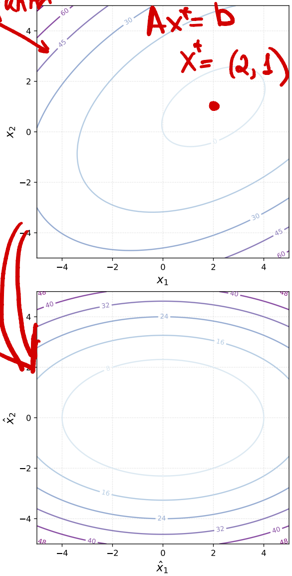
$$f(\hat{x}) = \frac{1}{2}(Q\hat{x} + x^*)^\top A (Q\hat{x} + x^*) - b^\top (Q\hat{x} + x^*)$$

всегда можно сделать координат



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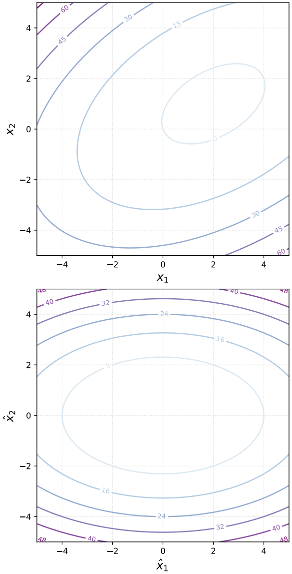
$$\begin{aligned} f(\hat{x}) &= \frac{1}{2}(Q\hat{x} + x^*)^\top A (Q\hat{x} + x^*) - b^\top (Q\hat{x} + x^*) \\ &= \frac{1}{2}\hat{x}^T Q^T A Q \hat{x} + (x^*)^T A Q \hat{x} + \frac{1}{2}(x^*)^T A (x^*)^T - b^T Q \hat{x} - b^T x^* \end{aligned}$$



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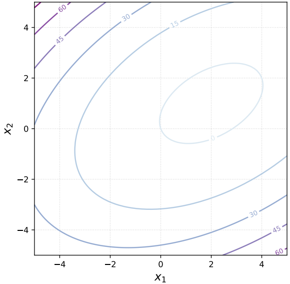
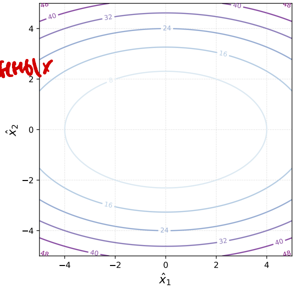
замена переменных

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



# 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 $\hat{x}$)

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

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

$n \times n$ $\quad$ $n \times 1$

↑ диагональная

$$y = \mathrm{diag}(d) \cdot x$$

$$y_i = d_i \cdot x_i$$

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\end{aligned}
$$

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

$\alpha^* = \dfrac{2}{\lambda_{min}(A) + \lambda_{max}(A)}$

L - константа Липшица градиента функции.

$\dfrac{L-\mu}{L+\mu} = \dfrac{\frac{L}{\mu} - 1}{\frac{L}{\mu} + 1} = \dfrac{\varkappa - 1}{\varkappa + 1}$

$\varkappa = \frac{L}{\mu} \geq 1$

# 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.

меньше - лучше

| $\kappa$ | $\rho$ | 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 |

$\kappa = 1$ $\kappa = 10$

# Polyak-Lojasiewicz smooth case

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

∀ сильно выпуклая f является PL-функцией

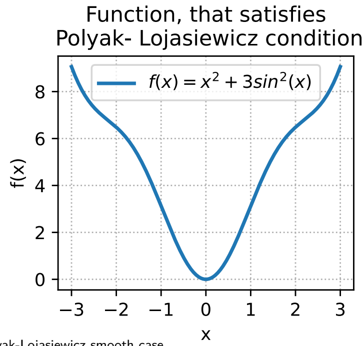
PL inequality holds if the following condition is satisfied for some $\mu > 0$,

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

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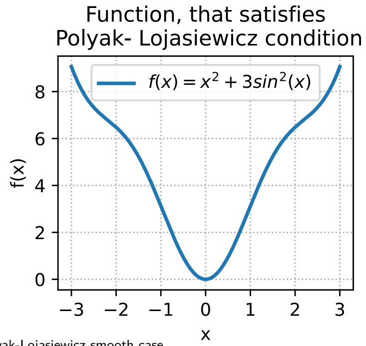
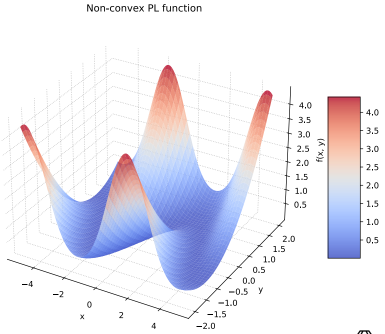
The following functions satisfy the PL condition but are not convex. Link to the code

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

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



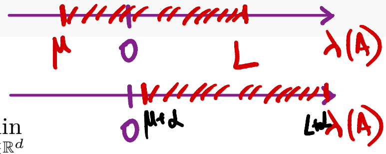
# Convergence analysis

пусть есть $f(x) = \frac{1}{2} x^T A x$

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

$\lambda_{max}(A) = L$

$g(x) = \frac{1}{2} x^T A x + \frac{\alpha}{2} \|x\|_2^2 = \frac{1}{2} x^T (A + \alpha \cdot I) x$




**Theorem**

Consider the Problem

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

and assume that $f$ is $\mu$-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:

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

сильно выпуклые функции

# Example: linear least squares

сходимость

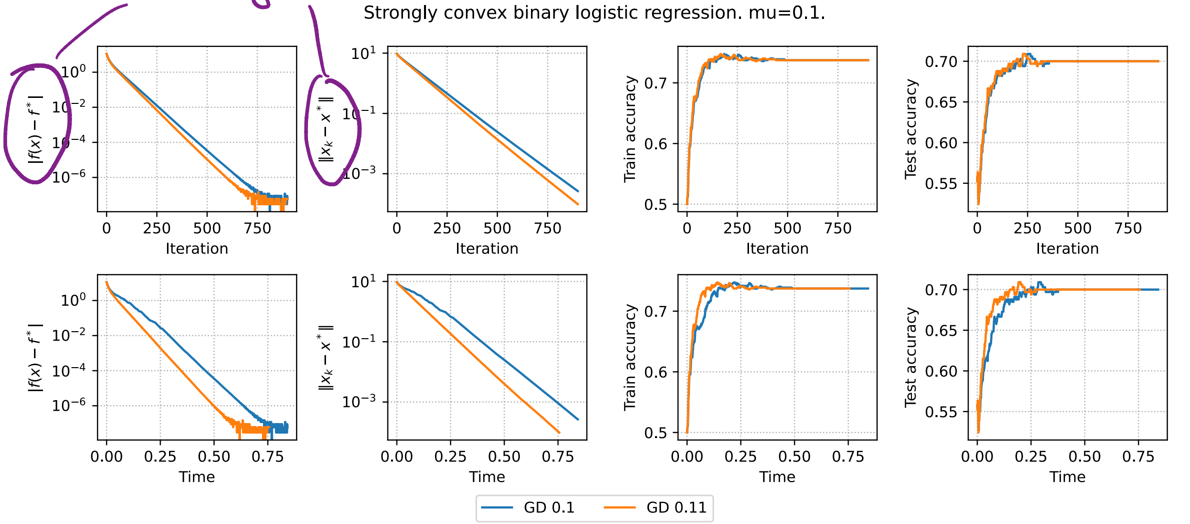
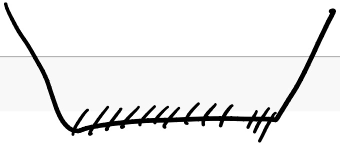



Figure 4: Convergence both in domain and in function value for regularized quadratics

# Smooth convex case

# Smooth convex case

НЕ сильно выпуклые



**Theorem**

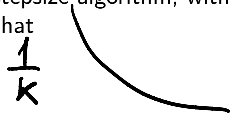
есть сходимость только по f(x)

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 $0 < \alpha \le \frac{1}{L}$. Then, for all $x^* \in \operatorname{argmin} f$, for all $k \in \mathbb{N}$ we have that

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




$$\rho^k \left(f(x^0) - f^*\right)$$

# Example: linear least squares

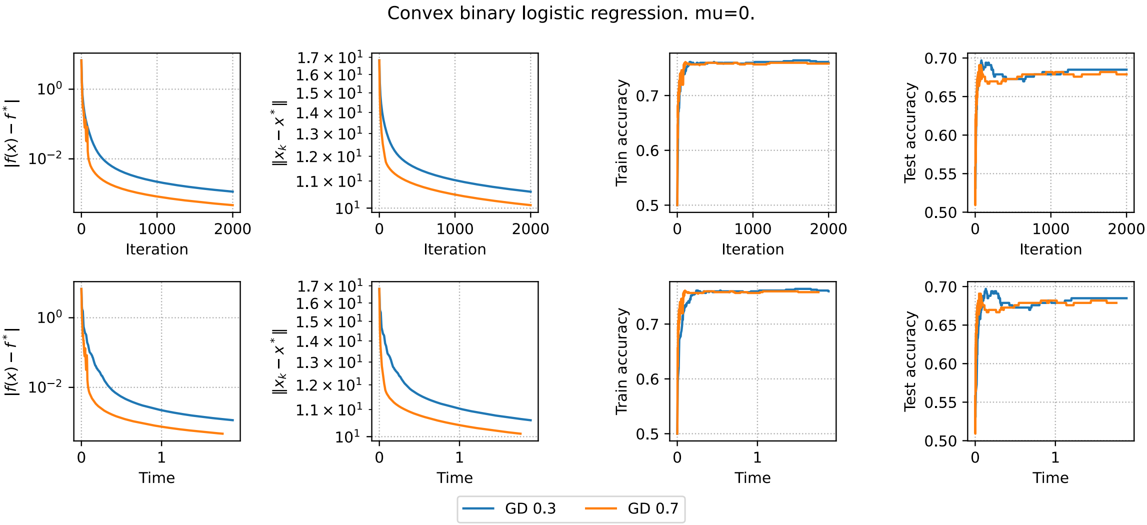



Figure 5: Convergence in function value for convex (but not strongly convex) quadratics

# Lower bounds

# 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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- The iteration of gradient descent:

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\begin{aligned}
x^{k+1} &= x^k - \alpha^k \nabla f(x^k) \\
&= x^{k-1} - \alpha^{k-1} \nabla f(x^{k-1}) - \alpha^k \nabla f(x^k) \\
&\vdots \\
&= x^0 - \sum_{i=0}^{k} \alpha^{k-i} \nabla f(x^{k-i})
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&\;\;\vdots \\
&= x^0 - \sum_{i=0}^{k} \alpha^{k-i} \nabla f(x^{k-i})
\end{aligned}
$$

- Consider a family of first-order methods, where

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

## Smooth convex case

GD: $\frac{1}{k}$ можно $\frac{1}{k^2}$

**Theorem**

There exists a function $f$ that is $L$-smooth and convex such that any method 2 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 $\mathcal{O}\left(\frac{1}{k^2}\right)$.

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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 $f$.

