



**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**

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# Gradient Descent

## 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:

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

Optimality conditions:

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

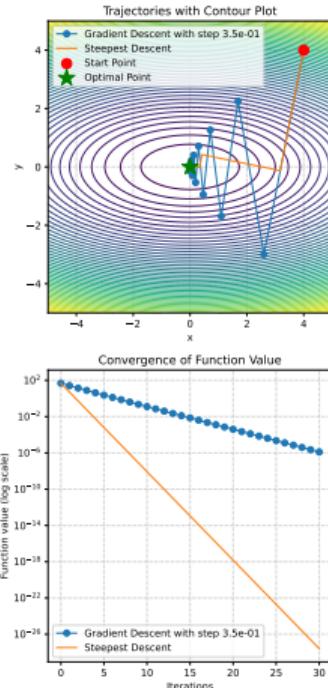


Figure 1: Steepest Descent

Open In Colab ♣

## Strongly convex quadratics

## Coordinate shift

Consider the following quadratic optimization problem:

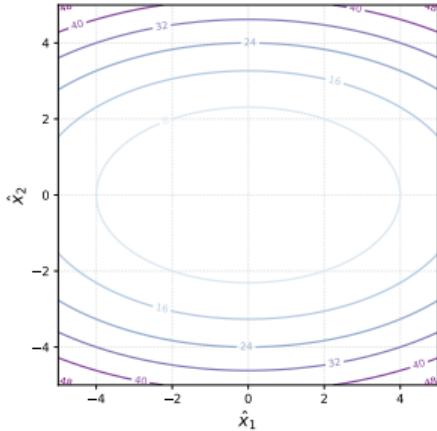
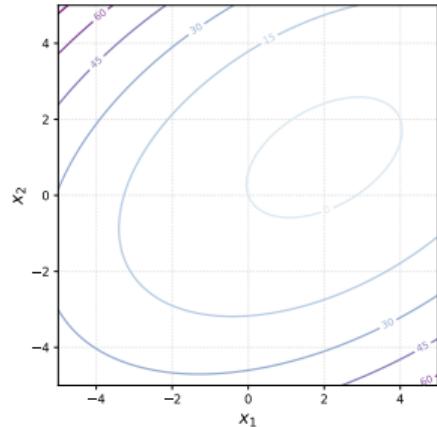
$$\min_{x \in \mathbb{R}^d} f(x) = \min_{x \in \mathbb{R}^d} \frac{1}{2} x^\top A x - b^\top x + c, \text{ where } A \in \mathbb{S}_{++}^d.$$

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- Firstly, without loss of generality we can set  $c = 0$ , which will not affect optimization process.



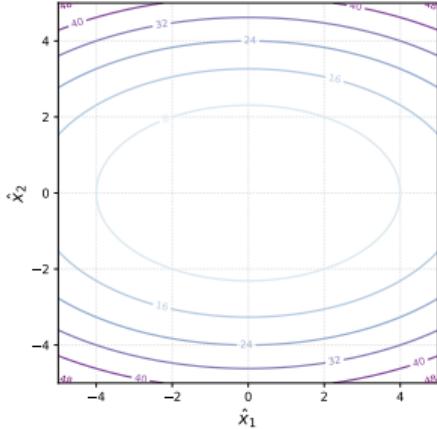
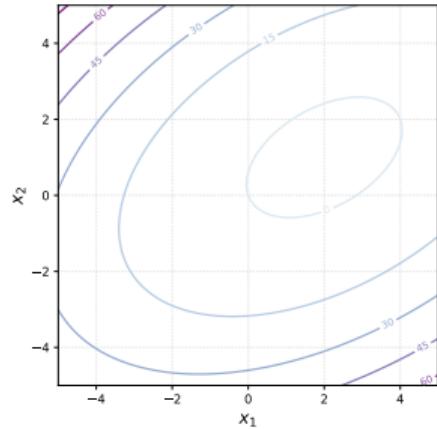
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$$A = Q \Lambda Q^T$$



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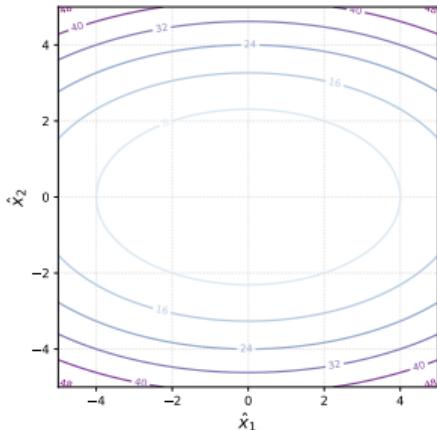
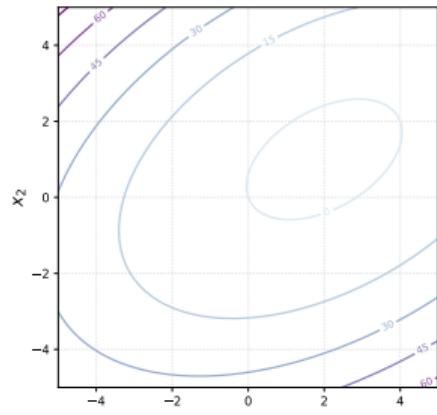
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- Let's show, that we can switch coordinates to make an analysis a little bit easier. Let  $\hat{x} = Q^T(x - x^*)$ , where  $x^*$  is the minimum point of initial function, defined by  $Ax^* = b$ . At the same time  $x = Q\hat{x} + x^*$ .



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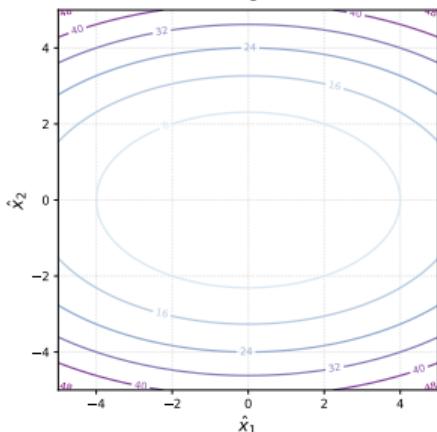
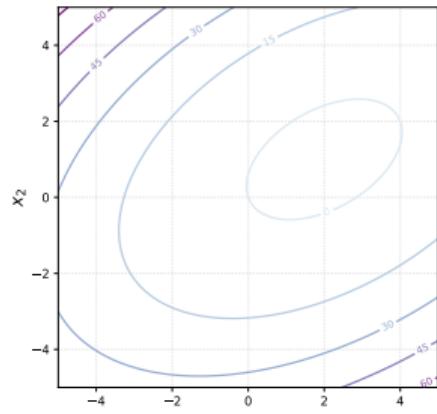
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$$f(\hat{x}) = \frac{1}{2} (Q\hat{x} + x^*)^\top A (Q\hat{x} + x^*) - b^\top (Q\hat{x} + x^*)$$



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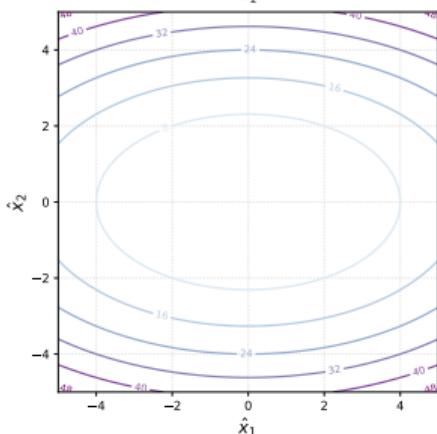
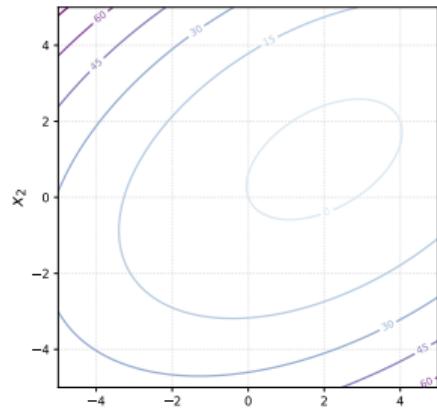
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$$\begin{aligned} f(\hat{x}) &= \frac{1}{2}(Q\hat{x} + x^*)^\top A(Q\hat{x} + x^*) - b^\top(Q\hat{x} + x^*) \\ &= \frac{1}{2}\hat{x}^T Q^T A Q \hat{x} + (x^*)^T A Q \hat{x} + \frac{1}{2}(x^*)^T A (x^*)^T - b^T Q \hat{x} - b^T x^* \end{aligned}$$



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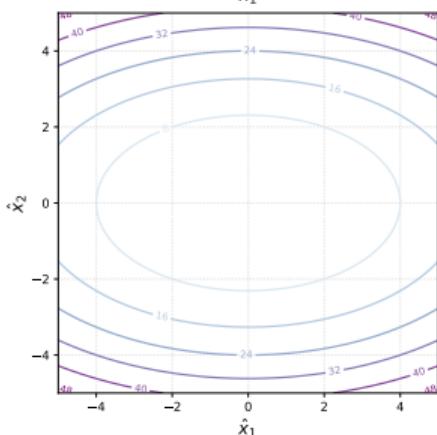
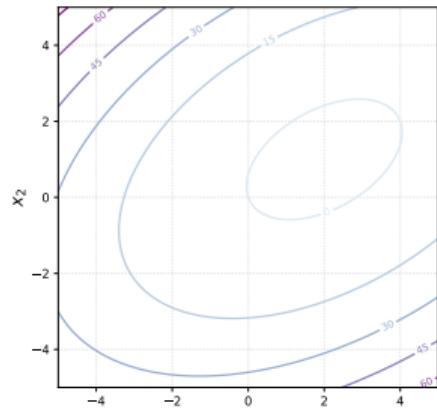
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## Convergence analysis

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  $\hat{x}$ )

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

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

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

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

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

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

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

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

## 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.

$\kappa$	$\rho$	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

## Polyak-Łojasiewicz smooth case

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

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

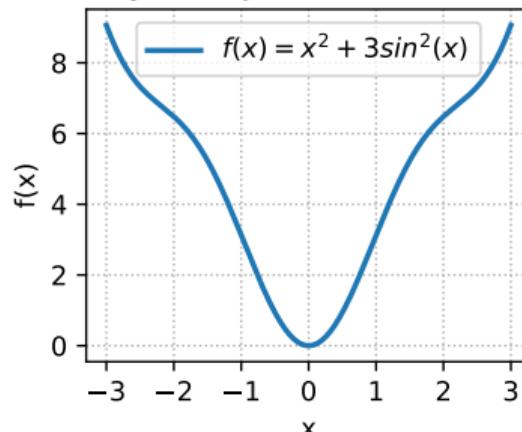
$$\|\nabla f(x)\|^2 \geq 2\mu(f(x) - f^*) \quad \forall x$$

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

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

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

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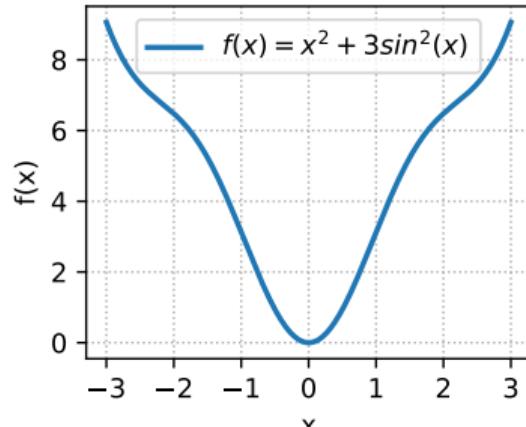
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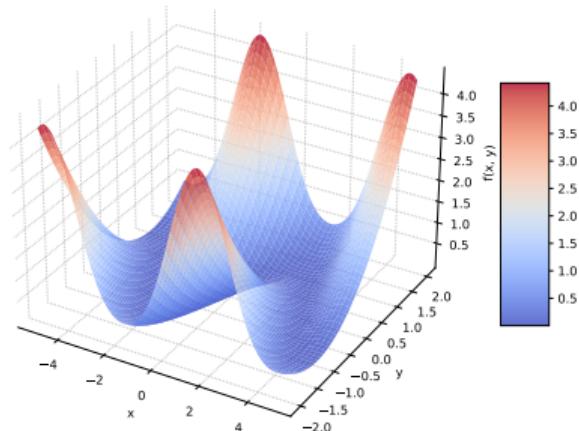
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$$f(x, y) = \frac{(y - \sin x)^2}{2}$$

Non-convex PL function



# Convergence analysis

## i Theorem

Consider the Problem

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

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:

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

## Example: linear least squares

Strongly convex binary logistic regression.  $\mu=0.1$ .

