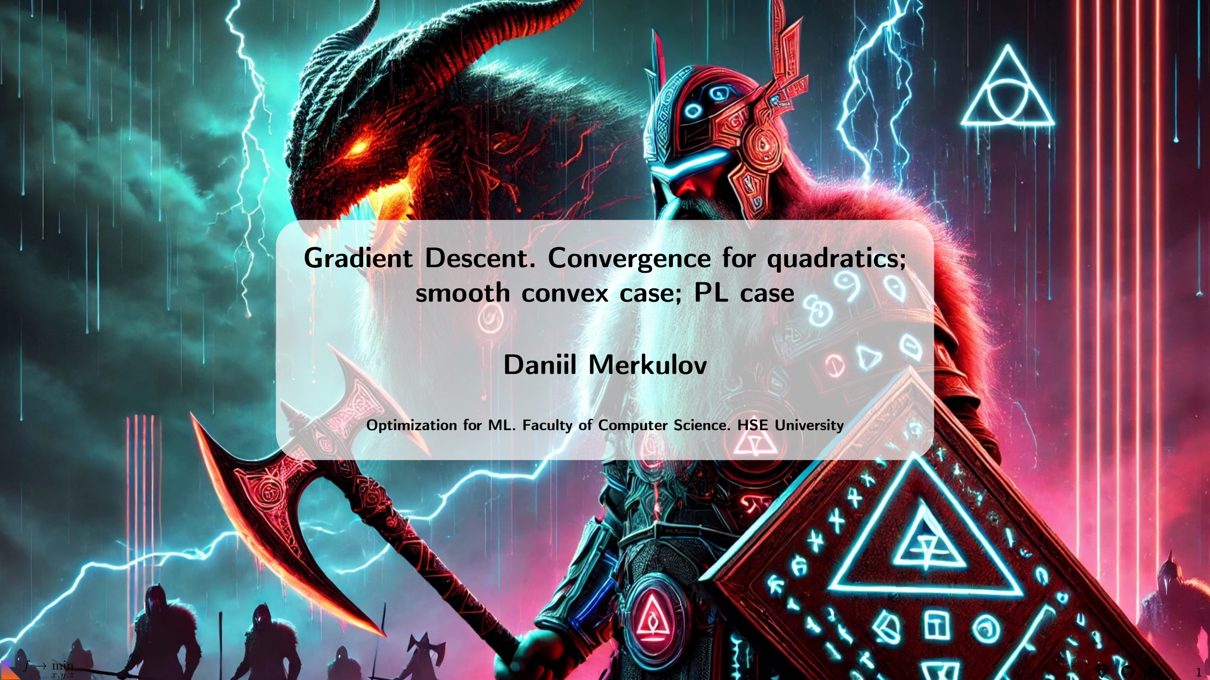

Gradient Descent. Convergence for quadratics; smooth convex case; PL case

Daniil Merkulov

Optimization for ML. Faculty of Computer Science. HSE University

Gradient Descent

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Thus, the direction of the antigradient