# Recap

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Gradient Descent: $\min\limits_{x \in \mathbb{R}^n} f(x)$ $\qquad x^{k+1} = x^k - \alpha^k \nabla f(x^k)$

Негладкий $\nabla f \nexists$

| convex (non-smooth) | smooth (non-convex) | smooth & convex | smooth & strongly convex (or PL) |
|---|---|---|---|
| $f(x^k) - f^* \sim \mathcal{O}\left(\dfrac{1}{\sqrt{k}}\right)$ | $\|\nabla f(x^k)\|^2 \sim \mathcal{O}\left(\dfrac{1}{k}\right)$ | $f(x^k) - f^* \sim \mathcal{O}\left(\dfrac{1}{k}\right)$ | $\|x^k - x^*\|^2 \sim \mathcal{O}\left(\left(1 - \dfrac{\mu}{L}\right)^k\right)$ |
| $k_\varepsilon \sim \mathcal{O}\left(\dfrac{1}{\varepsilon^2}\right)$ | $k_\varepsilon \sim \mathcal{O}\left(\dfrac{1}{\varepsilon}\right)$ | $k_\varepsilon \sim \mathcal{O}\left(\dfrac{1}{\varepsilon}\right)$ | $k_\varepsilon \sim \mathcal{O}\left(\kappa \log \dfrac{1}{\varepsilon}\right)$ |

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For smooth strongly convex we have:

$$
f(x^k) - f^* \leq \left(1 - \frac{\mu}{L}\right)^k (f(x^0) - f^*).
$$

Note also, that for any $x$

$$
1 - x \leq e^{-x}
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# Recap

Gradient Descent: $\min_{x \in \mathbb{R}^n} f(x)$ $\qquad x^{k+1} = x^k - \alpha^k \nabla f(x^k)$

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$$

Note also, that for any $x$

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1 - x \leq e^{-x}
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Finally we have

$$
\begin{aligned}
\varepsilon = f(x^{k_\varepsilon}) - f^* &\leq \left(1 - \frac{\mu}{L}\right)^{k_\varepsilon} (f(x^0) - f^*) \\
&\leq \exp\left(-k_\varepsilon \frac{\mu}{L}\right) (f(x^0) - f^*) \\
k_\varepsilon \geq \kappa \log \frac{f(x^0) - f^*}{\varepsilon} &= \mathcal{O}\left(\kappa \log \frac{1}{\varepsilon}\right)
\end{aligned}
$$

# Recap

Gradient Descent: $\min_{x \in \mathbb{R}^n} f(x)$ $\qquad x^{k+1} = x^k - \alpha^k \nabla f(x^k)$

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|---|---|---|---|
| $f(x^k) - f^* \sim \mathcal{O}\left(\frac{1}{\sqrt{k}}\right)$ | $\|\nabla f(x^k)\|^2 \sim \mathcal{O}\left(\frac{1}{k}\right)$ | $f(x^k) - f^* \sim \mathcal{O}\left(\frac{1}{k}\right)$ | $\|x^k - x^*\|^2 \sim \mathcal{O}\left(\left(1 - \frac{\mu}{L}\right)^k\right)$ |
| $k_\varepsilon \sim \mathcal{O}\left(\frac{1}{\varepsilon^2}\right)$ | $k_\varepsilon \sim \mathcal{O}\left(\frac{1}{\varepsilon}\right)$ | $k_\varepsilon \sim \mathcal{O}\left(\frac{1}{\varepsilon}\right)$ | $k_\varepsilon \sim \mathcal{O}\left(\kappa \log \frac{1}{\varepsilon}\right)$ |

For smooth strongly convex we have:

$$f(x^k) - f^* \leq \left(1 - \frac{\mu}{L}\right)^k (f(x^0) - f^*).$$

Note also, that for any $x$

$$1 - x \leq e^{-x}$$

Finally we have

$$\begin{aligned}
\varepsilon = f(x^{k_\varepsilon}) - f^* &\leq \left(1 - \frac{\mu}{L}\right)^{k_\varepsilon} (f(x^0) - f^*) \\
&\leq \exp\left(-k_\varepsilon \frac{\mu}{L}\right) (f(x^0) - f^*) \\
k_\varepsilon \geq \kappa \log \frac{f(x^0) - f^*}{\varepsilon} &= \mathcal{O}\left(\kappa \log \frac{1}{\varepsilon}\right)
\end{aligned}$$

**Question:** Can we do faster, than this using the first-order information?

# Recap

Gradient Descent: $\min_{x \in \mathbb{R}^n} f(x)$ $\quad x^{k+1} = x^k - \alpha^k \nabla f(x^k)$

| convex (non-smooth) | smooth (non-convex) | smooth & convex | smooth & strongly convex (or PL) |
|---|---|---|---|
| $f(x^k) - f^* \sim \mathcal{O}\left(\frac{1}{\sqrt{k}}\right)$ | $\|\nabla f(x^k)\|^2 \sim \mathcal{O}\left(\frac{1}{k}\right)$ | $f(x^k) - f^* \sim \mathcal{O}\left(\frac{1}{k}\right)$ | $\|x^k - x^*\|^2 \sim \mathcal{O}\left(\left(1 - \frac{\mu}{L}\right)^k\right)$ |
| $k_\varepsilon \sim \mathcal{O}\left(\frac{1}{\varepsilon^2}\right)$ | $k_\varepsilon \sim \mathcal{O}\left(\frac{1}{\varepsilon}\right)$ | $k_\varepsilon \sim \mathcal{O}\left(\frac{1}{\varepsilon}\right)$ | $k_\varepsilon \sim \mathcal{O}\left(\kappa \log \frac{1}{\varepsilon}\right)$ |

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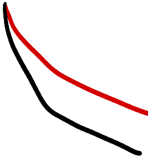
\end{aligned}
$$

**Question:** Can we do faster, than this using the first-order information? **Yes, we can.**

# Lower bounds

# Lower bounds

совпадает с базовым методом




| convex (non-smooth) | smooth (non-convex)[1] | smooth & convex[2] | smooth & strongly convex (or PL) |
|---|---|---|---|
| $\mathcal{O}\left(\dfrac{1}{\sqrt{k}}\right)$ | $\mathcal{O}\left(\dfrac{1}{k^2}\right)$ | $\mathcal{O}\left(\dfrac{1}{k^2}\right)$ | $\mathcal{O}\left(\left(1-\sqrt{\dfrac{\mu}{L}}\right)^k\right)$ |
| $k_\varepsilon \sim \mathcal{O}\left(\dfrac{1}{\varepsilon^2}\right)$ | $k_\varepsilon \sim \mathcal{O}\left(\dfrac{1}{\sqrt{\varepsilon}}\right)$ | $k_\varepsilon \sim \mathcal{O}\left(\dfrac{1}{\sqrt{\varepsilon}}\right)$ | $k_\varepsilon \sim \mathcal{O}\left(\sqrt{\kappa}\log\dfrac{1}{\varepsilon}\right)$ |

[1] Carmon, Duchi, Hinder, Sidford, 2017
[2] Nemirovski, Yudin, 1979

# Lower bounds

The iteration of gradient descent:

$$
\begin{aligned}
x^{k+1} &= x^k - \alpha^k \nabla f(x^k) \\
&= x^{k-1} - \alpha^{k-1} \nabla f(x^{k-1}) - \alpha^k \nabla f(x^k) \\
&\vdots \\
&= x^0 - \sum_{i=0}^{k} \alpha^{k-i} \nabla f(x^{k-i})
\end{aligned}
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\end{aligned}
$$

Consider a family of first-order methods, where

$$
x^{k+1} \in x^0 + \text{span}\left\{\nabla f(x^0), \nabla f(x^1), \ldots, \nabla f(x^k)\right\} \quad (2)
$$

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**Non-smooth convex case**

There exists a function $f$ that is $M$-Lipschitz and convex such that any first-order method of the form 2 satisfies

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

**Smooth and convex case**

There exists a function $f$ that is $L$-smooth and convex such that any first-order method of the form 2 satisfies

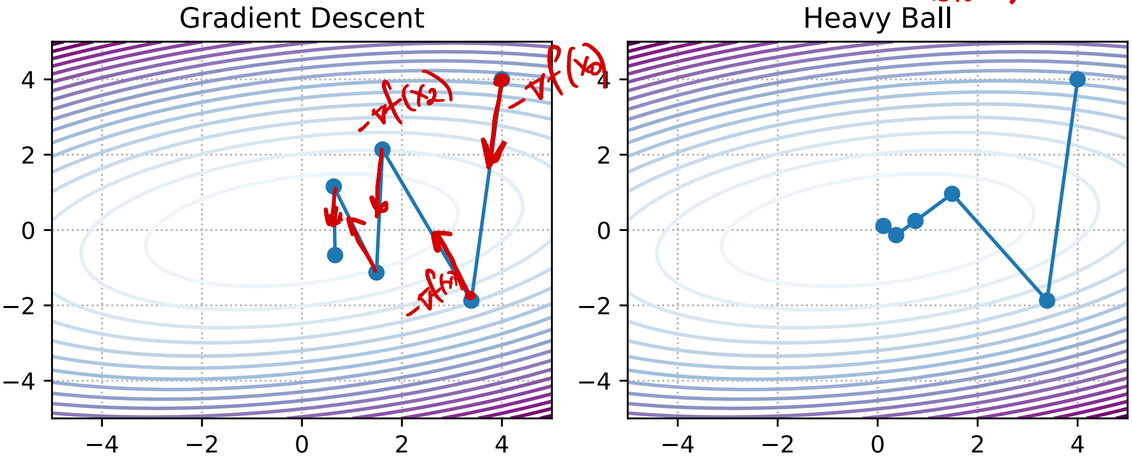
$$
\min_{i \in [1,k]} f(x^i) - f^* \geq \frac{3L\|x^0 - x^*\|_2^2}{32(1 + k)^2}
$$

# Strongly convex quadratic problem

# Oscillations and acceleration

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

momentum



$$x_{k+1} = x_k - \alpha \cdot \nabla f(x_k) + \beta(x_k - x_{k-1}) \ominus$$

$$x_k = x_{k-1} - \alpha \cdot \nabla f(x_{k-1}) + \beta(x_{k-1} - x_{k-2}) \Rightarrow x_k - x_{k-1} = -\alpha \nabla f(x_{k-1}) + \beta(x_{k-1} - x_{k-2})$$

$$0 < \beta < 1$$

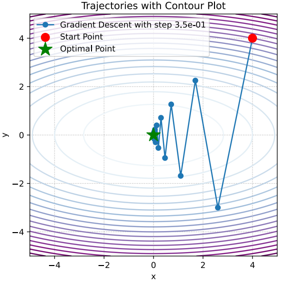
$$\beta^3 < \beta^2 < \beta < 1$$

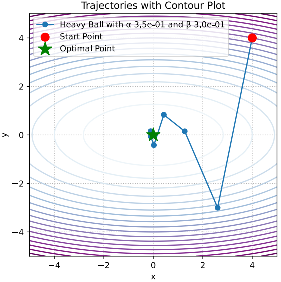
## Heavy ball

$$\ominus\ x_k - \alpha \cdot \nabla f(x_k) + \beta\left(-\alpha \nabla f(x_{k-1}) + \beta(x_{k-1} - x_{k-2})\right) =$$

$$= x_k - \alpha\left(\nabla f(x_k) + \beta \cdot \nabla f(x_{k-1}) + \beta^2 \cdot \nabla f(x_{k-2}) + \beta^3 \cdot \nabla f(x_{k-3}) + \ldots\right)$$

# Polyak Heavy ball method




Let's introduce the idea of momentum, proposed by Polyak in 1964. Recall that the momentum update is