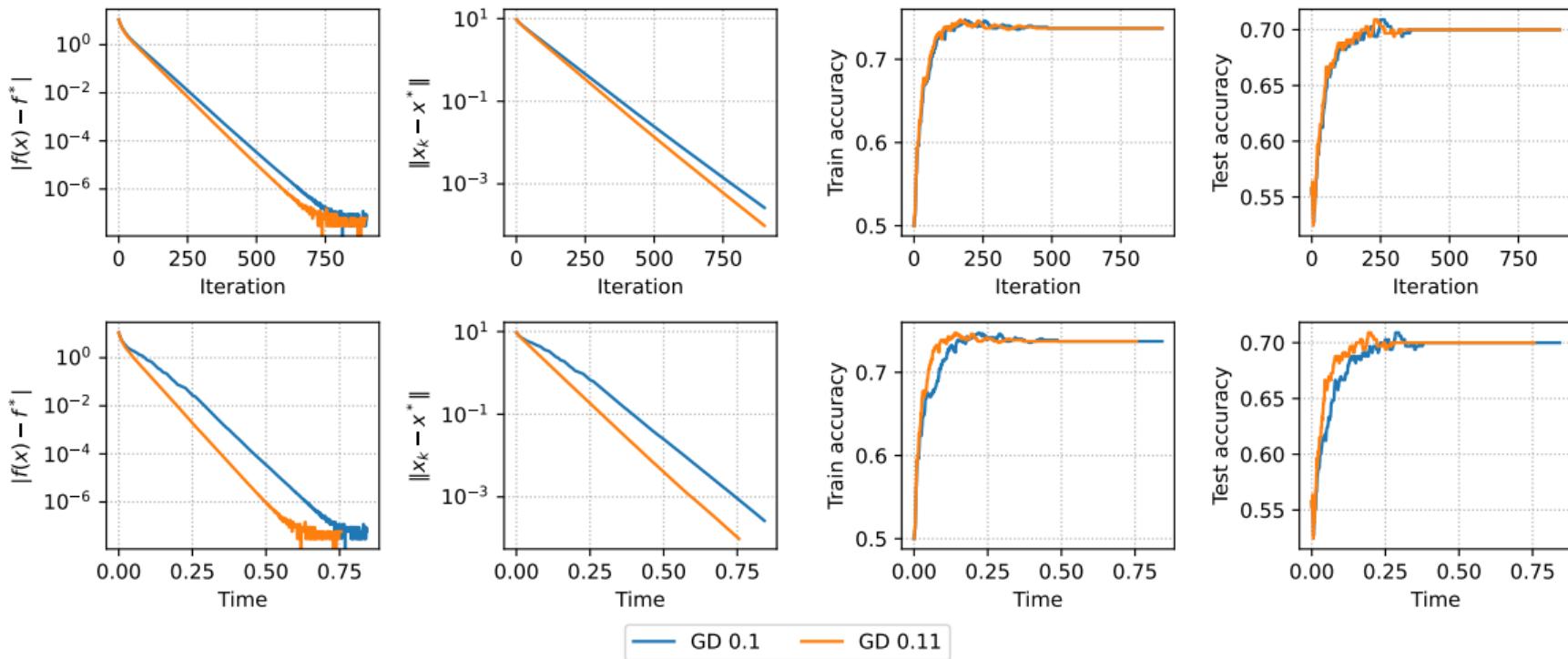


Figure 4: Convergence both in domain and in function value for regularized quadratics

## Smooth convex case

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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

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

## Example: linear least squares

Convex binary logistic regression. mu=0.

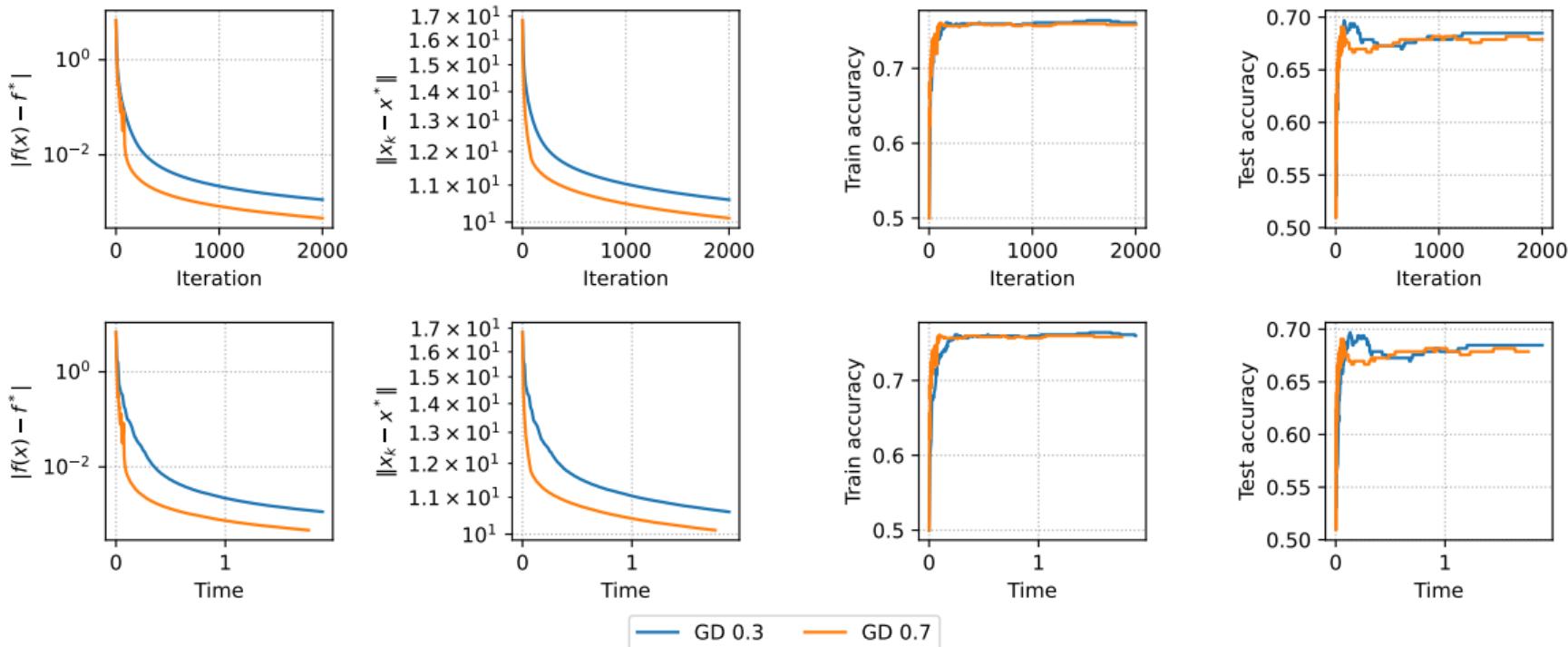


Figure 5: Convergence in function value for convex (but not strongly convex) quadratics

## Lower bounds

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

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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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- The key to the proof is to explicitly build a special function  $f$ .

## Recap

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Gradient Descent:

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

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

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

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

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

## Lower bounds

## Lower bounds

convex (non-smooth)	smooth (non-convex) <sup>1</sup>	smooth & convex <sup>2</sup>	smooth & strongly convex (or PL)
$\mathcal{O}\left(\frac{1}{\sqrt{k}}\right)$	$\mathcal{O}\left(\frac{1}{k^2}\right)$	$\mathcal{O}\left(\frac{1}{k^2}\right)$	$\mathcal{O}\left(\left(1 - \sqrt{\frac{\mu}{L}}\right)^k\right)$
$k_\varepsilon \sim \mathcal{O}\left(\frac{1}{\varepsilon^2}\right)$	$k_\varepsilon \sim \mathcal{O}\left(\frac{1}{\sqrt{\varepsilon}}\right)$	$k_\varepsilon \sim \mathcal{O}\left(\frac{1}{\sqrt{\varepsilon}}\right)$	$k_\varepsilon \sim \mathcal{O}\left(\sqrt{\kappa} \log \frac{1}{\varepsilon}\right)$

<sup>1</sup>Carmon, Duchi, Hinder, Sidford, 2017

<sup>2</sup>Nemirovski, Yudin, 1979

## Lower bounds

The iteration of gradient descent:

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

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

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## Lower bounds

The iteration of gradient descent:

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

Consider a family of first-order methods, where

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

### i 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

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

### i Smooth and convex case

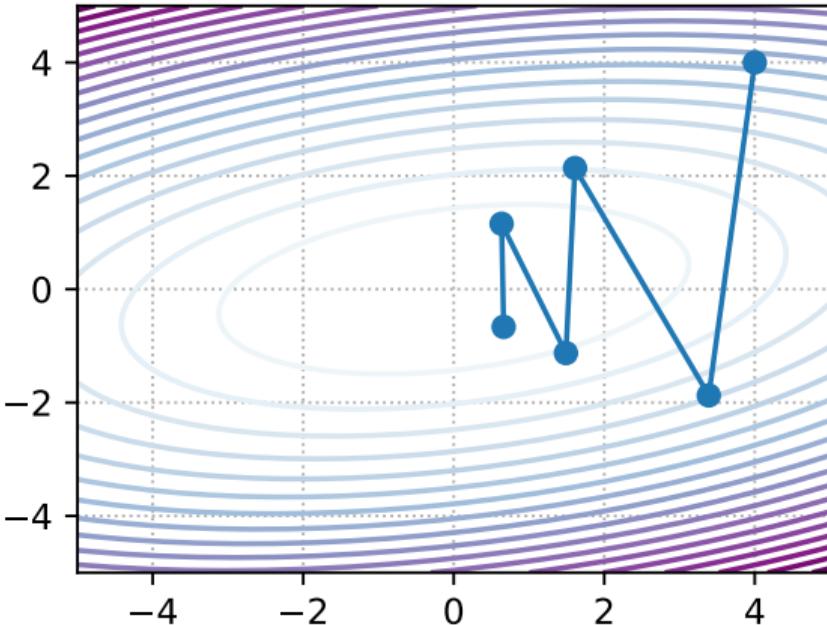
There exists a function  $f$  that is  $L$ -smooth and convex such that any first-order method of the form 2 satisfies