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

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

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

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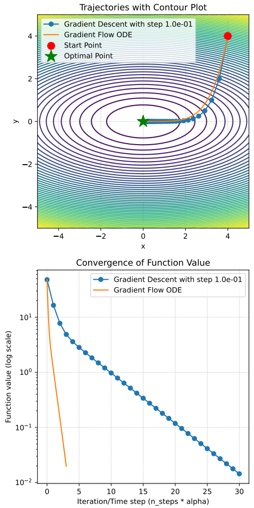
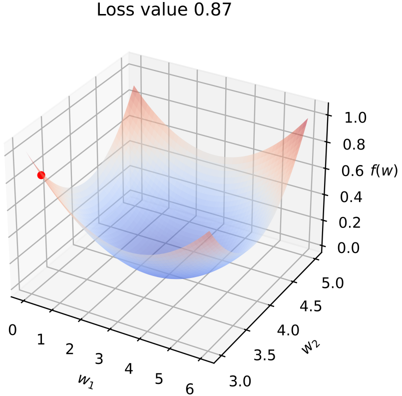
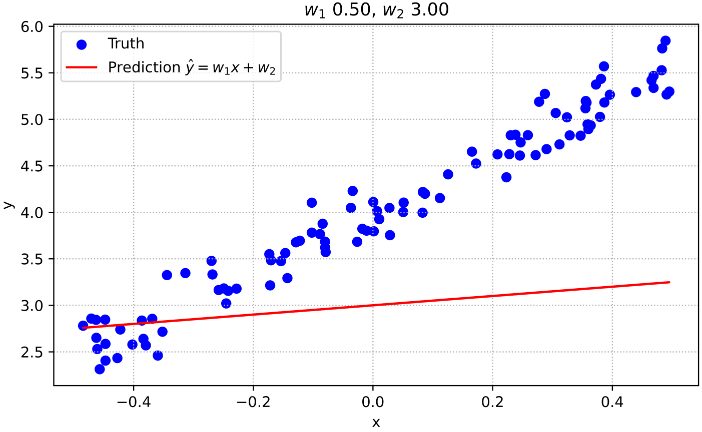


Рисунок 1: Gradient flow trajectory

Convergence of Gradient Descent algorithm

Heavily depends on the choice of the learning rate α:





Exact line search aka steepest descent

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

More theoretical than practical approach. It also allows you to analyze the convergence, but often exact line search can be difficult if the function calculation takes too long or costs a lot. An interesting theoretical property of this method is that each following iteration is orthogonal to the previous one:

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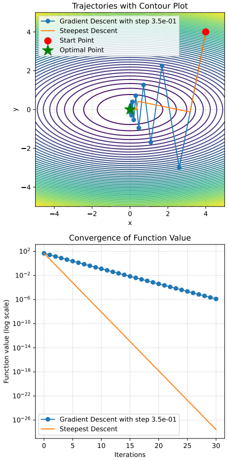

Рисунок 2: Steepest Descent

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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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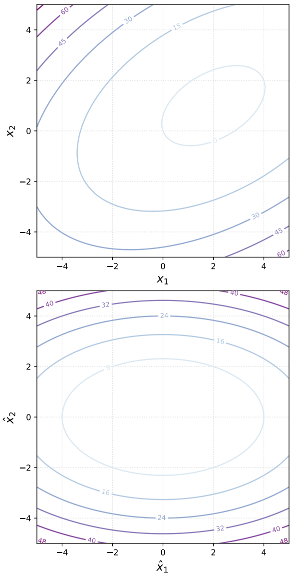

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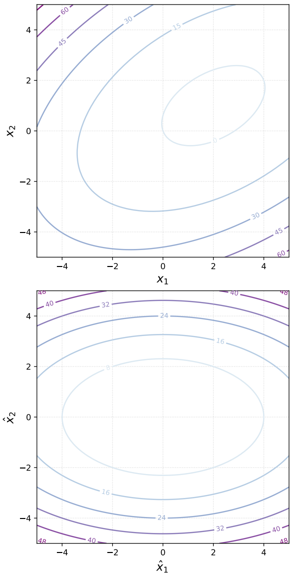

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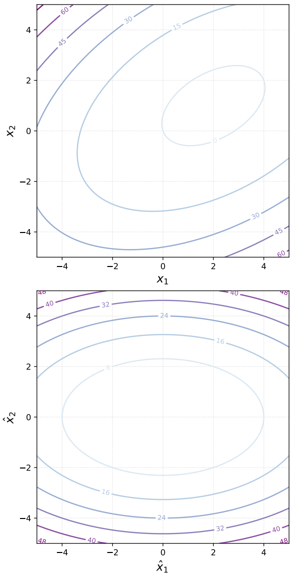