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

optimal hyperparameters for strongly convex quadratics:

$$\alpha^*, \beta^* = \arg\min_{\alpha,\beta} \max_{\lambda \in [\mu, L]} \rho(M) \quad \alpha^* = \frac{4}{(\sqrt{L} + \sqrt{\mu})^2}; \quad \beta^* = \left(\frac{\sqrt{L} - \sqrt{\mu}}{\sqrt{L} + \sqrt{\mu}}\right)^2.$$

# Heavy Ball quadratics convergence

$\varkappa = 10^2 \quad \frac{\varkappa-1}{\varkappa+1} = \frac{99}{101} \approx 0.98$

$\sqrt{\varkappa} \approx 10^1 \quad \frac{\sqrt{\varkappa}-1}{\sqrt{\varkappa}+1} = \frac{10-1}{10+1} \approx 0.9$

**Theorem**

Assume that $f$ is quadratic $\mu$-strongly convex $L$-smooth quadratics, then Heavy Ball method with parameters

$$
\alpha = \frac{4}{(\sqrt{L}+\sqrt{\mu})^2}, \beta = \frac{\sqrt{L}-\sqrt{\mu}}{\sqrt{L}+\sqrt{\mu}}
$$

converges linearly:

$$
\|x_k - x^*\|_2 \leq \left( \frac{\sqrt{\kappa}-1}{\sqrt{\kappa}+1} \right)^k \|x_0 - x^*\|
$$

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

# Heavy Ball Global Convergence [3]

**Theorem**

Assume that $f$ is smooth and convex and that

$$\beta \in [0,1), \quad \alpha \in \left(0, \dfrac{2(1-\beta)}{L}\right).$$

Then, the sequence $\{x_k\}$ generated by Heavy-ball iteration satisfies

$$f(\overline{x}_T) - f^\star \leq \begin{cases} \frac{\|x_0 - x^\star\|^2}{2(T+1)}\left(\frac{L\beta}{1-\beta} + \frac{1-\beta}{\alpha}\right), & \text{if } \alpha \in \left(0, \dfrac{1-\beta}{L}\right], \\ \frac{\|x_0 - x^\star\|^2}{2(T+1)(2(1-\beta)-\alpha L)}\left(L\beta + \frac{(1-\beta)^2}{\alpha}\right), & \text{if } \alpha \in \left[\dfrac{1-\beta}{L}, \dfrac{2(1-\beta)}{L}\right), \end{cases}$$

where $\overline{x}_T$ is the Cesaro average of the iterates, i.e.,

$$\overline{x}_T = \frac{1}{T+1}\sum_{k=0}^{T} x_k.$$

[3] Global convergence of the Heavy-ball method for convex optimization, Euhanna Ghadimi et.al.

# Heavy Ball Global Convergence [4]

**Theorem**

Assume that $f$ is smooth and strongly convex and that

$$\alpha \in (0, \frac{2}{L}), \quad 0 \leq \beta < \frac{1}{2}\left( \frac{\mu\alpha}{2} + \sqrt{\frac{\mu^2\alpha^2}{4} + 4(1 - \frac{\alpha L}{2})} \right).$$

where $\alpha_0 \in (0, 1/L]$. Then, the sequence $\{x_k\}$ generated by Heavy-ball iteration converges linearly to a unique optimizer $x^\star$. In particular,

$$f(x_k) - f^\star \leq q^k (f(x_0) - f^\star),$$

where $q \in [0, 1)$.

[4] Global convergence of the Heavy-ball method for convex optimization, Euhanna Ghadimi et.al.

# Heavy ball method summary

- Ensures accelerated convergence for strongly convex quadratic problems

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# Heavy ball method summary

On the importance of momentum

- Ensures accelerated convergence for strongly convex quadratic problems
- Local accelerated convergence was proved in the original paper.
- Recently was proved, that there is no global accelerated convergence for the method.
- Method was not extremely popular until the ML boom
- Nowadays, it is de-facto standard for practical acceleration of gradient methods, even for the non-convex problems (neural network training)

# Nesterov accelerated gradient

# The concept of Nesterov Accelerated Gradient method

GD

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

2P

HB

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

3P

$$\begin{cases} y_{k+1} = x_k + \beta(x_k - x_{k-1}) \\ x_{k+1} = y_{k+1} - \alpha \nabla f(y_{k+1}) \end{cases}$$

# The concept of Nesterov Accelerated Gradient method

NAG: $x_{k+1} = x_k + \beta(x_k - x_{k-1}) - \alpha\nabla f(x_k + \beta(x_k - x_{k-1}))$

GD

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

HB

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

$$\begin{cases} y_{k+1} = x_k + \beta(x_k - x_{k-1}) \\ x_{k+1} = y_{k+1} - \alpha \nabla f(y_{k+1}) \end{cases}$$

nesterov = true

Let's define the following notation

$$x^+ = x - \alpha \nabla f(x) \qquad \text{Gradient step}$$

$$d_k = \beta_k (x_k - x_{k-1}) \qquad \text{Momentum term}$$

Then we can write down:

$$x_{k+1} = x_k^+ \qquad \text{Gradient Descent}$$

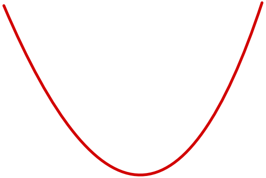
$$x_{k+1} = x_k^+ + d_k \qquad \text{Heavy Ball}$$

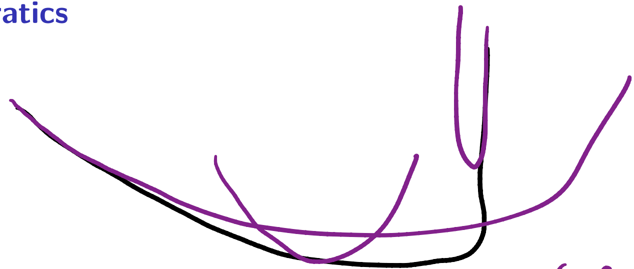
$$x_{k+1} = (x_k + d_k)^+ \qquad \text{Nesterov accelerated gradient}$$

сначала град. шаг, потом мом.

сначала momentum, потом град. шаг

# NAG convergence for quadratics





$$\mu = \min_{x \in \mathbb{R}^n} \lambda_{min}(\nabla^2 f(x))$$

$$L = \max_{x \in \mathbb{R}^n} \lambda_{max}(\nabla^2 f(x))$$

# General case convergence

**Theorem**

Let $f : \mathbb{R}^n \to \mathbb{R}$ is convex and $L$-smooth. The Nesterov Accelerated Gradient Descent (NAG) algorithm is designed to solve the minimization problem starting with an initial point $x_0 = y_0 \in \mathbb{R}^n$ and $\lambda_0 = 0$. The algorithm iterates the following steps:

$$
\begin{aligned}
&\textbf{Gradient update:} && y_{k+1} = x_k - \frac{1}{L}\nabla f(x_k) \\
&\textbf{Extrapolation:} && x_{k+1} = (1-\gamma_k)y_{k+1} + \gamma_k y_k \\
&\textbf{Extrapolation weight:} && \lambda_{k+1} = \frac{1+\sqrt{1+4\lambda_k^2}}{2} \\
&\textbf{Extrapolation weight:} && \gamma_k = \frac{1-\lambda_k}{\lambda_{k+1}}
\end{aligned}
$$

The sequences $\{f(y_k)\}_{k\in\mathbb{N}}$ produced by the algorithm will converge to the optimal value $f^*$ at the rate of $\mathcal{O}\left(\frac{1}{k^2}\right)$, specifically:

$$
f(y_k) - f^* \leq \frac{2L\|x_0 - x^*\|^2}{k^2}
$$

# General case convergence

**Theorem**

Let $f : \mathbb{R}^n \to \mathbb{R}$ is $\mu$-strongly convex and $L$-smooth. The Nesterov Accelerated Gradient Descent (NAG) algorithm is designed to solve the minimization problem starting with an initial point $x_0 = y_0 \in \mathbb{R}^n$ and $\lambda_0 = 0$. The algorithm iterates the following steps:

**Gradient update:** $$y_{k+1} = x_k - \frac{1}{L}\nabla f(x_k)$$

**Extrapolation:** $$x_{k+1} = (1 - \gamma_k)y_{k+1} + \gamma_k y_k$$

**Extrapolation weight:** $$\gamma_k = \frac{\sqrt{L} - \sqrt{\mu}}{\sqrt{L} + \sqrt{\mu}}$$

The sequences $\{f(y_k)\}_{k \in \mathbb{N}}$ produced by the algorithm will converge to the optimal value $f^*$ linearly:

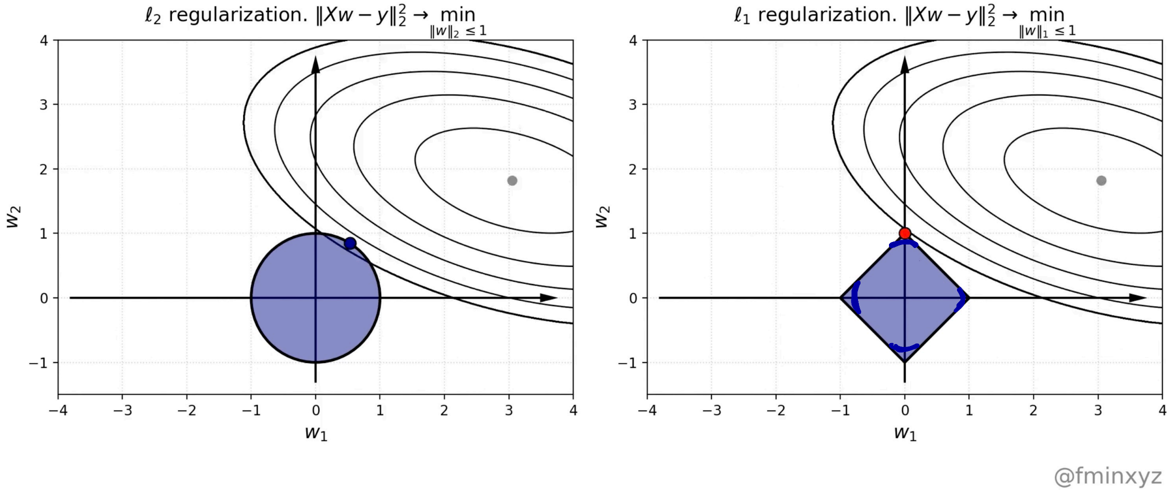
$$f(y_k) - f^* \leq \frac{\mu + L}{2}\|x_0 - x^*\|_2^2 \exp\left(-\frac{k}{\sqrt{\kappa}}\right)$$

# Non-smooth problems

# $\ell_1$-regularized linear least squares

$\ell_1 + \ell_2$

$\ell_1$ induces sparsity



# Norms are not smooth

$$\min_{x \in \mathbb{R}^n} f(x),$$

A classical convex optimization problem is considered. We assume that $f(x)$ is a convex function, but now we do not require smoothness.