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

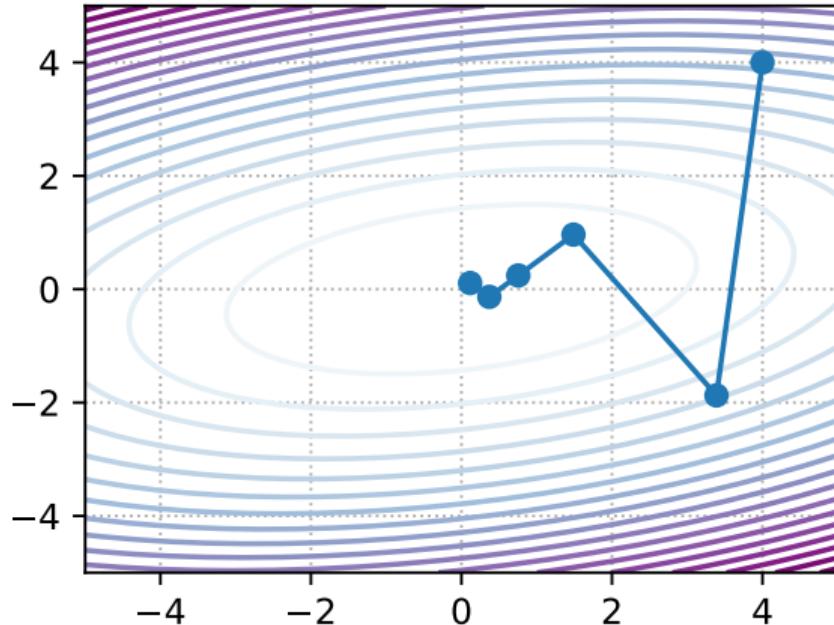
## Strongly convex quadratic problem

## Oscillations and acceleration

Gradient Descent



Heavy Ball



## Heavy ball

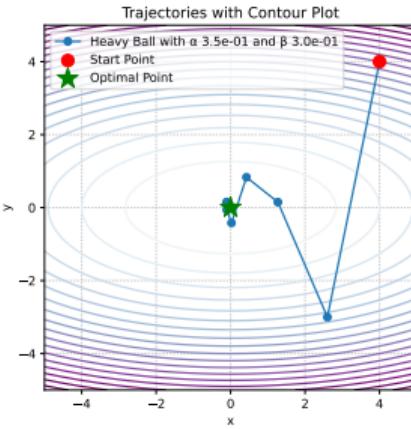
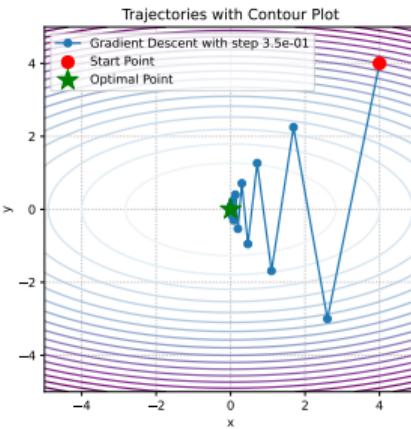
# Polyak Heavy ball method

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

### i Theorem

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

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

converges linearly:

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

# Heavy Ball Global Convergence <sup>3</sup>

## i Theorem

Assume that  $f$  is smooth and convex and that

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

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

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

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

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

<sup>3</sup>Global convergence of the Heavy-ball method for convex optimization, Euhanna Ghadimi et.al.

## Heavy Ball Global Convergence <sup>4</sup>

### i 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  $x^*$ . In particular,

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

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

<sup>4</sup>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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- 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

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

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Let's define the following notation

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

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

Then we can write down:

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

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

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

## NAG convergence for quadratics

## General case convergence

### i Theorem

Let  $f : \mathbb{R}^n \rightarrow \mathbb{R}$  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:

**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:**  $\lambda_{k+1} = \frac{1 + \sqrt{1 + 4\lambda_k^2}}{2}$

**Extrapolation weight:**  $\gamma_k = \frac{1 - \lambda_k}{\lambda_{k+1}}$

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

### i Theorem

Let  $f : \mathbb{R}^n \rightarrow \mathbb{R}$  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:

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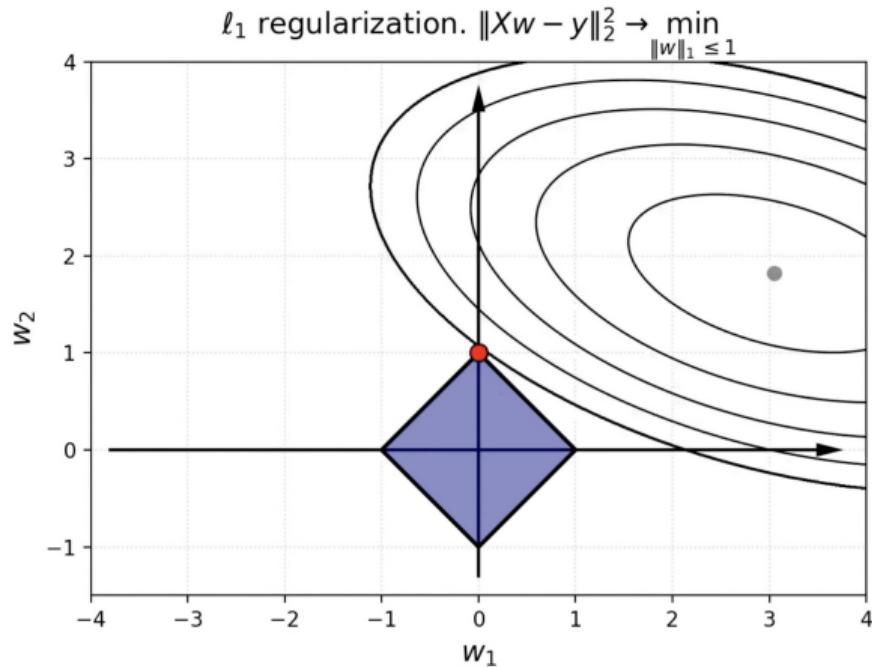
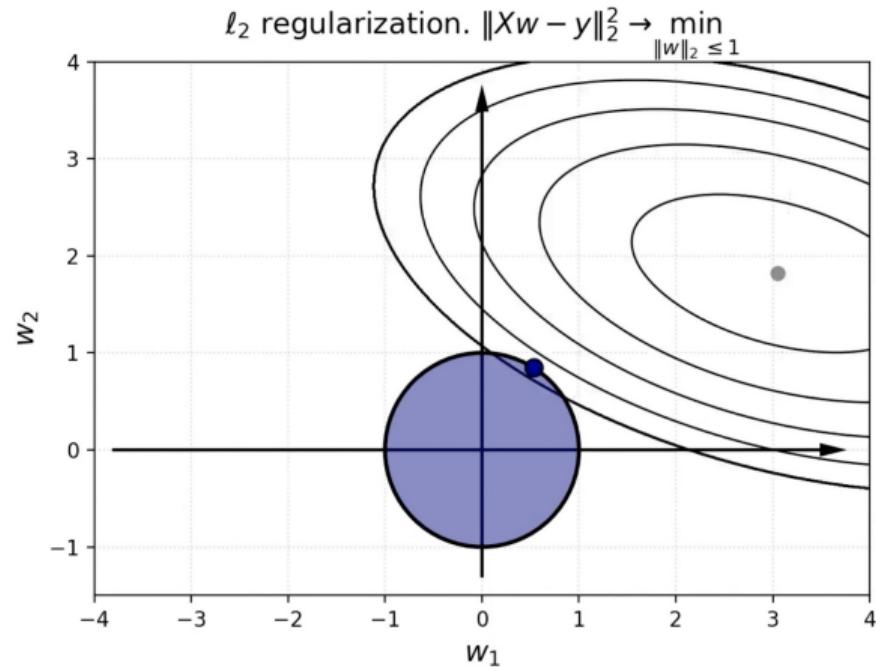
The sequences  $\{f(y_k)\}_{k \in \mathbb{N}}$  produced by the algorithm will converge to the optimal value  $f^*$  linearly:

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

## Non-smooth problems

## $\ell_1$ -regularized linear least squares

$\ell_1$  induces sparsity



@fminxyz

## 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.

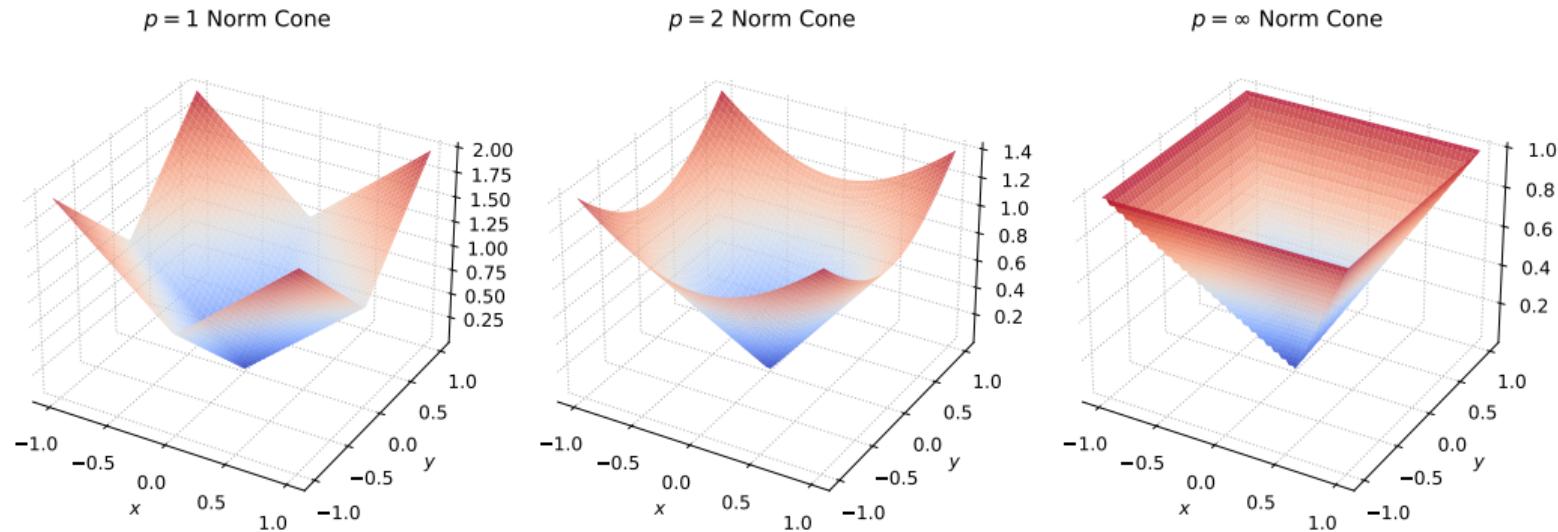


Figure 6: Norm cones for different  $p$ -norms are non-smooth

## Wolfe's example

Wolfe's example

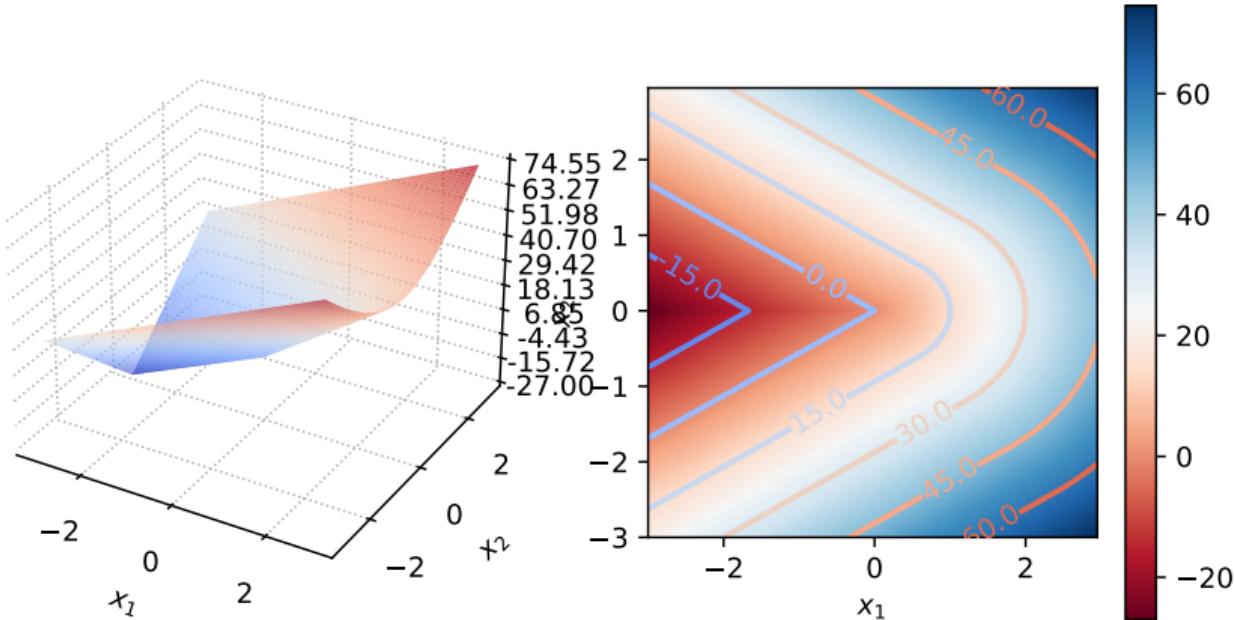
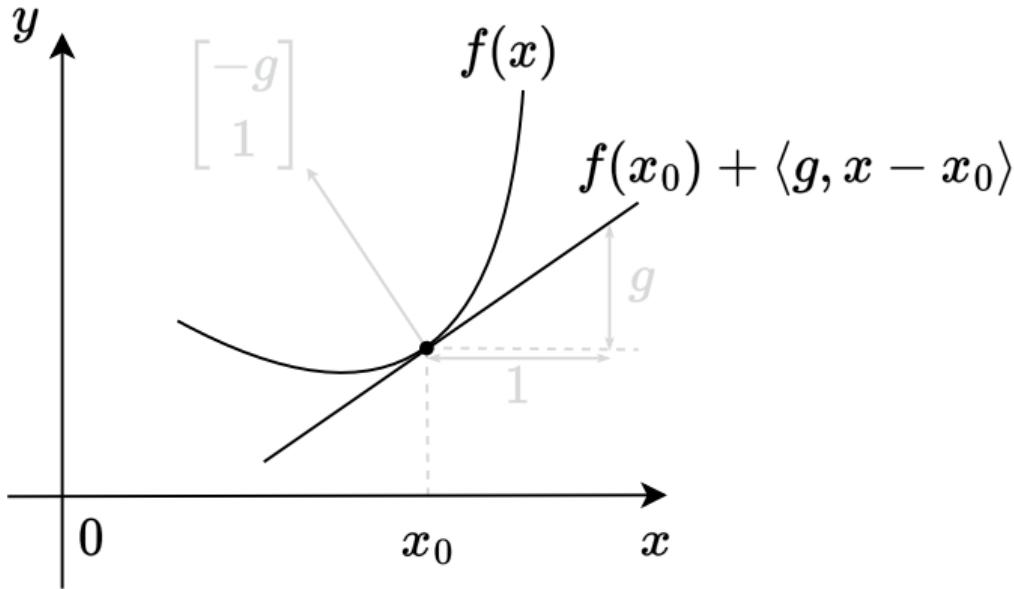


Figure 7: Wolfe's example. [Open in Colab](#)

## Subgradient calculus

## Convex function linear lower bound

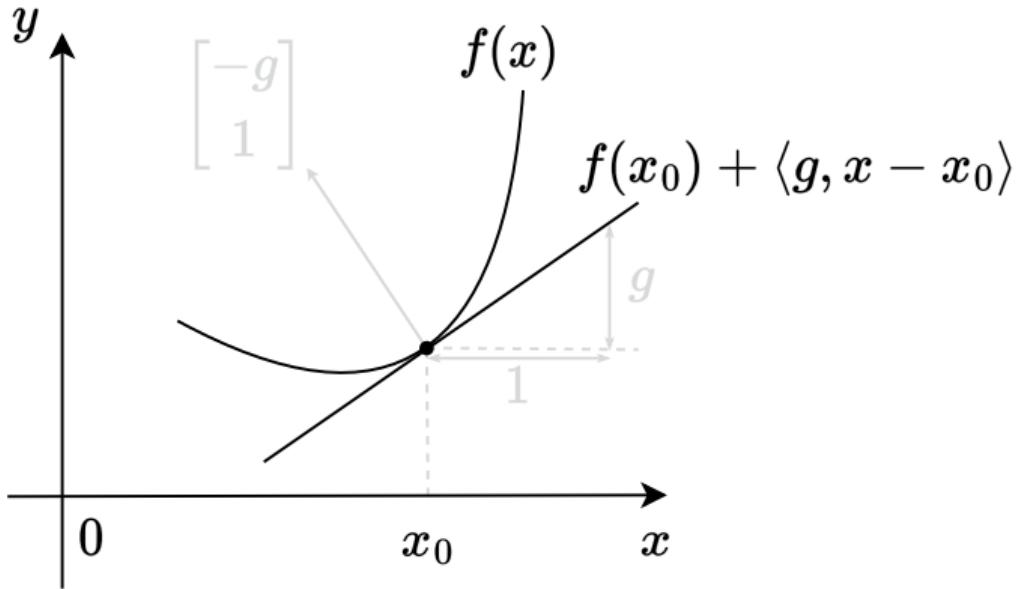


An important property of a continuous convex function  $f(x)$  is that at any chosen point  $x_0$  for all  $x \in \text{dom } f$  the inequality holds:

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

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

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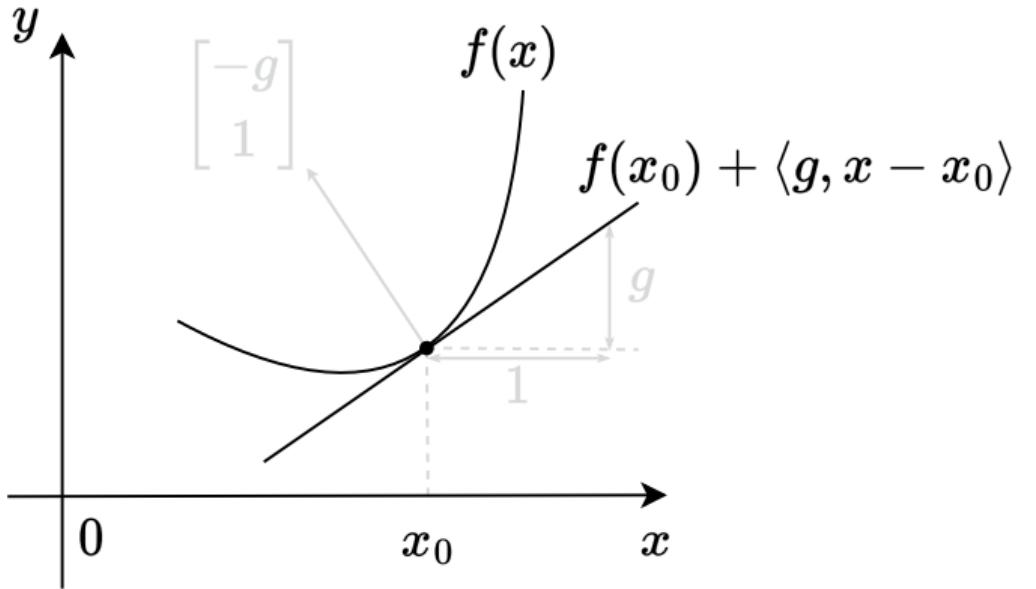
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for some vector  $g$ , i.e., the tangent to the graph of the function is the *global* estimate from below for the function.

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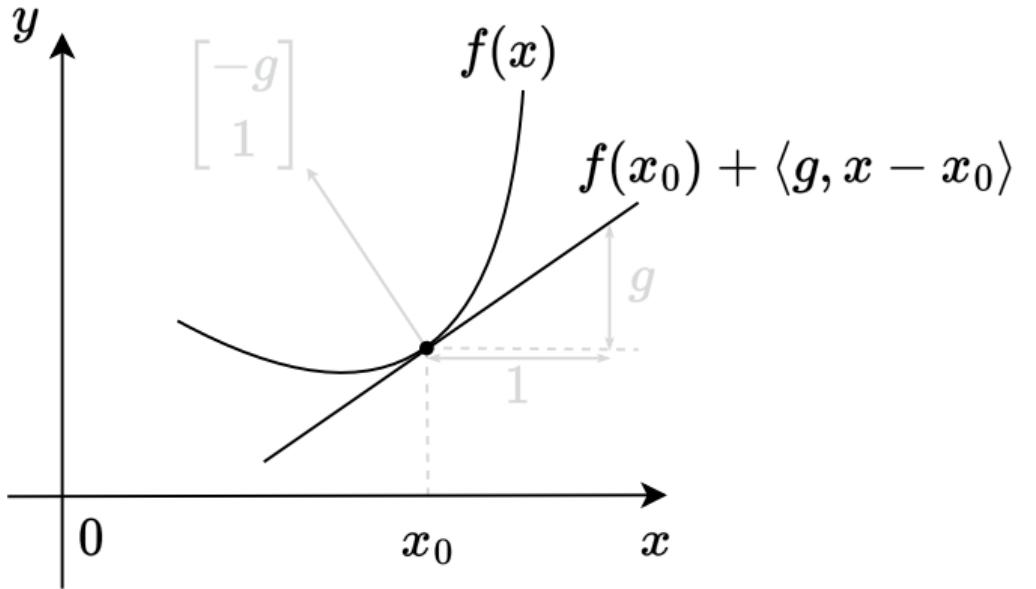
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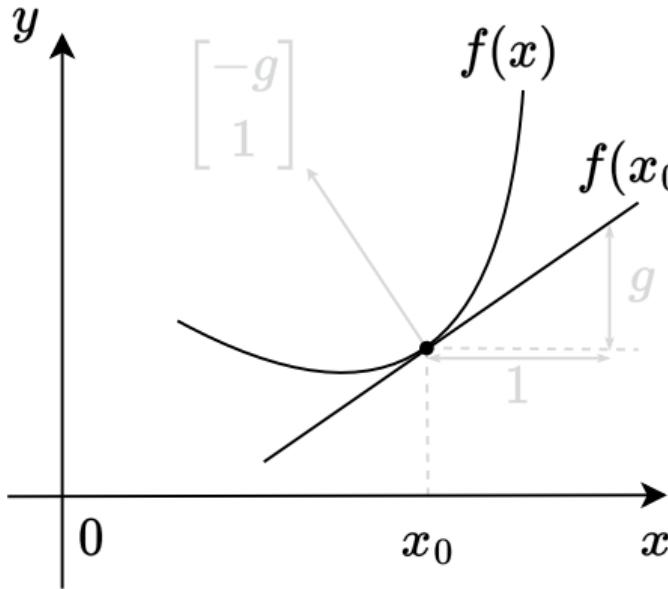
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- If  $f(x)$  is differentiable, then  $g = \nabla f(x_0)$
- Not all continuous convex functions are differentiable.