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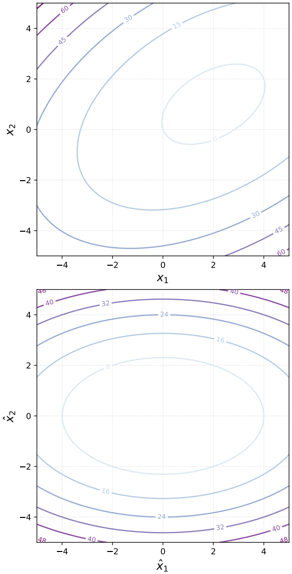

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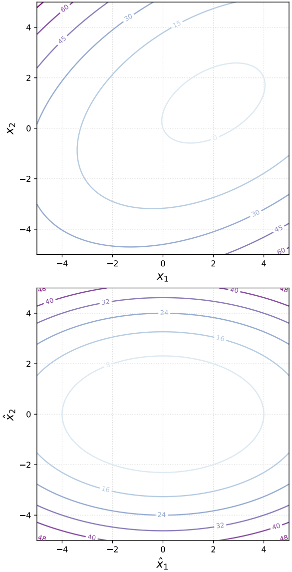

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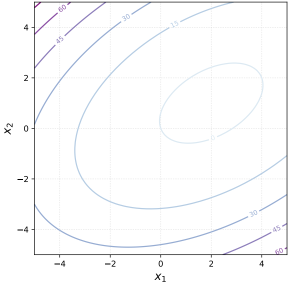

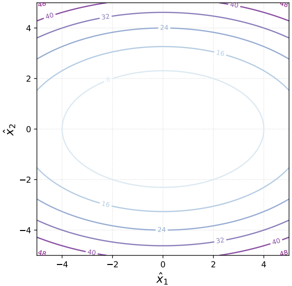

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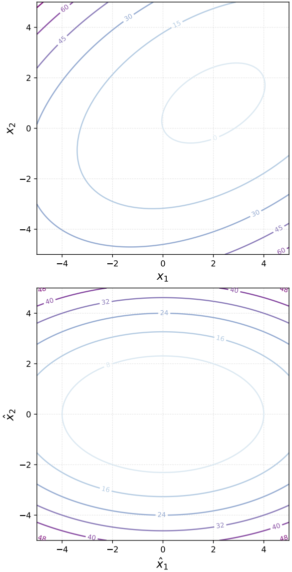

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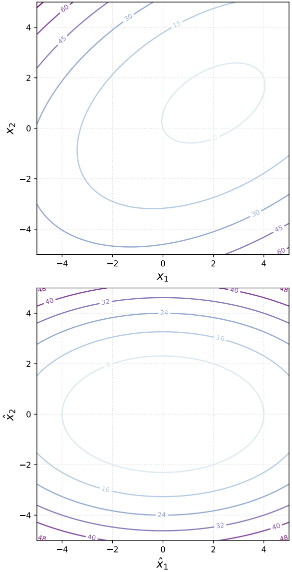

Convergence analysis

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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&= (I - \alpha^k \Lambda) x^k
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x^{k+1}_{(i)} &= (1 - \alpha^k \lambda_{(i)}) x^k_{(i)} \text{ For } i\text{-th coordinate}
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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
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Remember, that $\lambda_{\text{min}} = \mu > 0, \lambda_{\text{max}} = L \geq \mu$.

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

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

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

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&|1 - \alpha\mu| < 1 \\
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&\alpha < \frac{2}{\mu} \qquad \alpha\mu > 0
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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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$\alpha < \frac{2}{L}$ is needed for convergence.