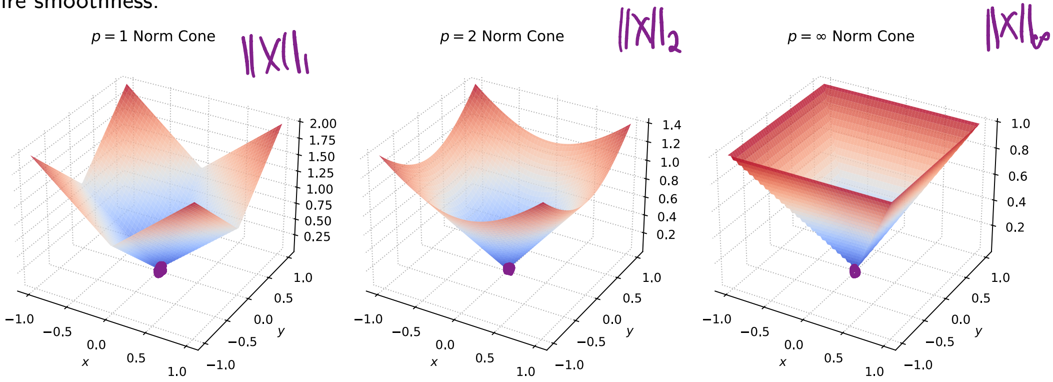



Figure 6: Norm cones for different $p$ - norms are non-smooth

# Wolfe's example

$\|x\|_2 \leq 1$

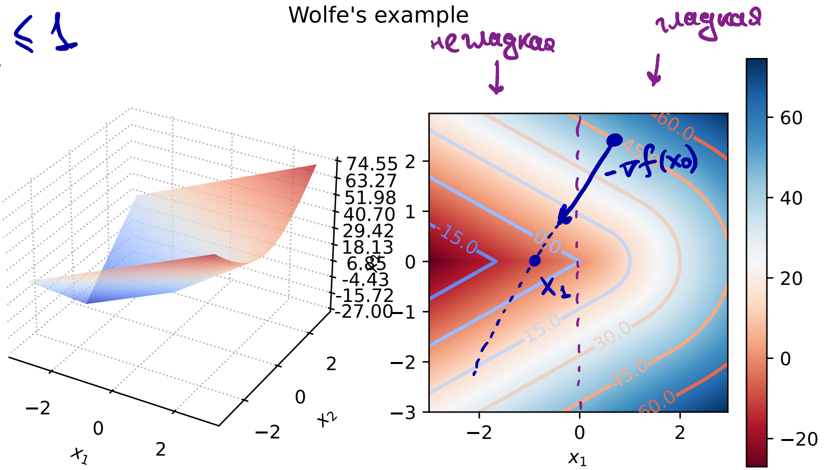



Figure 7: Wolfe's example. Open in Colab

Субградиентный метод

$$x_{k+1} = x_k - \alpha_k g_k$$

$g_k$ — субградиент

## Subgradient calculus

для выпуклых негладких функций

# Convex function linear lower bound

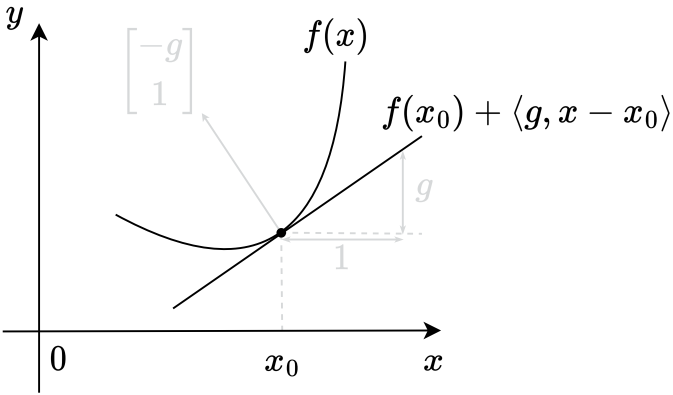
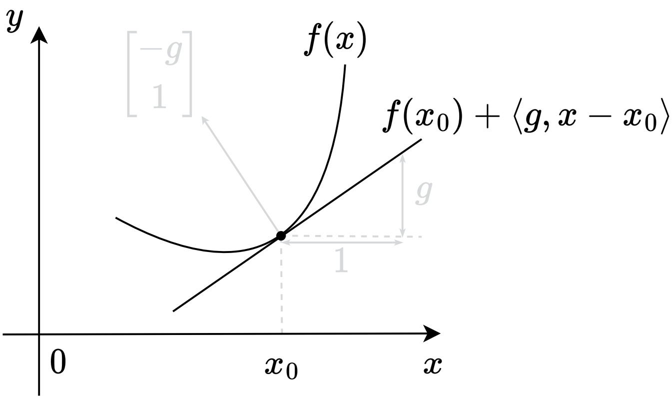



Figure 8: Taylor linear approximation serves as a global lower bound for a convex function

An important property of a continuous convex function $f(x)$ is that at any chosen point $x_0$ for all $x \in \text{dom } f$ the inequality holds:

$$f(x) \geq f(x_0) + \langle g, x - x_0 \rangle$$

# Convex function linear lower bound

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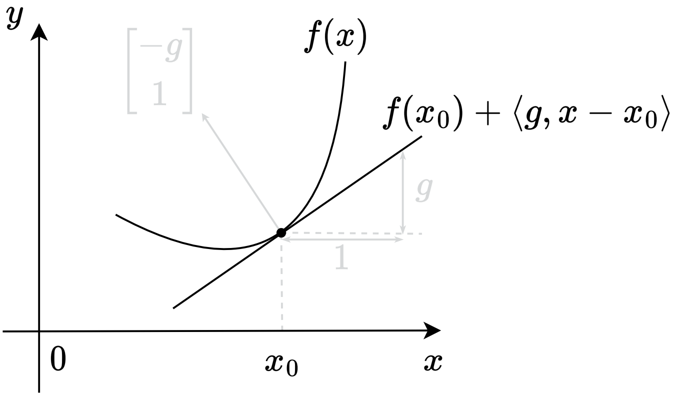
for some vector $g$, i.e., the tangent to the graph of the function is the *global* estimate from below for the function.

- If $f(x)$ is differentiable, then $g = \nabla f(x_0)$

# Convex function linear lower bound

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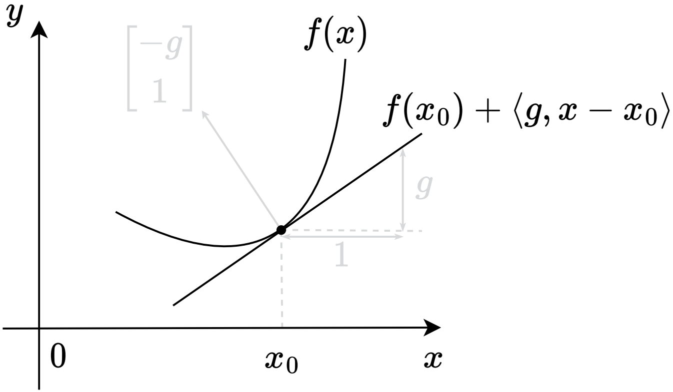


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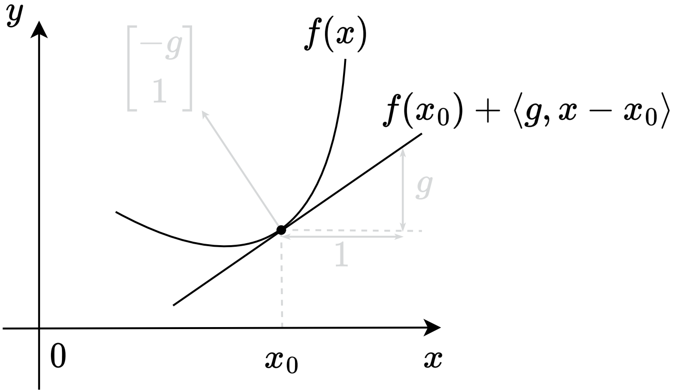


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- If $f(x)$ is differentiable, then $g = \nabla f(x_0)$
- Not all continuous convex functions are differentiable.

We wouldn't want to lose such a nice property.

## Subgradient and subdifferential

A vector $g$ is called the **subgradient** of a function $f(x) : S \to \mathbb{R}$ at a point $x_0$ if $\forall x \in S$:

$$f(x) \geq f(x_0) + \langle g, x - x_0 \rangle$$

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The set of all subgradients of a function $f(x)$ at a point $x_0$ is called the **subdifferential** of $f$ at $x_0$ and is denoted by $\partial f(x_0)$.

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The set of all subgradients of a function $f(x)$ at a point $x_0$ is called the **subdifferential** of $f$ at $x_0$ and is denoted by $\partial f(x_0)$.

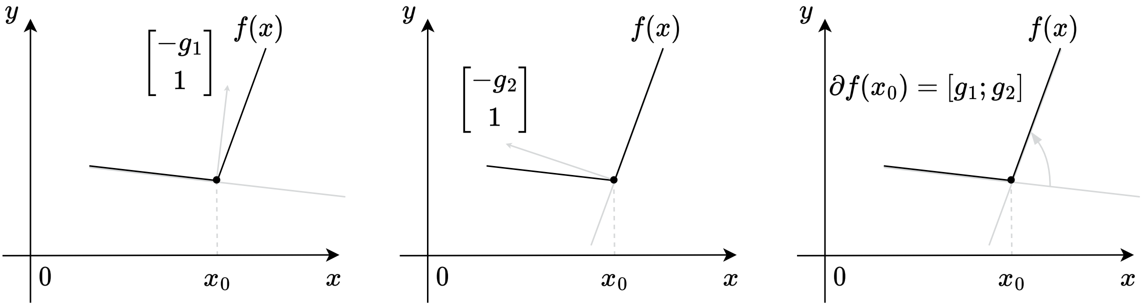


Figure 9: Subdifferential is a set of all possible subgradients

# Subgradient and subdifferential

Find $\partial f(x)$, if $f(x) = |x|$

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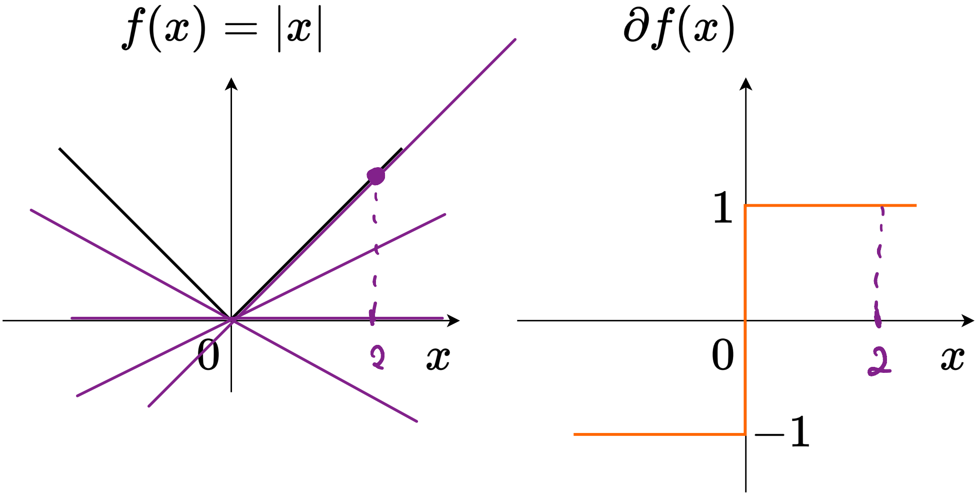
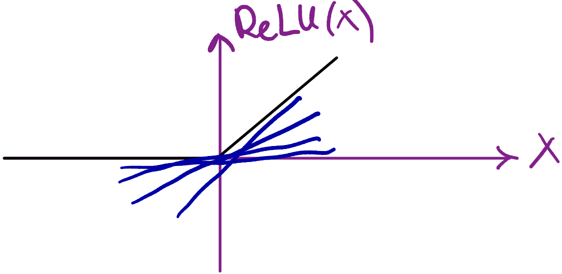


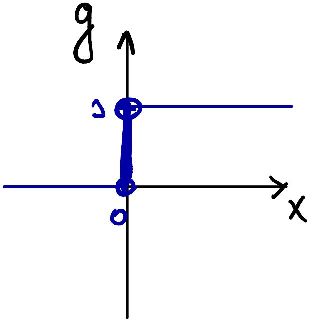
# Subgradient Method

# Algorithm

A vector $g$ is called the **subgradient** of the function $f(x) : S \to \mathbb{R}$ at the point $x_0$ if $\forall x \in S$:

$$f(x) \geq f(x_0) + \langle g, x - x_0 \rangle$$



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The idea is very simple: let's replace the gradient $\nabla f(x_k)$ in the gradient descent algorithm with a subgradient $g_k$ at point $x_k$:

$$x_{k+1} = x_k - \alpha_k g_k,$$

where $g_k$ is an arbitrary subgradient of the function $f(x)$ at the point $x_k$, $g_k \in \partial f(x_k)$

# Convergence results

GD: $\frac{1}{K}$ AGD: $\frac{1}{K^2}$

**Theorem**

Let $f$ be a convex $G$-Lipschitz function. For a fixed step size $\alpha = \frac{\|x_0 - x^*\|_2}{G}\sqrt{\frac{1}{K}}$, subgradient method satisfies

$\frac{1}{\sqrt{K}}$

$$
f(\overline{x}) - f^* \leq \frac{G\|x_0 - x^*\|_2}{\sqrt{K}} \qquad \overline{x} = \frac{1}{K}\sum_{k=0}^{K-1} x_i
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- $\mathcal{O}\left(\frac{1}{\sqrt{T}}\right)$ is slow, but already hits the lower bound ($\mathcal{O}\left(\frac{1}{T}\right)$ in the strongly convex case).