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

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

## Subgradient and subdifferential

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

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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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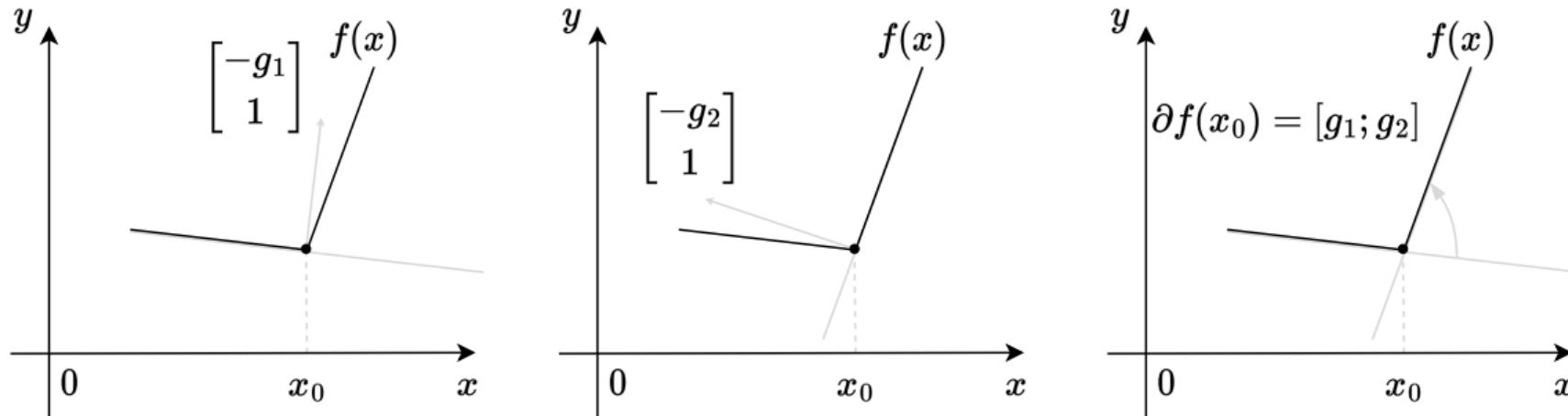


Figure 9: Subdifferential is a set of all possible subgradients

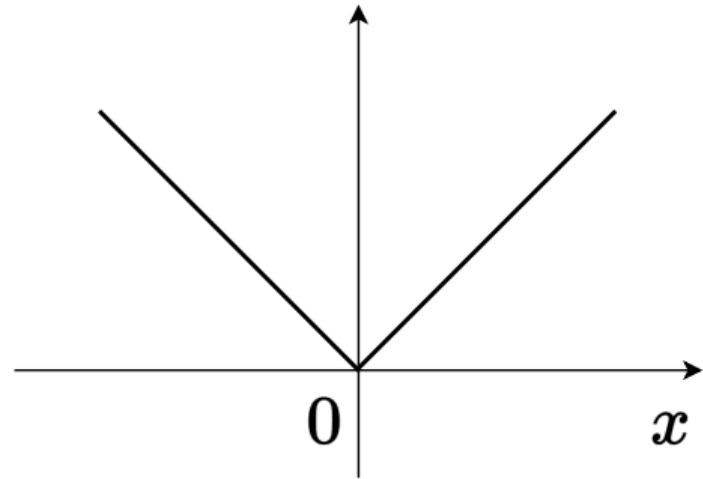
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Find  $\partial f(x)$ , if  $f(x) = |x|$

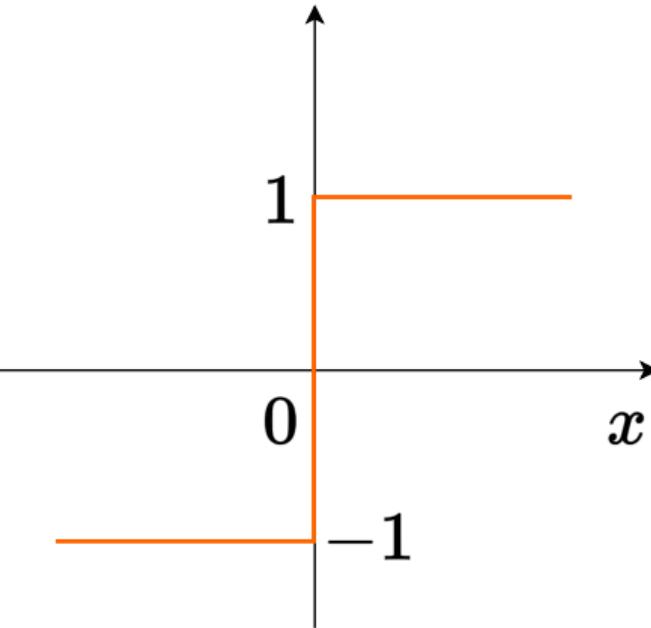
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$$\partial f(x)$$



## Subgradient Method

## Algorithm

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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

### i 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

$$f(\bar{x}) - f^* \leq \frac{G\|x_0 - x^*\|_2}{\sqrt{K}} \quad \bar{x} = \frac{1}{K} \sum_{k=0}^{K-1} x_i$$

- $\mathcal{O}\left(\frac{1}{\sqrt{T}}\right)$  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 can just use several diminishing 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

### i Theorem

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

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

### i Theorem

Let  $f$  be a convex  $G$ -Lipschitz function and  $f_k^{\text{best}} = \min_{i=1,\dots,k} f(x^i)$ . 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

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

## Applications

# Linear Least Squares with $l_1$ -regularization

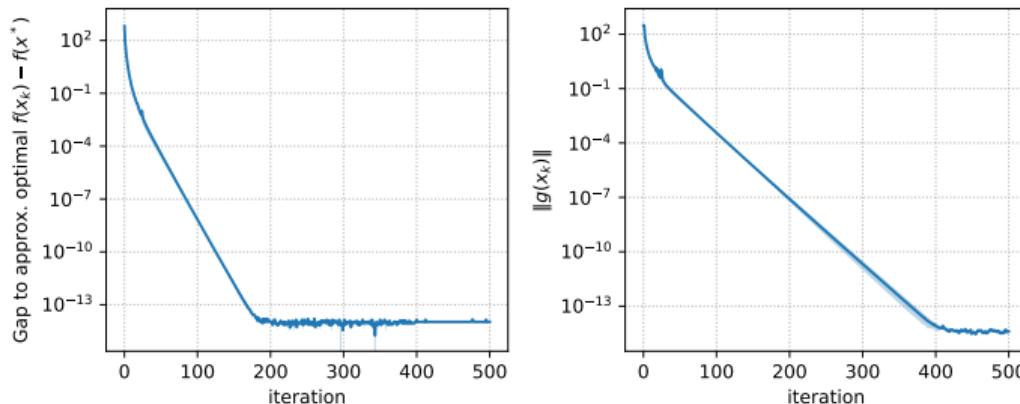
$$\min_{x \in \mathbb{R}^n} \frac{1}{2} \|Ax - b\|_2^2 + \lambda \|x\|_1$$

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.

LLS with  $l_1$  regularization. 2 runs.  $\lambda = 1$



## Regularized logistic regression

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

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

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  $i = 1, \dots, n$ . Consider the regularized problem:

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

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

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

## Subgradient method

Subgradient Method:

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

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convex (non-smooth)

$$f(x_k) - f^* \sim \mathcal{O}\left(\frac{1}{\sqrt{k}}\right)$$

$$k_\varepsilon \sim \mathcal{O}\left(\frac{1}{\varepsilon^2}\right)$$

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## i Theorem

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

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

where

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

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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:

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

where

- $\alpha = \frac{R}{G\sqrt{k}}$
- $R = \|x_0 - x^*\|$

# Subgradient method

Subgradient Method:

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

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- $R = \|x_0 - x^*\|$
- $\bar{x} = \frac{1}{k} \sum_{i=0}^{k-1} x_i$

## Non-smooth convex optimization lower bounds

convex (non-smooth)	strongly convex (non-smooth)
$f(x_k) - f^* \sim \mathcal{O}\left(\frac{1}{\sqrt{k}}\right)$	$f(x_k) - f^* \sim \mathcal{O}\left(\frac{1}{k}\right)$
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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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## Proximal operator visualization

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

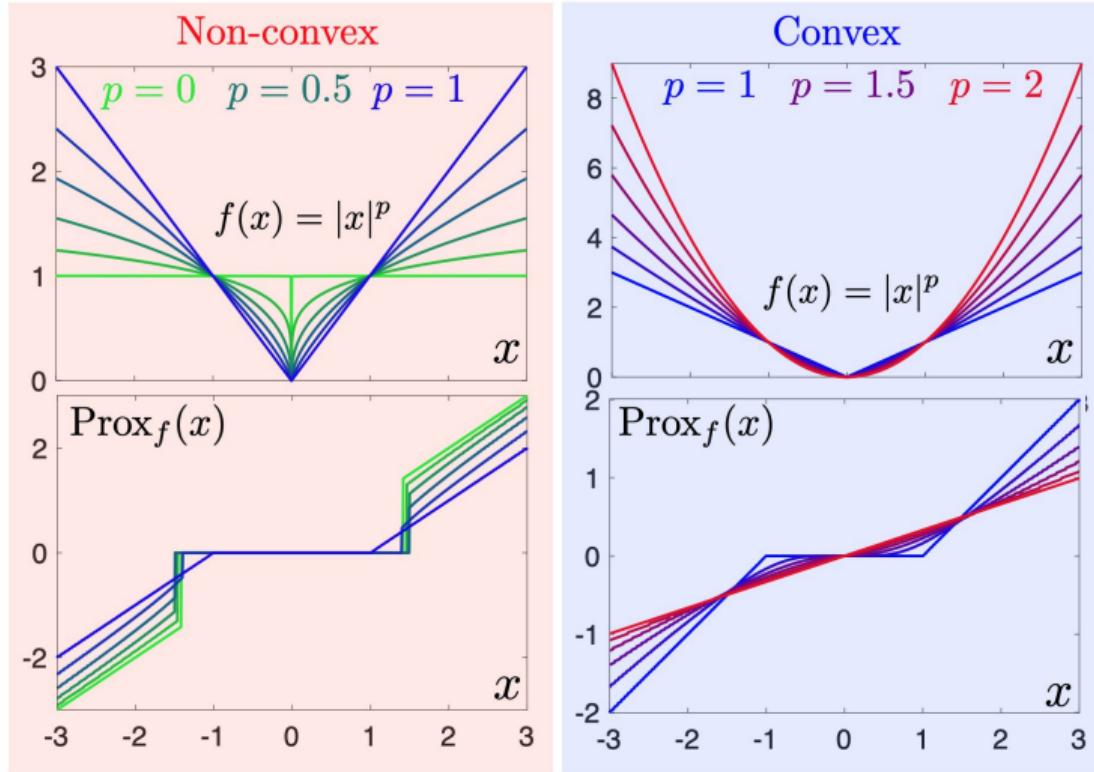


Figure 12: Source

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## From projections to proximity

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!

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

## Composite optimization

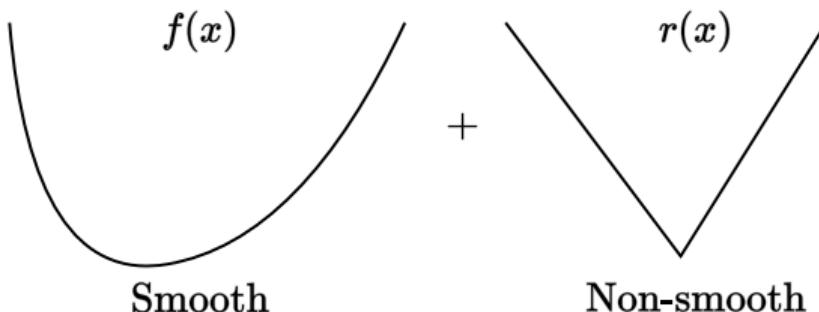
# Regularized / Composite Objectives

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

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



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Optimality conditions:

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

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

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

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**i** Another form of proximal operator

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## 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.

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- $r(x) = \mathbb{I}_S(x).$

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## Proximal Gradient Method. Convex case

# Convergence

## i Theorem

Consider the proximal gradient method

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

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

## i Theorem

Consider the proximal gradient method

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

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

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

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

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

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$$y_k = x_k + \frac{k-1}{k+2}(x_k - x_{k-1})$$

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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.

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- **Application:**

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

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- **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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- **Application:**

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

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- Proximal method is a general modern framework for many numerical methods. Further development includes accelerated, stochastic, primal-dual modifications and etc.