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

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

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x^{k+1}_{(i)} &= \left(\frac{L - \mu}{L + \mu} \right)^k x^0_{(i)} \\
\|x^{k+1}\|_2 &\leq \left(\frac{L - \mu}{L + \mu} \right)^k \|x^0\|_2
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\end{aligned}
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$$
x^{k+1}_{(i)} = \left(\frac{L - \mu}{L + \mu} \right)^k x^0_{(i)}
$$

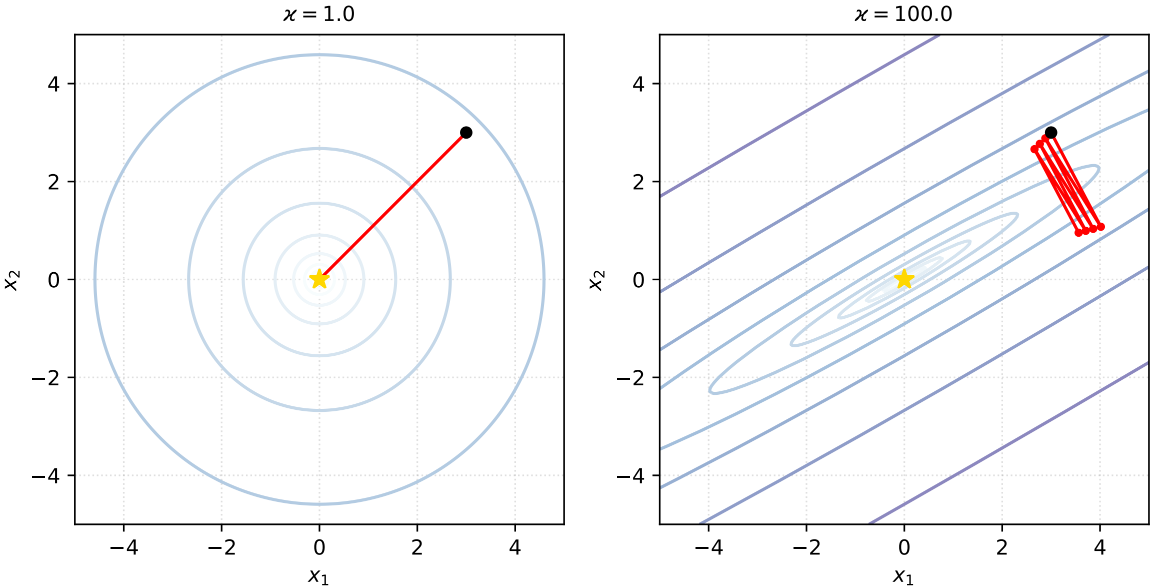
$$
\|x^{k+1}\|_2 \leq \left(\frac{L - \mu}{L + \mu} \right)^k \|x^0\|_2 \quad f(x^{k+1}) \leq \left(\frac{L - \mu}{L + \mu} \right)^{2k} f(x^0
$$

Convergence analysis

So, we have a linear convergence in the domain with rate $\frac{\varkappa-1}{\varkappa+1} = 1 - \frac{2}{\varkappa+1}$, where $\varkappa = \frac{L}{\mu}$ is sometimes called condition number of the quadratic problem.

$\varkappa$	ρ	Iterations to decrease domain gap 10 times	Iterations to decrease function gap 10 times
1.1	0.05	1	1
2	0.33	3	2
5	0.67	6	3
10	0.82	12	6
50	0.96	58	29
100	0.98	116	58
500	0.996	576	288
1000	0.998	1152	576

Condition number $\varkappa$



Polyak-Lojasiewicz smooth case

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

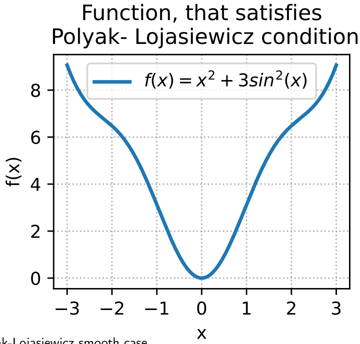
PL inequality holds if the following condition is satisfied for some $\mu > 0$,