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- Proved result requires pre-defined step size strategy, which is not practical (usually one cas just use several diminishes strategies).
- There is no monotonic decrease of objective.
- Convergence is slower, than for the gradient descent (smooth case). However, if we will go deeply for the problem structure, we can improve convergence (proximal gradient method).

# Convergence results

если запускать субградиентный метод с $\alpha = const$, он не будет сходится

G - константа Липшица $f(x)$

**Theorem**

Let $f$ be a convex $G$-Lipschitz function and $f_k^{\text{best}} = \min\limits_{i=1,\ldots,k} f(x^i)$. For a fixed step size $\alpha$, subgradient method satisfies

$$\lim_{k\to\infty} f_k^{\text{best}} \leq f^* + \frac{G^2\alpha}{2}$$

**Theorem**

Let $f$ be a convex $G$-Lipschitz function and $f_k^{\text{best}} = \min\limits_{i=1,\ldots,k} f(x^i)$. For a diminishing step size $\alpha_k$ (square summable but not summable. Important here that step sizes go to zero, but not too fast), subgradient method satisfies

$$\lim_{k\to\infty} f_k^{\text{best}} \leq f^*$$

## Applications

стратегии выбора шага субград. метода

1. если $\alpha = const$, то НЕТ сходимости $f_k^{best} - f^* \leq \frac{R^2}{2k\alpha} + G^2\alpha$

2. уменьшающийся $\alpha$ $\quad \alpha = \frac{R}{G\sqrt{k}} \sim \frac{A}{\sqrt{k}}$; $\alpha \sim \frac{A}{k}$

$R$ — $\|x^0 - x^*\|$

3. Шаг Поляка: $\alpha_k = \frac{f(x^k) - f^*}{\|g_k\|^2}$

$f^*$ неизв, но можно оценить

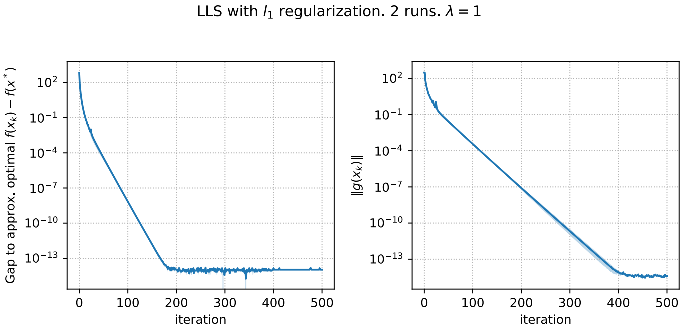
# Linear Least Squares with $l_1$-regularization

$$\min_{x \in \mathbb{R}^n} \frac{1}{2}\|Ax - b\|_2^2 + \lambda \|x\|_1$$

Algorithm will be written as:

$$x_{k+1} = x_k - \alpha_k \left( A^\top (Ax_k - b) + \lambda \text{sign}(x_k) \right)$$

where signum function is taken element-wise.



# Regularized logistic regression

Given $(x_i, y_i) \in \mathbb{R}^p \times \{0,1\}$ for $i = 1, \ldots, n$, the logistic regression function is defined as:

$$f(\theta) = \sum_{i=1}^{n} \left( -y_i x_i^T \theta + \log(1 + \exp(x_i^T \theta)) \right)$$

This is a smooth and convex function with its gradient given by:

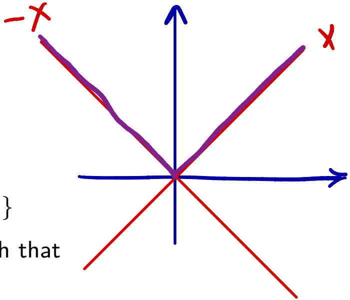
$$\nabla f(\theta) = \sum_{i=1}^{n} (y_i - s_i(\theta))\, x_i$$

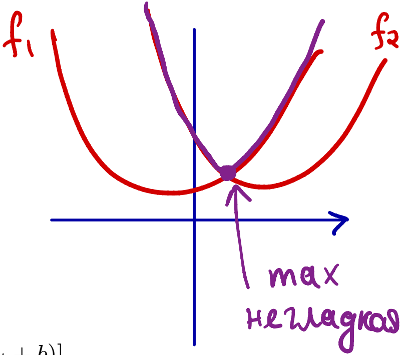
where $s_i(\theta) = \frac{\exp(x_i^T \theta)}{1+\exp(x_i^T \theta)}$, for $i = 1, \ldots, n$. Consider the regularized problem:

$$f(\theta) + \lambda r(\theta) \to \min_{\theta}$$

where $r(\theta) = \|\theta\|_2^2$ for the ridge penalty, or $r(\theta) = \|\theta\|_1$ for the lasso penalty.

# Support Vector Machines




Let $D = \{(x_i, y_i) \mid x_i \in \mathbb{R}^n, y_i \in \{\pm 1\}\}$

We need to find $\theta \in \mathbb{R}^n$ and $b \in \mathbb{R}$ such that

$$\min_{\theta \in \mathbb{R}^n, b \in \mathbb{R}} \frac{1}{2}\|\theta\|_2^2 + C\sum_{i=1}^{m} \text{max}[0, 1 - y_i(\theta^\top x_i + b)]$$

$$|X| = \max(-X; X)$$

# Subgradient method

Subgradient Method: $\min_{x \in \mathbb{R}^n} f(x)$ $x_{k+1} = x_k - \alpha_k g_k, \quad g_k \in \partial f(x_k)$

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Assume that $f$ is $G$-Lipschitz and convex, then Subgradient method converges as:

$$f(\overline{x}) - f^* \leq \frac{GR}{\sqrt{k}},$$

where

- $\alpha = \frac{R}{G\sqrt{k}}$

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# Non-smooth convex optimization lower bounds

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- However, we can achieve standard gradient descent rate $\mathcal{O}\left(\frac{1}{k}\right)$ (and even accelerated version $\mathcal{O}\left(\frac{1}{k^2}\right)$) if we will exploit the structure of the problem.

# Proximal operator

# Proximal mapping intuition

Consider Gradient Flow ODE:

$$\frac{dx}{dt} = -\nabla f(x)$$

Explicit Euler discretization:

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Leads to ordinary Gradient Descent method

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**! Proximal operator**

$$\text{prox}_{\alpha f}(x_k) = \text{arg}\min_{x \in \mathbb{R}^n} \left[f(x) + \frac{1}{2\alpha}\|x - x_k\|_2^2\right] = \text{argmin}_{x \in \mathbb{R}^n} \left[\alpha f(x) + \frac{1}{2}\|x - x_k\|^2\right]$$

# Proximal operator visualization

$$\text{Prox}_f(x) = \underset{x'}{\text{argmin}} \, \frac{1}{2}\|x - x'\|^2 + f(x')$$

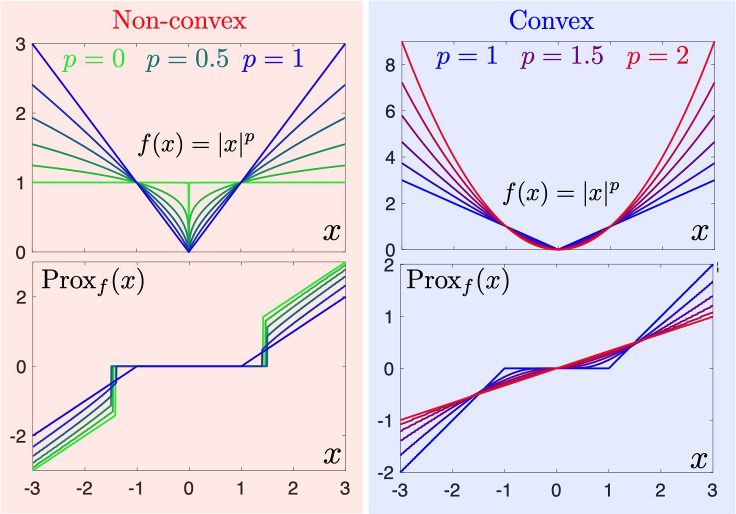


Figure 12: Source

# Proximal mapping intuition

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(I + \alpha \nabla f)(x_{k+1}) &= x_k
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  Thus, we have a usual gradient descent with $\alpha \to 0$: $x_{k+1} = x_k - \alpha \nabla f(x_k)$

- **Newton from proximal method.** Now let's consider proximal mapping of a second order Taylor approximation of the function $f^{II}_{x_k}(x)$:

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$$
x_{k+1} = \text{prox}_{f^{II}_{x_k}, \alpha}(x_k) = \text{arg}\min_{x \in \mathbb{R}^n} \left[ f(x_k) + \langle \nabla f(x_k), x - x_k \rangle + \frac{1}{2} \langle \nabla^2 f(x_k)(x - x_k), x - x_k \rangle + \frac{1}{2\alpha} \|x - x_k\|_2^2 \right]
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x_{k+1} = \text{prox}_{f^{II}_{x_k}, \alpha}(x_k) = \arg\min_{x \in \mathbb{R}^n} \left[ f(x_k) + \langle \nabla f(x_k), x - x_k \rangle + \frac{1}{2} \langle \nabla^2 f(x_k)(x - x_k), x - x_k \rangle + \frac{1}{2\alpha} \|x - x_k\|_2^2 \right]
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$$
\nabla f(x_k) + \nabla^2 f(x_k)(x - x_k) + \frac{1}{\alpha}(x - x_k) \Big|_{x = x_{k+1}} = 0
$$

# Proximal mapping intuition

- **GD from proximal method.** Back to the discretization:

$$
\begin{aligned}
x_{k+1} + \alpha \nabla f(x_{k+1}) &= x_k \\
(I + \alpha \nabla f)(x_{k+1}) &= x_k \\
x_{k+1} = (I + \alpha \nabla f)^{-1} x_k &\stackrel{\alpha \to 0}{\approx} (I - \alpha \nabla f) x_k
\end{aligned}
$$