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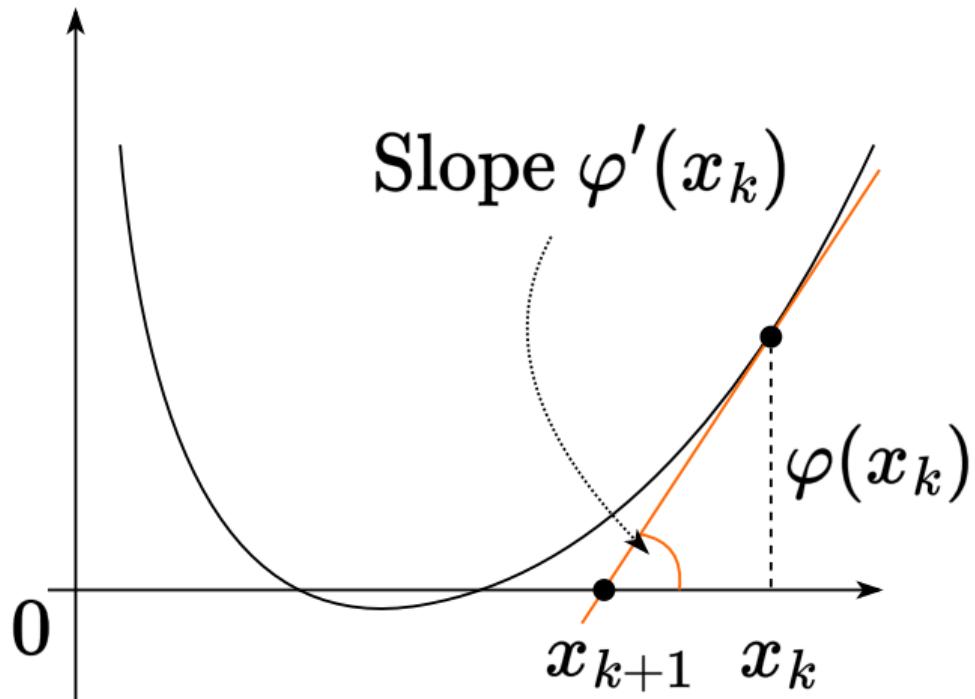
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- Further reading: Proximal operator splitting, Douglas-Rachford splitting, Best approximation problem, Three operator splitting.

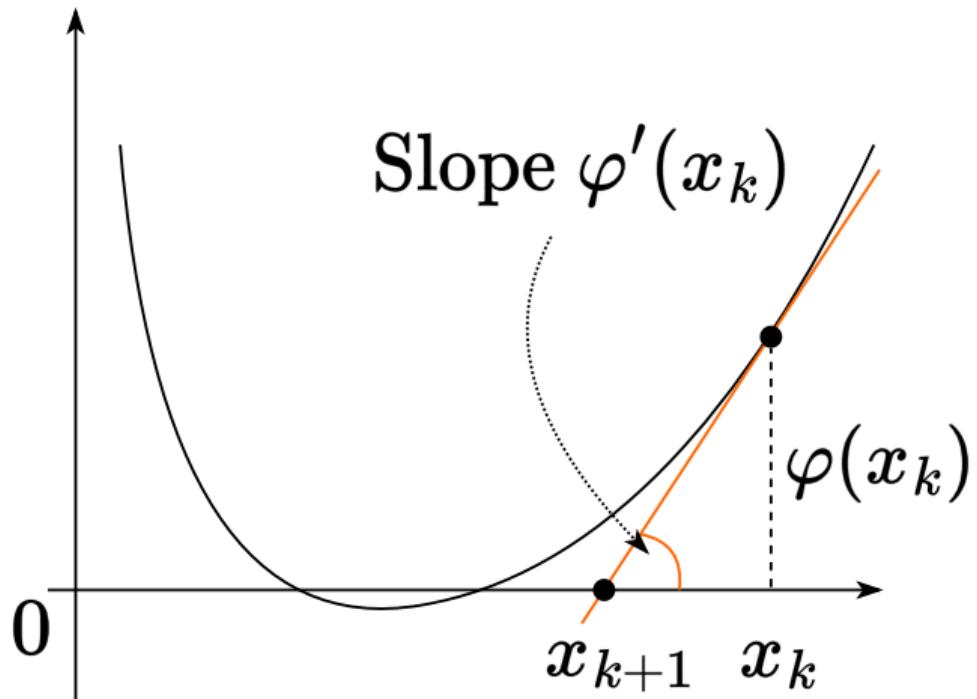
## Newton method

## Idea of Newton method of root finding

Consider the function  $\varphi(x) : \mathbb{R} \rightarrow \mathbb{R}$ .

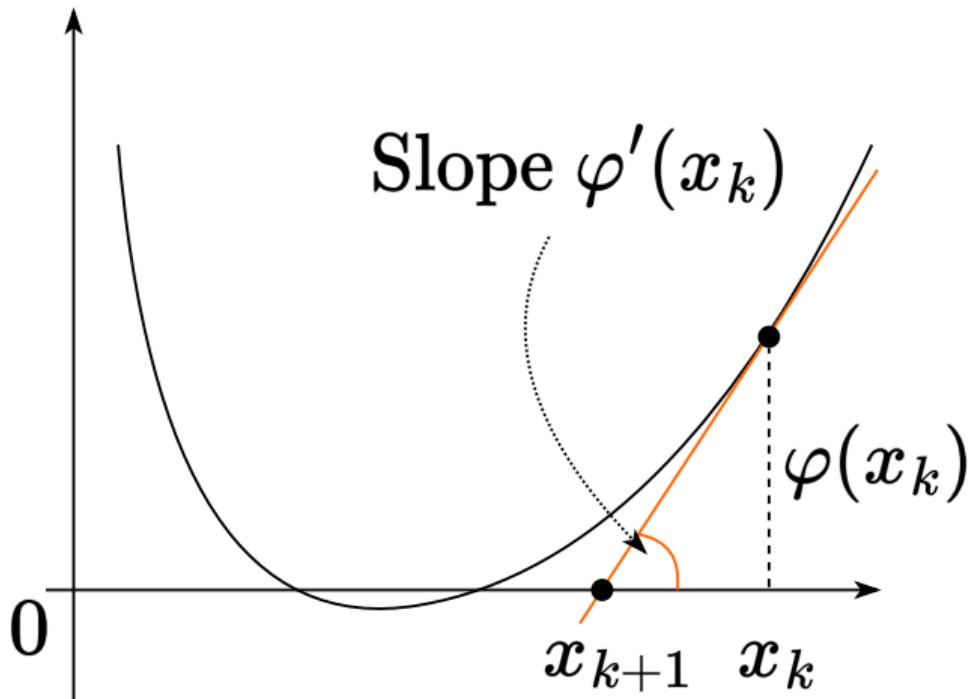


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The whole idea came from building a linear approximation at the point  $x_k$  and find its root, which will be the new iteration point:

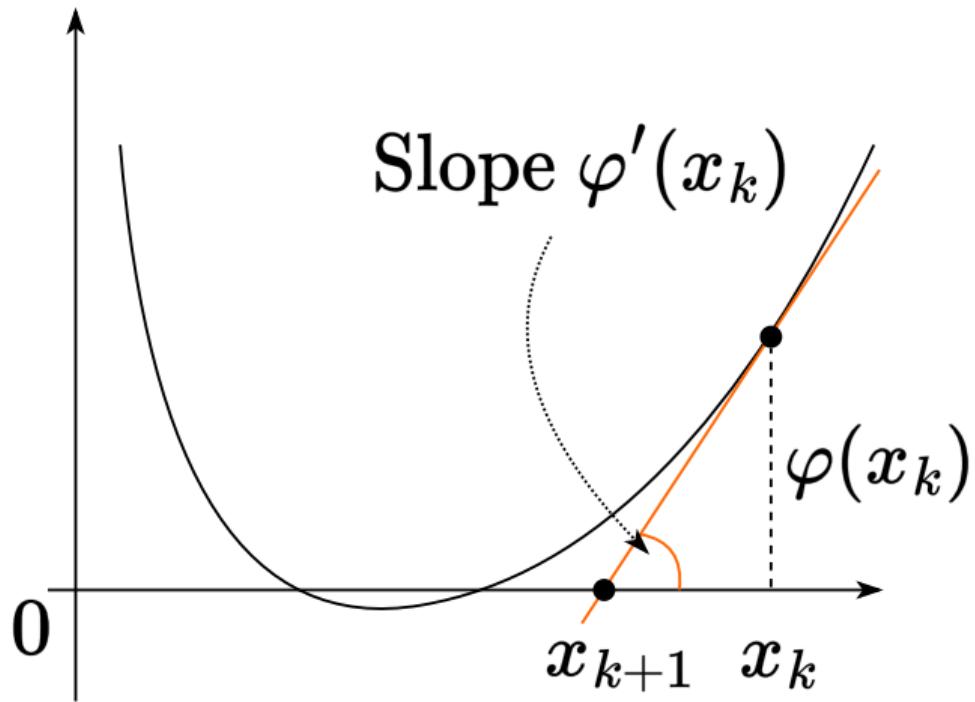
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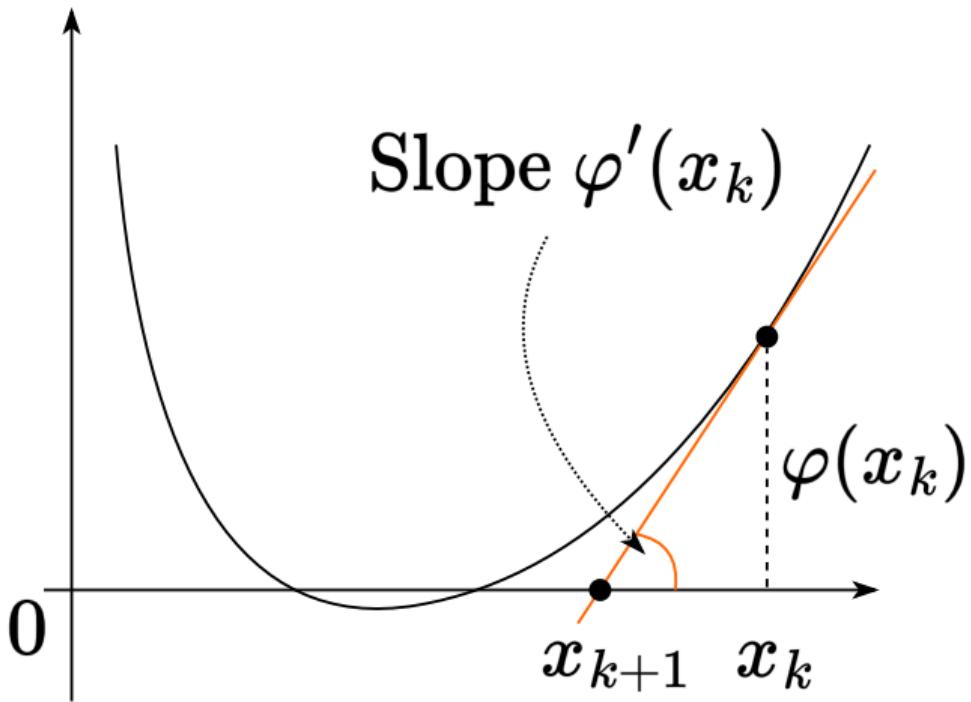