  Thus, we have a usual gradient descent with $\alpha \to 0$: $x_{k+1} = x_k - \alpha \nabla f(x_k)$

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$$

$$
x_{k+1} = x_k - \left[ \nabla^2 f(x_k) + \frac{1}{\alpha} I \right]^{-1} \nabla f(x_k)
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Let $\mathbb{I}_S$ be the indicator function for closed, convex $S$. Recall orthogonal projection $\pi_S(y)$

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Proximity: Replace $\mathbb{I}_S$ by some convex function!

$$\text{prox}_r(y) = \text{prox}_{r,1}(y) := \arg\min \frac{1}{2}\|x - y\|^2 + r(x)$$

# Composite optimization

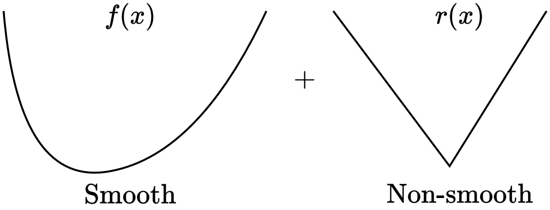
# Regularized / Composite Objectives

Many nonsmooth problems take the form

$$\min_{x \in \mathbb{R}^n} \varphi(x) = f(x) + r(x)$$

- **Lasso, L1-LS, compressed sensing**

$$f(x) = \frac{1}{2}\|Ax - b\|_2^2, r(x) = \lambda\|x\|_1$$



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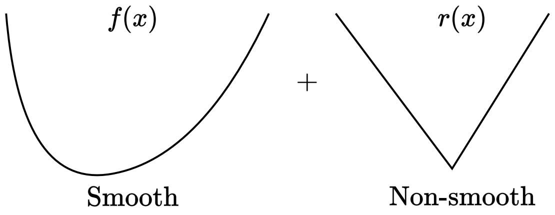
$$f(x) = \frac{1}{2}\|Ax - b\|_2^2, r(x) = \lambda\|x\|_1$$

- **L1-Logistic regression, sparse LR**

$$f(x) = -y \log h(x) - (1-y) \log(1-h(x)), r(x) = \lambda\|x\|_1$$



# Proximal mapping intuition

Optimality conditions:

$$0 \in \nabla f(x^*) + \partial r(x^*)$$

$$\min_{x \in \mathbb{R}^n} \varphi(x)$$

$$\varphi(x) = f(x) + r(x)$$

# Proximal mapping intuition

Optimality conditions:

$$0 \in \nabla f(x^*) + \partial r(x^*)$$
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0 &\in \nabla f(x^*) + \partial r(x^*) \\
0 &\in \alpha \nabla f(x^*) + \alpha \partial r(x^*) \\
x^* &\in \alpha \nabla f(x^*) + (I + \alpha \partial r)(x^*)
\end{aligned}
$$

$+x^*$

# Proximal mapping intuition

Optimality conditions:

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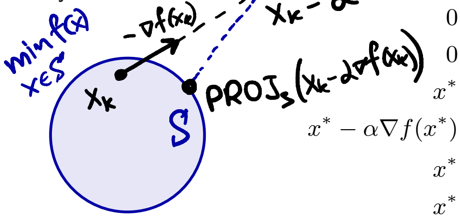


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$$

$\min_{x \in \mathbb{R}^n} [f(x) + r(x)]$

Which leads to the proximal gradient method:

$$
x_{k+1} = \text{prox}_{r,\alpha}(x_k - \alpha \nabla f(x_k))
$$

градиентный

проксимальный градиентный метод

And this method converges at a rate of $\mathcal{O}(\frac{1}{k})$!

$$
x_{k+1} = \text{PROJ}_S(x_k - \alpha \nabla f(x_k))
$$

# Proximal mapping intuition

Optimality conditions:

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And this method converges at a rate of $\mathcal{O}(\frac{1}{k})$!

**Another form of proximal operator**

$$
\text{prox}_{f,\alpha}(x_k) = \text{prox}_{\alpha f}(x_k) = \text{arg}\min_{x \in \mathbb{R}^n} \left[ \alpha f(x) + \frac{1}{2} \|x - x_k\|_2^2 \right] \qquad \text{prox}_f(x_k) = \text{arg}\min_{x \in \mathbb{R}^n} \left[ f(x) + \frac{1}{2} \|x - x_k\|_2^2 \right]
$$

# Proximal operators examples

Типичный пример: $\ell_1$ - рег.

$$\min_{x \in \mathbb{R}^n} f(x) + \underbrace{\lambda \|x\|_1}_{r(x)}$$

by def: $\text{PROX}_{r(x)}(x_k) = \arg\min_{x \in \mathbb{R}^n} \left[ r(x) + \frac{1}{2}\|x - x_k\|_2^2 \right]$

- $r(x) = \lambda \|x\|_1$, $\lambda > 0$

$$[\text{prox}_r(x)]_i = [|x_i| - \lambda]_+ \cdot \text{sign}(x_i),$$

which is also known as soft-thresholding operator.

$$\text{PROX}_{\lambda\|x\|_1}(x_k) = \arg\min_{x \in \mathbb{R}^n} \left[ \lambda \|x\|_1 + \frac{1}{2}\|x_k - x\|_2^2 \right] =$$

$$\arg\min_{x \in \mathbb{R}^n} \lambda \left( \sum_{i=1}^n |x_i| \right) + \frac{1}{2} \sum_{i=1}^n (x_{k_i} - x_i)^2 =$$

$$\arg\min_{x \in \mathbb{R}^n} \sum_{i=1}^n \left[ \lambda |x_i| + \frac{1}{2}(x_{k_i} - x_i)^2 \right] \Rightarrow$$

# Proximal operators examples

пусть $x_i < 0$, $|x_i| = -x_i$

$$-\lambda x_i + \frac{1}{2}(x_{k_i} - x_i)^2 \to \min_{x_i}$$

$$-\lambda - (x_{k_i} - x_i) = 0 \longrightarrow x_i = x_{k_i} + \lambda$$

$$x_{k_i} < -\lambda$$

пусть $x_i = 0$, тогда $x_i = 0$

- $r(x) = \lambda\|x\|_1$, $\lambda > 0$

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$$\lambda|x_i| + \frac{1}{2}(x_{k_i} - x_i)^2 \to \min_{x_i}$$

пусть $x_i > 0$ $|x_i| = x_i$

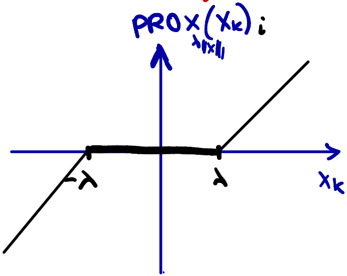
$$\lambda x_i + \frac{1}{2}(x_{k_i} - x_i)^2 \to \min_{x_i}$$

$$\lambda + \frac{1}{2}\cdot 2(x_{k_i} - x_i)\cdot(-1) = 0$$

$$x_{k_i} - x_i = \lambda$$

$$\boxed{x_i = x_{k_i} - \lambda}$$

$$\lambda < x_{k_i}$$



# Proximal operators examples

- $r(x) = \lambda\|x\|_1,\ \lambda > 0$
$$[\text{prox}_r(x)]_i = [|x_i| - \lambda]_+ \cdot \text{sign}(x_i),$$
which is also known as soft-thresholding operator.
- $r(x) = \frac{\lambda}{2}\|x\|_2^2,\ \lambda > 0$
$$\text{prox}_r(x) = \frac{x}{1+\lambda}.$$

# Proximal operators examples

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- $r(x) = \mathbb{I}_S(x)$.
$$\text{prox}_r(x_k - \alpha\nabla f(x_k)) = \text{proj}_r(x_k - \alpha\nabla f(x_k))$$

# Proximal Gradient Method. Convex case

# Convergence

**Theorem**

Consider the proximal gradient method

$$x_{k+1} = \text{prox}_{\alpha r}\left(x_k - \alpha \nabla f(x_k)\right)$$

For the criterion $\varphi(x) = f(x) + r(x)$, we assume:

- $f$ is convex, differentiable, $\text{dom}(f) = \mathbb{R}^n$, and $\nabla f$ is Lipschitz continuous with constant $L > 0$.
- $r$ is convex, and $\text{prox}_{\alpha r}(x_k) = \text{arg}\min\limits_{x \in \mathbb{R}^n} \left[\alpha r(x) + \frac{1}{2}\|x - x_k\|_2^2\right]$ can be evaluated.

Proximal gradient descent with fixed step size $\alpha = 1/L$ satisfies

$$\varphi(x_k) - \varphi^* \leq \frac{L\|x_0 - x^*\|^2}{2k},$$

Proximal gradient descent has a convergence rate of $O(1/k)$ or $O(1/\varepsilon)$. This matches the gradient descent rate! (But remember the proximal operation cost)

# Proximal Gradient Method. Strongly convex case

# Convergence

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For the criterion $\varphi(x) = f(x) + r(x)$, we assume:

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Proximal gradient descent with fixed step size $\alpha \leq 1/L$ satisfies

$$\|x_{k+1} - x^*\|_2^2 \leq (1 - \alpha\mu)^k \, \|x_0 - x^*\|_2^2$$

This is exactly gradient descent convergence rate. Note, that the original problem is even non-smooth!

# Accelerated Proximal Method

**Accelerated Proximal Method**

Let $x_0 = y_0 \in \text{dom}(r)$. For $k \geq 1$:

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x_k &= \text{prox}_{\alpha_k h}(y_{k-1} - \alpha_k \nabla f(y_{k-1})) \\
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- Uses extra "memory" for interpolation
- Same computational cost as ordinary prox-grad
- Convergence rate theoretically optimal

# Example: ISTA

## Iterative Shrinkage-Thresholding Algorithm (ISTA)

ISTA is a popular method for solving optimization problems involving L1 regularization, such as Lasso. It combines gradient descent with a shrinkage operator to handle the non-smooth L1 penalty effectively.

- **Algorithm**:

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where $\text{prox}_{\lambda\alpha\|\cdot\|_1}(v)$ applies soft thresholding to each component of $v$.

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- **Application**:
  - Efficient for sparse signal recovery, image processing, and compressed sensing.

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FISTA improves upon ISTA's convergence rate by incorporating a momentum term, inspired by Nesterov's accelerated gradient method.

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$$
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t_k &= \frac{1 + \sqrt{1 + 4t_{k-1}^2}}{2}, \\
y_k &= x_k + \frac{t_{k-1} - 1}{t_k}(x_k - x_{k-1}).
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- **Convergence**:
  - Improves the convergence rate to $O(1/k^2)$.

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FISTA improves upon ISTA's convergence rate by incorporating a momentum term, inspired by Nesterov's accelerated gradient method.

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  - Improves the convergence rate to $O(1/k^2)$.
- **Application**:
  - Especially useful for large-scale problems in machine learning and signal processing where the L1 penalty induces sparsity.

# Example: Matrix Completion

## Solving the Matrix Completion Problem

Matrix completion problems seek to fill in the missing entries of a partially observed matrix under certain assumptions, typically low-rank. This can be formulated as a minimization problem involving the nuclear norm (sum of singular values), which promotes low-rank solutions.

- **Problem Formulation**:

$$\min_X \frac{1}{2}\|P_\Omega(X) - P_\Omega(M)\|_F^2 + \lambda\|X\|_*,$$

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  - Widely used in recommender systems, image recovery, and other domains where data is naturally matrix-formed but partially observed.

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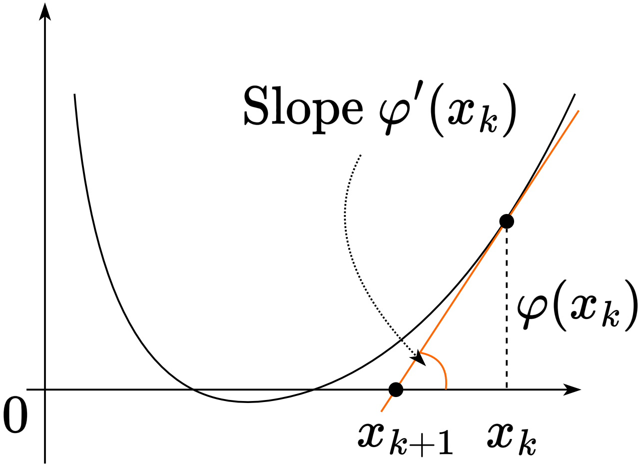
- Further reading: Proximal operator splitting, Douglas-Rachford splitting, Best approximation problem, Three operator splitting.

# Newton method

# Idea of Newton method of root finding

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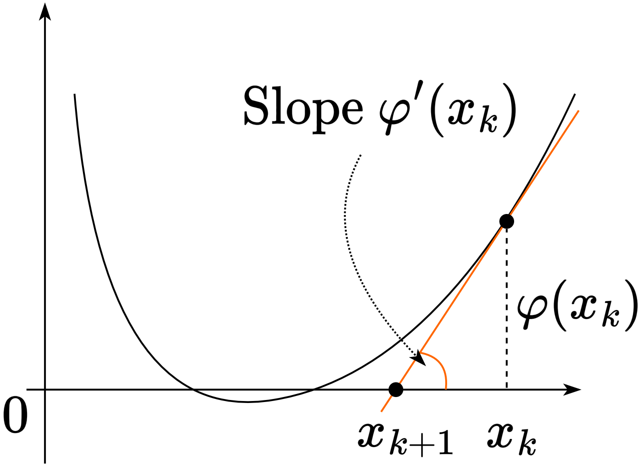


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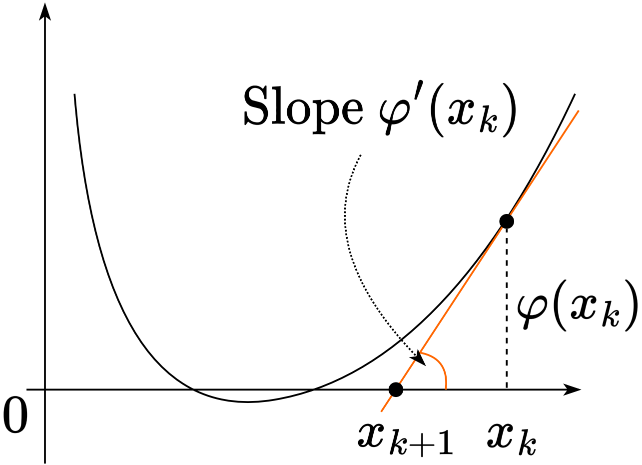


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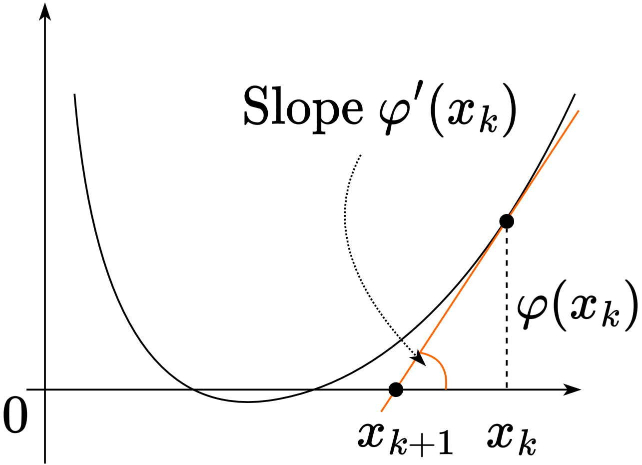


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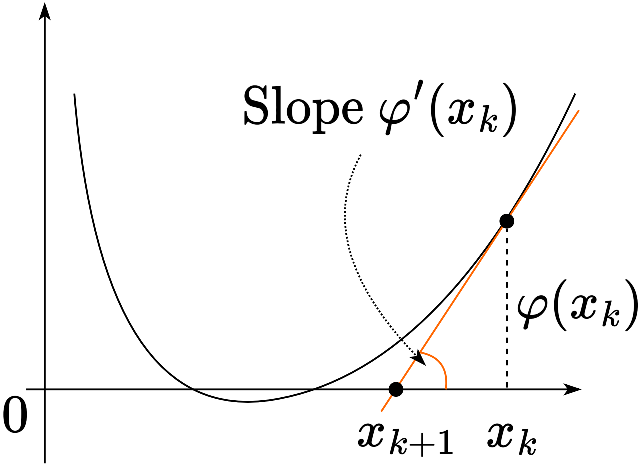


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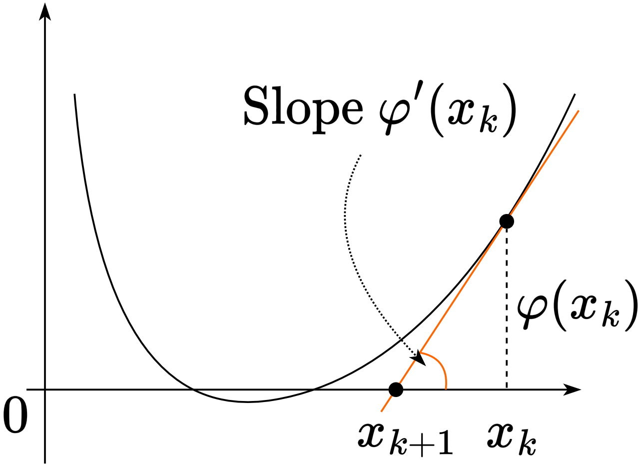


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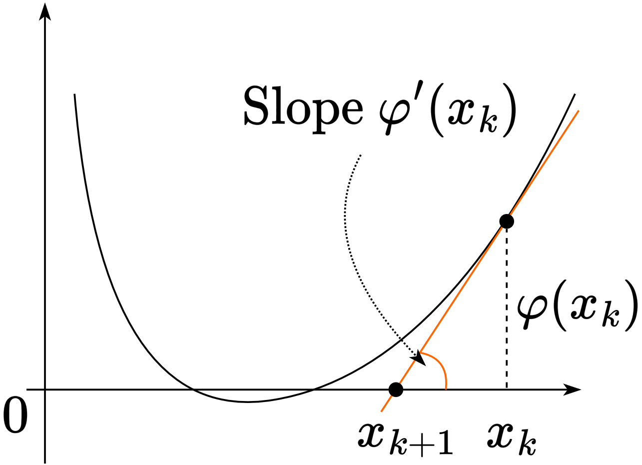


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[a] Literally we aim to solve the problem of finding stationary points $\nabla f(x) = 0$

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Let us immediately note the limitations related to the necessity of the Hessian's non-degeneracy (for the method to exist), as well as its positive definiteness (for the convergence guarantee).

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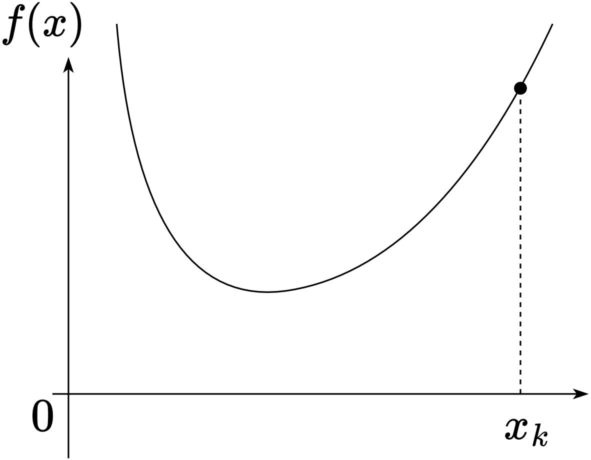

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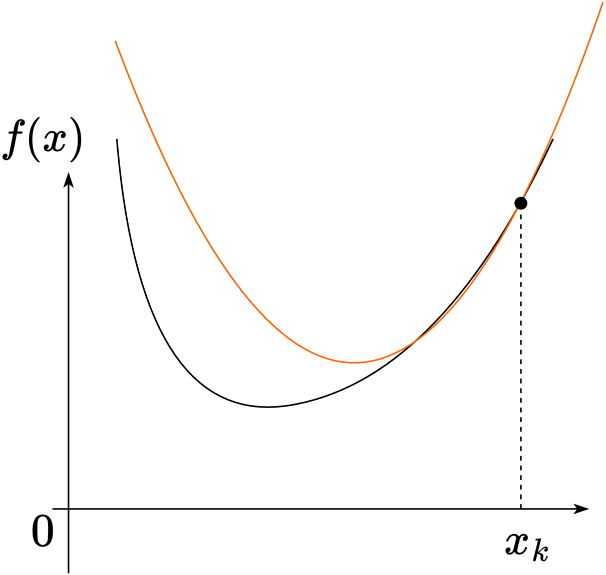

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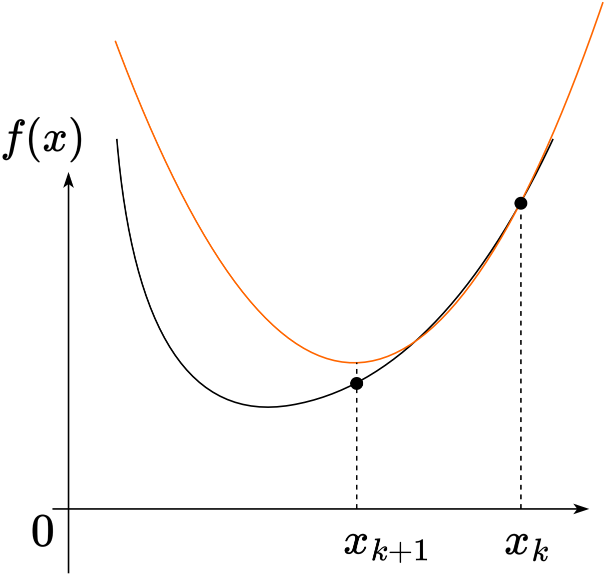

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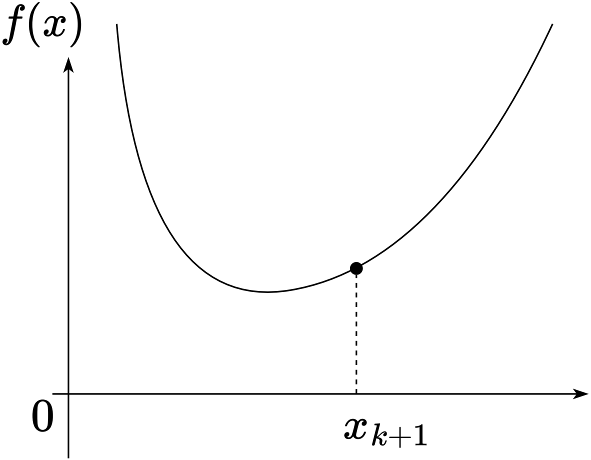