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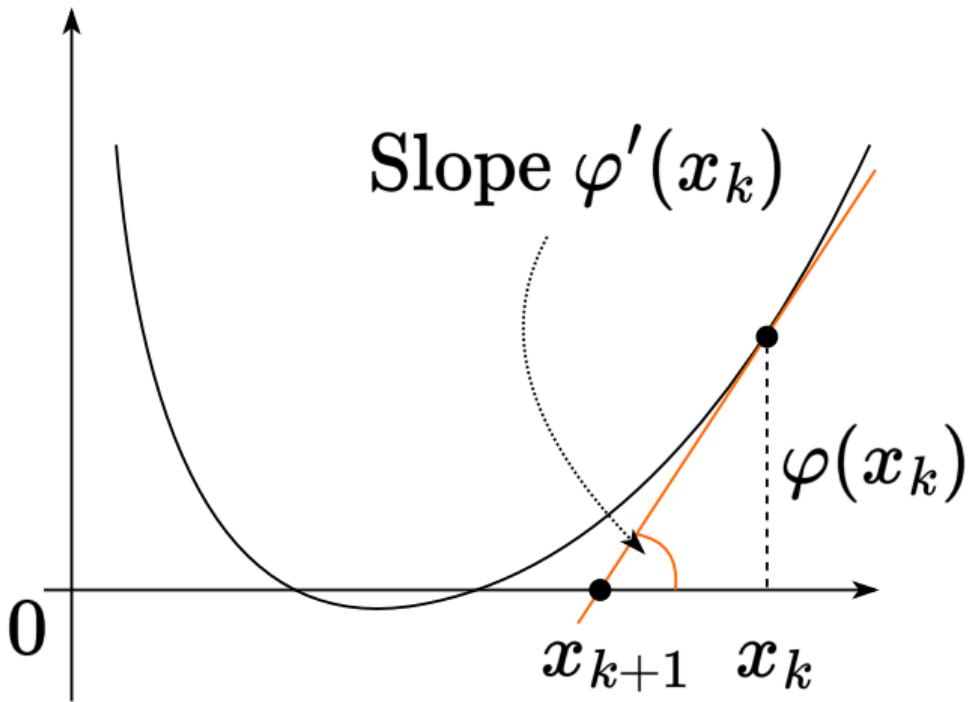
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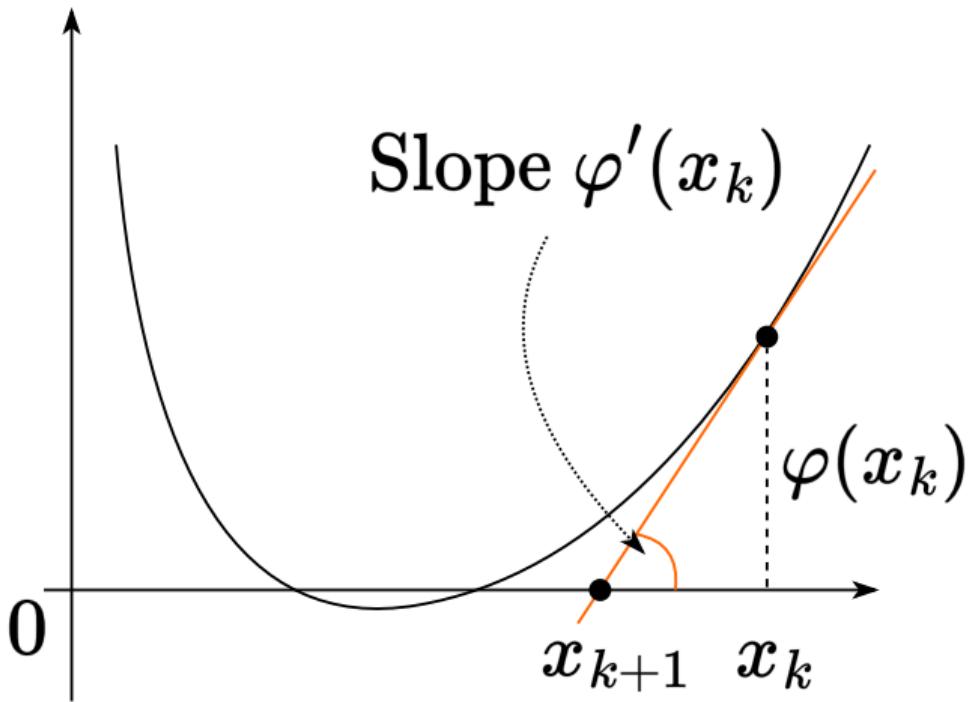
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<sup>a</sup>Literally we aim to solve the problem of finding stationary points  $\nabla f(x) = 0$

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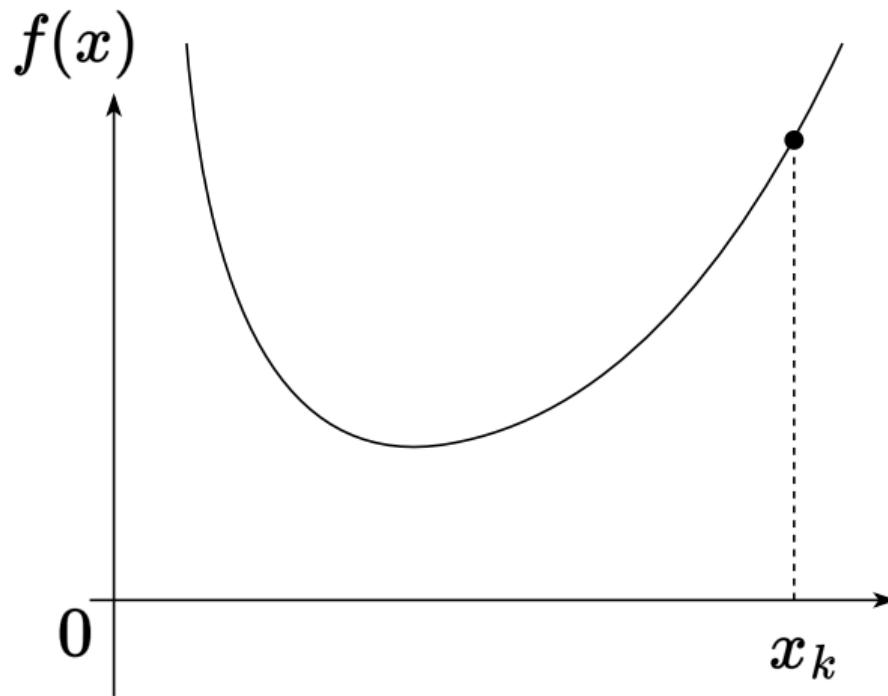
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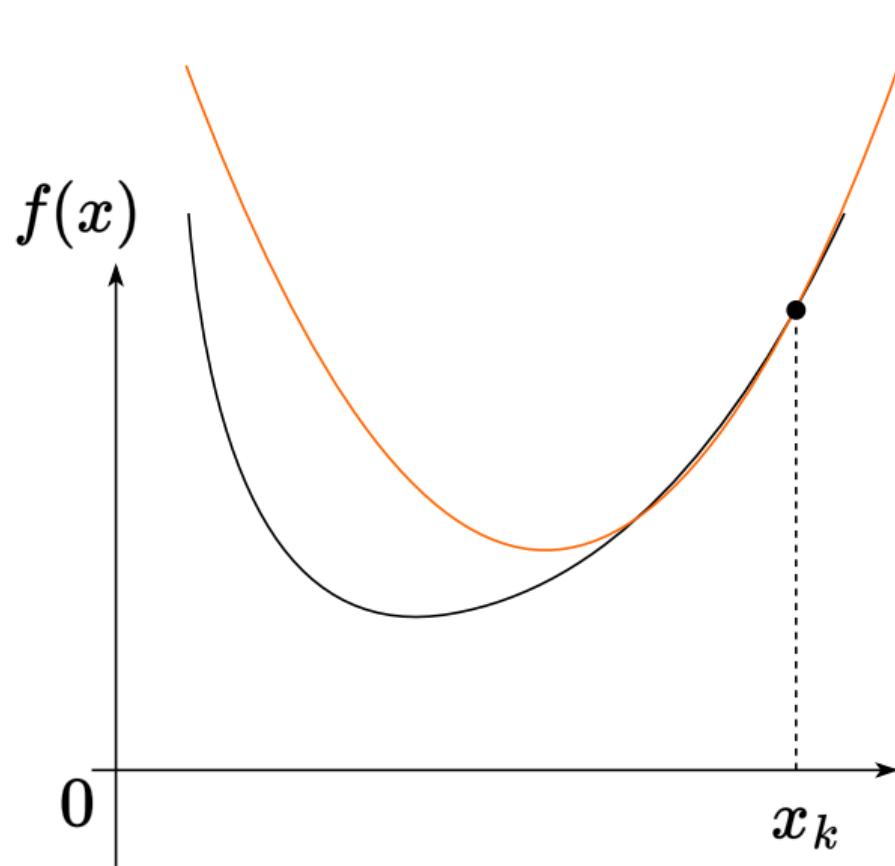
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Let us immediately note the limitations related to the necessity of the Hessian's non-degeneracy (for the method to exist), as well as its positive definiteness (for the convergence guarantee).