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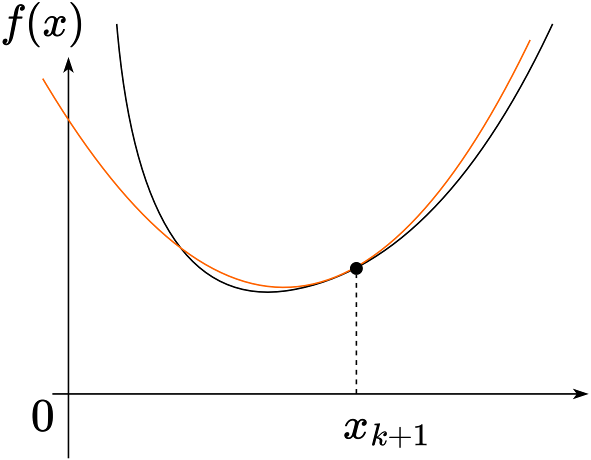

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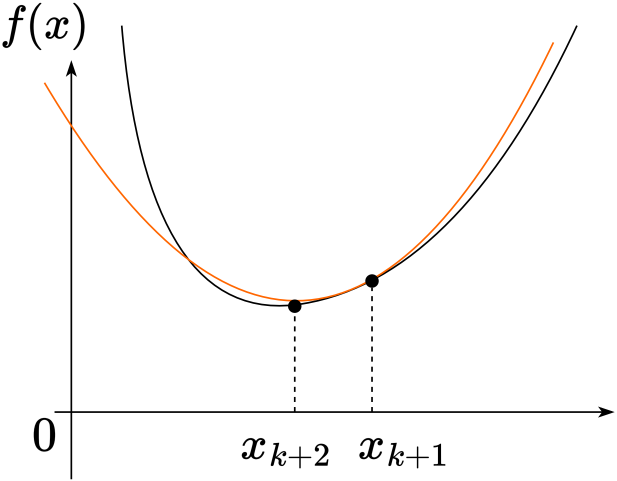

# Convergence

**Theorem**

Let $f(x)$ be a strongly convex twice continuously differentiable function at $\mathbb{R}^n$, for the second derivative of which inequalities are executed: $\mu I_n \preceq \nabla^2 f(x) \preceq L I_n$. Then Newton's method with a constant step locally converges to solving the problem with superlinear speed. If, in addition, Hessian is $M$-Lipschitz continuous, then this method converges locally to $x^*$ at a quadratic rate.

We have an important result: Newton's method for the function with Lipschitz positive-definite Hessian converges **quadratically** near ($\|x_0 - x^*\| < \frac{2\mu}{3M}$) to the solution.

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An important property of Newton's method is **affine invariance**. Given a function $f$ and a nonsingular matrix $A \in \mathbb{R}^{n \times n}$, let $x = Ay$, and define $g(y) = f(Ay)$. Note, that $\nabla g(y) = A^T \nabla f(x)$ and $\nabla^2 g(y) = A^T \nabla^2 f(x) A$. The Newton steps on $g$ are expressed as:

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# Affine Invariance of Newton's Method

An important property of Newton's method is **affine invariance**. Given a function $f$ and a nonsingular matrix $A \in \mathbb{R}^{n \times n}$, let $x = Ay$, and define $g(y) = f(Ay)$. Note, that $\nabla g(y) = A^T \nabla f(x)$ and $\nabla^2 g(y) = A^T \nabla^2 f(x) A$. The Newton steps on $g$ are expressed as:

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This shows that the progress made by Newton's method is independent of problem scaling. This property is not shared by the gradient descent method!

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- the Hessian can be degenerate at $x^*$
- the hessian may not be positively determined $\to$ direction $-(f''(x))^{-1}f'(x)$ may not be a descending direction

# Newton method problems

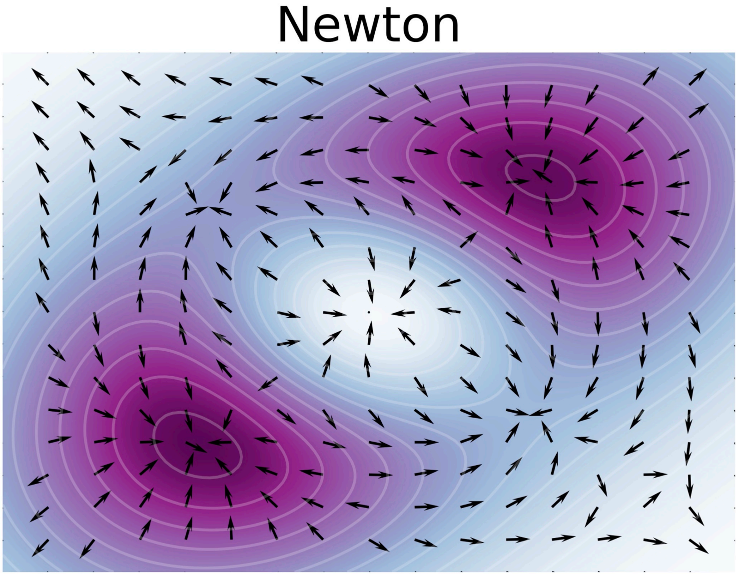


Figure 19: Animation

# Newton method problems

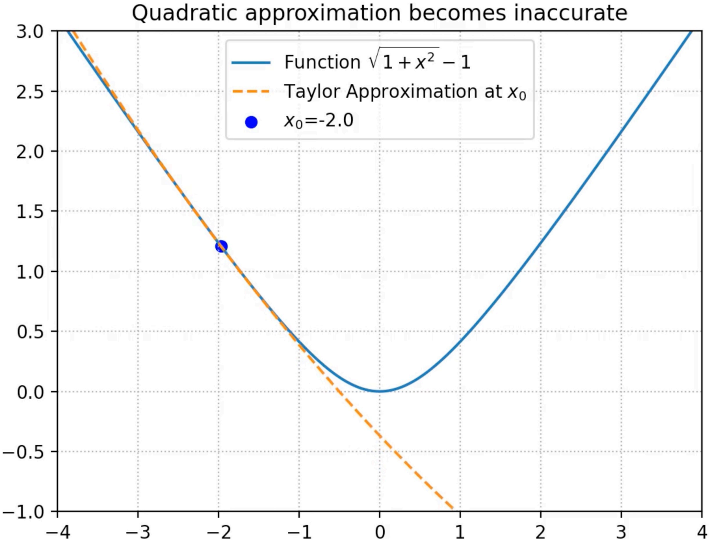


Figure 20: Animation

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i.e. at each iteration it is necessary to **compute** hessian and gradient and **solve** linear system.

Note here that if we take a single matrix of $B_k = I_n$ as $B_k$ at each step, we will exactly get the gradient descent method.

The general scheme of quasi-Newton methods is based on the selection of the $B_k$ matrix so that it tends in some sense at $k \to \infty$ to the truth value of the Hessian $\nabla^2 f(x_k)$.

# Quasi-Newton Method Template

Let $x_0 \in \mathbb{R}^n$, $B_0 \succ 0$. For $k = 1, 2, 3, \dots$, repeat:

1. Solve $B_k d_k = -\nabla f(x_k)$

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In addition to the secant equation, we want:

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- $B_{k+1}$ to be "close" to $B_k$
- $B_k \succ 0 \Rightarrow B_{k+1} \succ 0$

# Symmetric Rank-One Update

Let's try an update of the form:

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This only holds if $u$ is a multiple of $\Delta y_k - B_k d_k$. Putting $u = \Delta y_k - B_k d_k$, we solve the above,

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which leads to

$$B_{k+1} = B_k + \frac{(\Delta y_k - B_k d_k)(\Delta y_k - B_k d_k)^T}{(\Delta y_k - B_k d_k)^T d_k}$$

called the symmetric rank-one (SR1) update or Broyden method.

# Symmetric Rank-One Update with inverse

How can we solve

$$B_{k+1}d_{k+1} = -\nabla f(x_{k+1}),$$

in order to take the next step? In addition to propagating $B_k$ to $B_{k+1}$, let's propagate inverses, i.e., $C_k = B_k^{-1}$ to $C_{k+1} = (B_{k+1})^{-1}$.

## Sherman-Morrison Formula:

The Sherman-Morrison formula states:

$$(A + uv^T)^{-1} = A^{-1} - \frac{A^{-1}uv^T A^{-1}}{1 + v^T A^{-1}u}$$

Thus, for the SR1 update, the inverse is also easily updated:

$$C_{k+1} = C_k + \frac{(d_k - C_k\Delta y_k)(d_k - C_k\Delta y_k)^T}{(d_k - C_k\Delta y_k)^T\Delta y_k}$$

In general, SR1 is simple and cheap, but it has a key shortcoming: it does not preserve positive definiteness.

# Davidon-Fletcher-Powell Update

We could have pursued the same idea to update the inverse $C$:

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Multiplying by $\Delta y_k$, using the secant equation $d_k = C_k \Delta y_k$, and solving for $a$, $b$, yields:

$$C_{k+1} = C_k - \frac{C_k \Delta y_k \Delta y_k^T C_k}{\Delta y_k^T C_k \Delta y_k} + \frac{d_k d_k^T}{\Delta y_k^T d_k}$$

## Woodbury Formula Application

Woodbury then shows:

$$B_{k+1} = \left(I - \frac{\Delta y_k d_k^T}{\Delta y_k^T d_k}\right) B_k \left(I - \frac{d_k \Delta y_k^T}{\Delta y_k^T d_k}\right) + \frac{\Delta y_k \Delta y_k^T}{\Delta y_k^T d_k}$$

This is the Davidon-Fletcher-Powell (DFP) update. Also cheap: $O(n^2)$, preserves positive definiteness. Not as popular as BFGS.

# Broyden-Fletcher-Goldfarb-Shanno update

Let's now try a rank-two update:

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Putting $u = \Delta y_k$, $v = B_k d_k$, and solving for a, b we get:

$$B_{k+1} = B_k - \frac{B_k d_k d_k^T B_k}{d_k^T B_k d_k} + \frac{\Delta y_k \Delta y_k^T}{d_k^T \Delta y_k}$$

called the Broyden-Fletcher-Goldfarb-Shanno (BFGS) update.

# Broyden-Fletcher-Goldfarb-Shanno update with inverse

## Woodbury Formula

The Woodbury formula, a generalization of the Sherman-Morrison formula, is given by:

$$(A + UCV)^{-1} = A^{-1} - A^{-1}U(C^{-1} + VA^{-1}U)^{-1}VA^{-1}$$

# Broyden-Fletcher-Goldfarb-Shanno update with inverse

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$$(A + UCV)^{-1} = A^{-1} - A^{-1}U(C^{-1} + VA^{-1}U)^{-1}VA^{-1}$$

Applied to our case, we get a rank-two update on the inverse $C$:

$$C_{k+1} = C_k + \frac{(d_k - C_k \Delta y_k) d_k^T}{\Delta y_k^T d_k} + \frac{d_k (d_k - C_k \Delta y_k)^T}{\Delta y_k^T d_k} - \frac{(d_k - C_k \Delta y_k)^T \Delta y_k}{(\Delta y_k^T d_k)^2} d_k d_k^T$$

$$C_{k+1} = \left( I - \frac{d_k \Delta y_k^T}{\Delta y_k^T d_k} \right) C_k \left( I - \frac{\Delta y_k d_k^T}{\Delta y_k^T d_k} \right) + \frac{d_k d_k^T}{\Delta y_k^T d_k}$$

This formulation ensures that the BFGS update, while comprehensive, remains computationally efficient, requiring $O(n^2)$ operations. Importantly, BFGS update preserves positive definiteness. Recall this means $B_k \succ 0 \Rightarrow B_{k+1} \succ 0$. Equivalently, $C_k \succ 0 \Rightarrow C_{k+1} \succ 0$

# Code

- Open In Colab

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