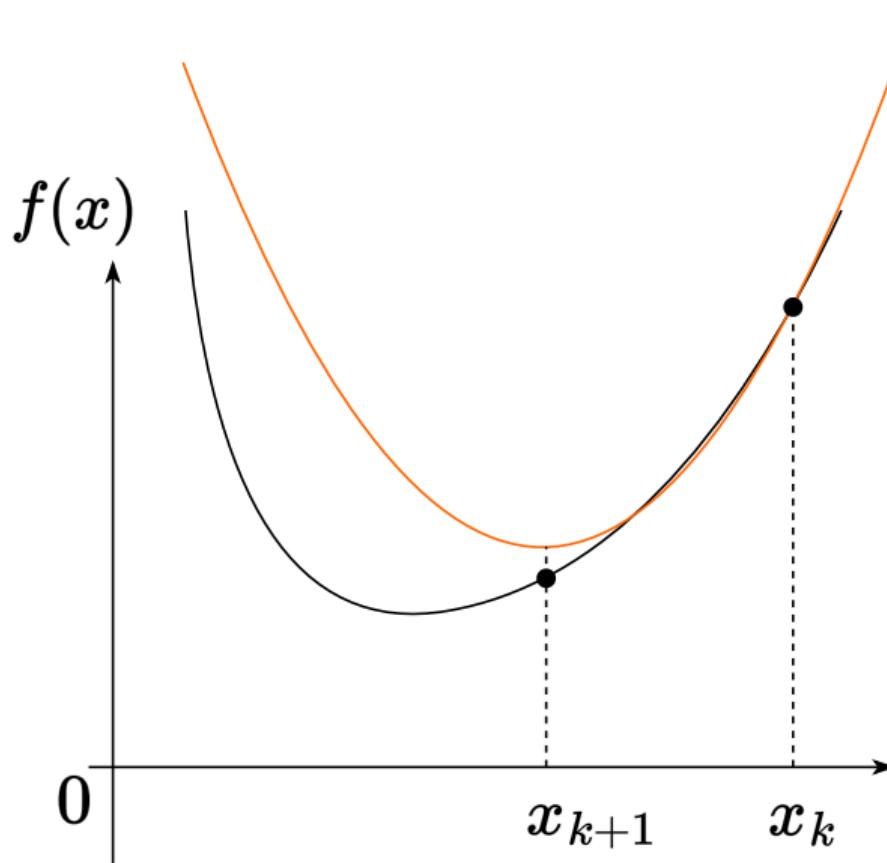
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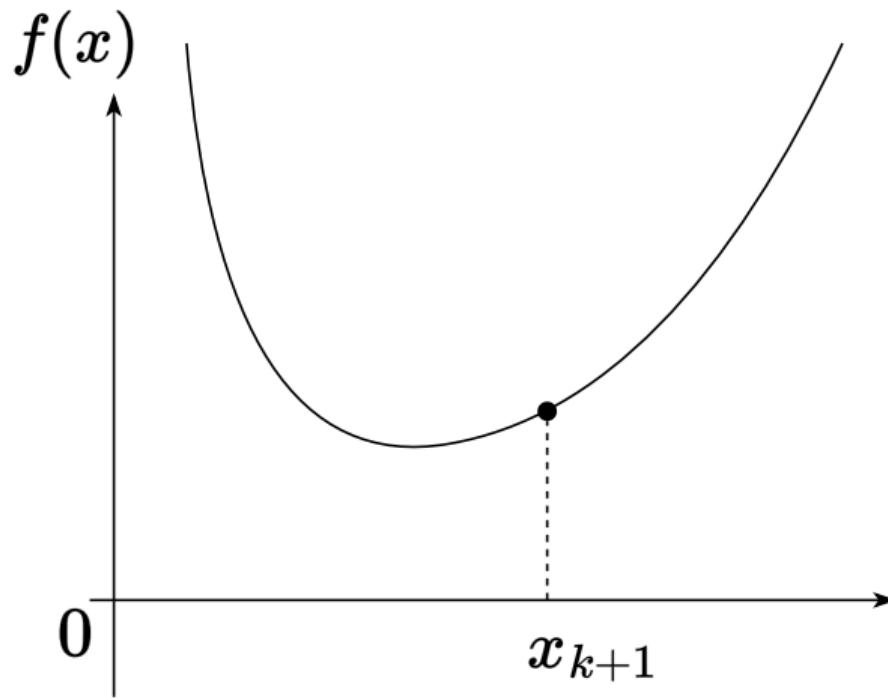
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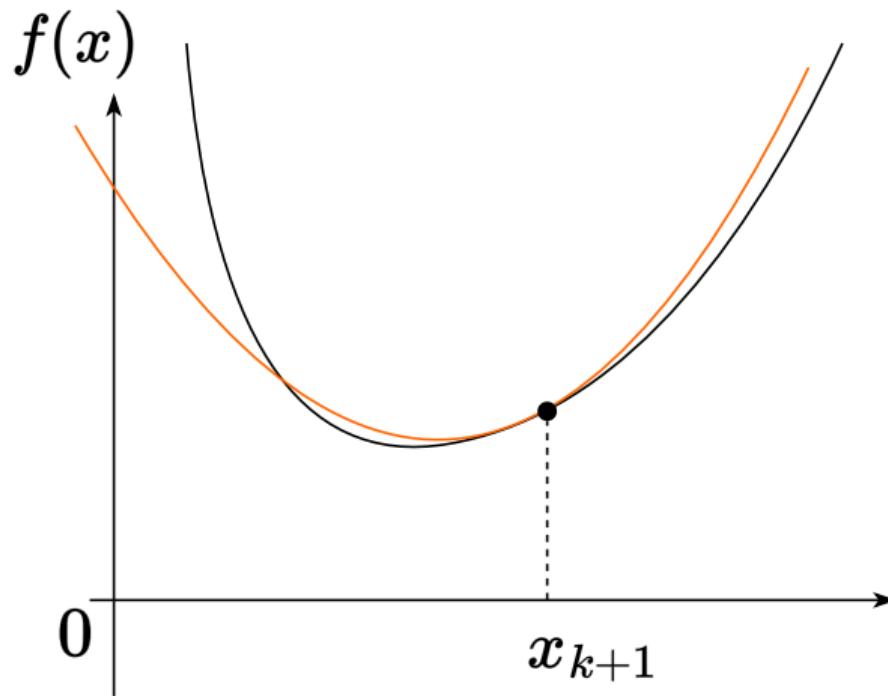
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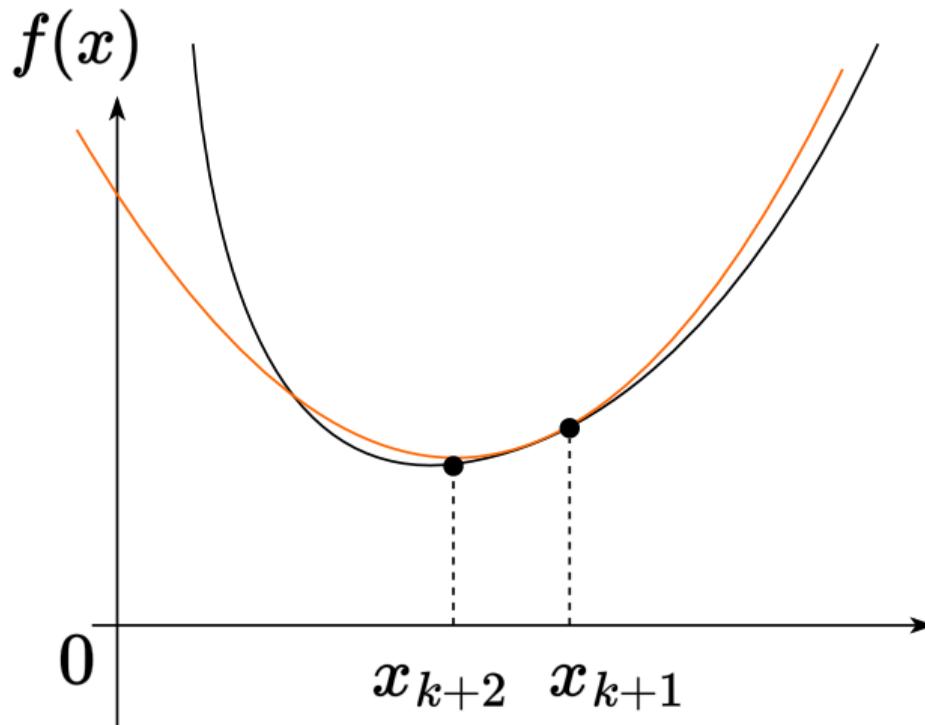
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# Convergence

## 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.

## 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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$$\begin{aligned} y_{k+1} &= y_k - A^{-1} (\nabla^2 f(Ay_k))^{-1} \nabla f(Ay_k) \\ Ay_{k+1} &= Ay_k - (\nabla^2 f(Ay_k))^{-1} \nabla f(Ay_k) \end{aligned}$$

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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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What's nice:

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

## Newton method problems

# Newton

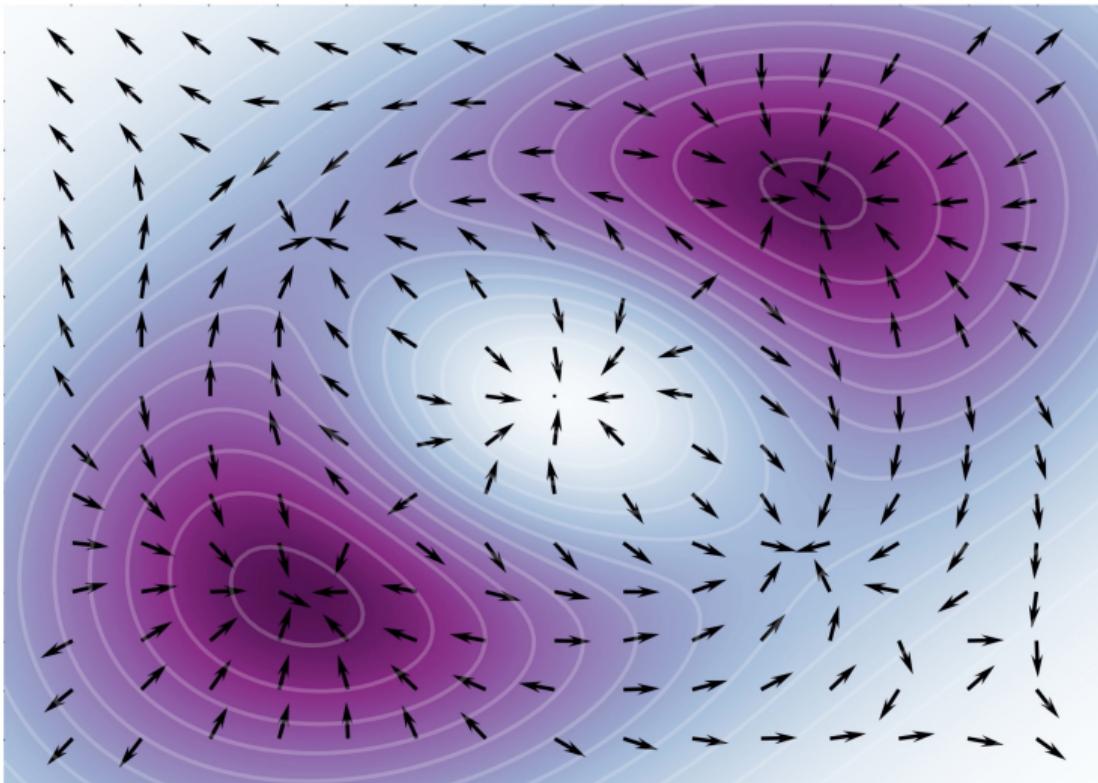


Figure 19: Animation

## Newton method problems

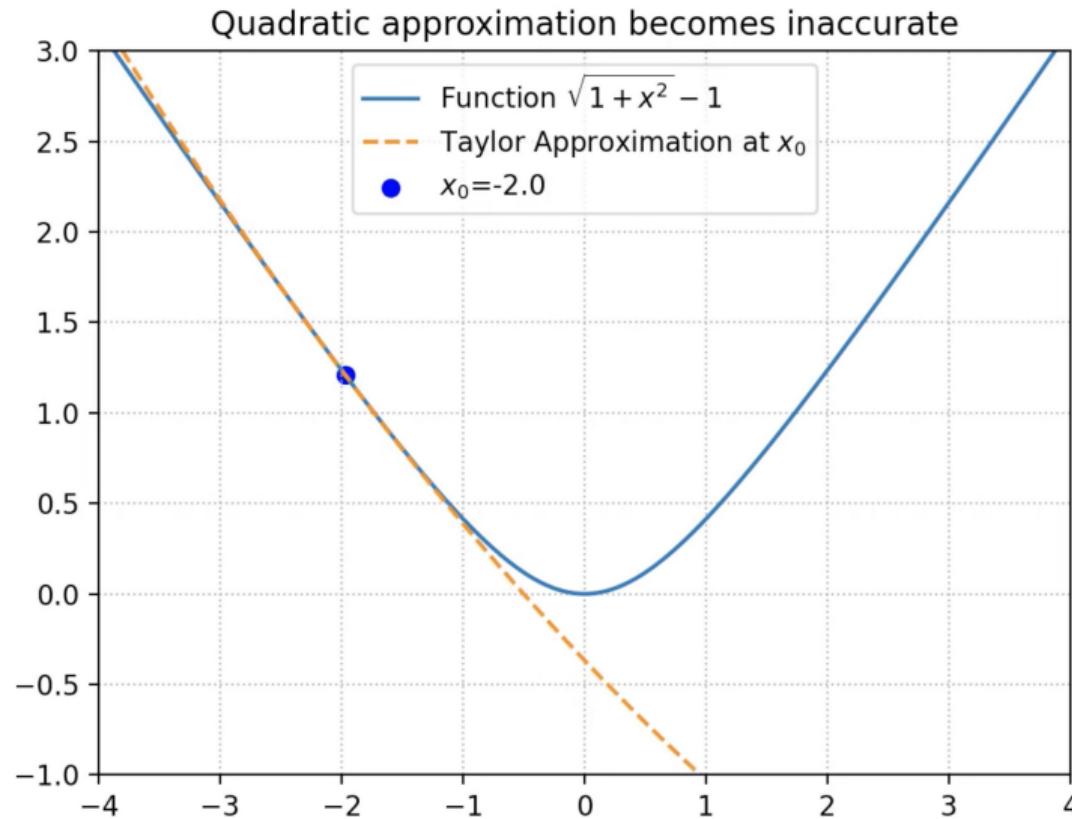


Figure 20: Animation

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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  $k \rightarrow \infty$  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:

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- $B_k \succ 0 \Rightarrow B_{k+1} \succ 0$

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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:

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

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

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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

### Woodbury Formula

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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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