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

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

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



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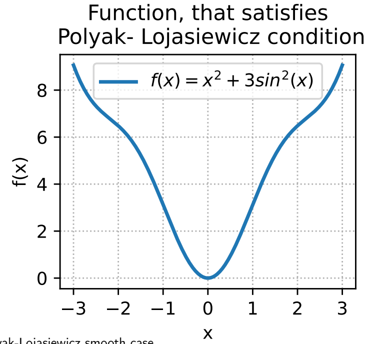
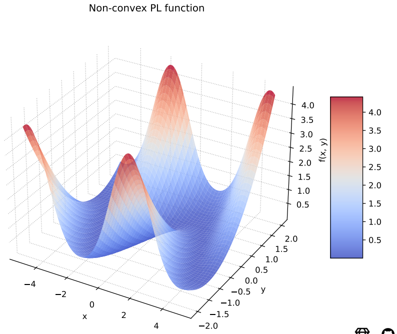
The following functions satisfy the PL condition but are not convex. Link to the code

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

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





Convergence analysis

Theorem

Consider the Problem

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

and assume that f is μ-Polyak-Lojasiewicz and L-smooth, for some $L \geq \mu > 0$.
Consider $(x^k)_{k \in \mathbb{N}}$ a sequence generated by the gradient descent constant stepsize algorithm, with a stepsize satisfying $0 < \alpha \leq \frac{1}{L}$. Then:

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

Convergence analysis

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

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

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

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

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

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

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

Any μ-strongly convex differentiable function is a PL-function

Theorem

If a function $f(x)$ is differentiable and μ-strongly convex, then it is a PL function.

Proof

By first order strong convexity criterion:

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

Putting $y = x^*$:

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

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f(x) - f(x^*) &\leq \nabla f(x)^T(x-x^*) - \frac{\mu}{2}\|x^*-x\|_2^2 = \\
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&= \left(\nabla f(x)^T - \frac{\mu}{2}(x^* - x)\right)^T (x - x^*) = \\
&= \frac{1}{2}\left(\frac{2}{\sqrt{\mu}}\nabla f(x)^T - \sqrt{\mu}(x^* - x)\right)^T \sqrt{\mu}(x - x^*) =
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Let $a = \frac{1}{\sqrt{\mu}}\nabla f(x)$ and
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Let $a = \frac{1}{\sqrt{\mu}}\nabla f(x)$ and
$b = \sqrt{\mu}(x - x^*) - \frac{1}{\sqrt{\mu}}\nabla f(x)$
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Any μ-strongly convex differentiable function is a PL-function

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

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

Smooth convex case

Smooth convex case

Theorem

Consider the Problem

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

and assume that f is convex and L-smooth, for some $L > 0$.
Let $(x^k)_{k \in \mathbb{N}}$ be the sequence of iterates generated by the gradient descent constant stepsize algorithm, with a stepsize satisfying $0 < \alpha \leq \frac{1}{L}$. Then, for all $x^* \in \operatorname{argmin} f$, for all $k \in \mathbb{N}$ we have that

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

Convergence analysis

- As it was before, we first use smoothness:

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

Typically, for the convergent gradient descent algorithm the higher the learning rate the faster the convergence. That is why we often will use $\alpha = \frac{1}{L}$.

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- After that we add convexity:

$$
\tag{2}
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f(y) \geq f(x) + \langle \nabla f(x), y - x \rangle \tag{2}
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f(x^k) - f^* &\leq \langle \nabla f(x^k), x^k - x^* \rangle
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Convergence analysis

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

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Let $a = x^k - x^*$ and $b = x^k - x^* - \alpha \nabla f(x^k)$.

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

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

Convergence analysis

- Now we put Уравнение 2 to Уравнение 1:

$$
\begin{aligned}
f(x^{k+1}) &\leq f(x^k) - \frac{\alpha}{2}\|\nabla f(x^k)\|^2 \leq f^* + \langle \nabla f(x^k), x^k - x^* \rangle - \frac{\alpha}{2}\|\nabla f(x^k)\|^2 \\
&= f^* + \langle \nabla f(x^k), x^k - x^* - \frac{\alpha}{2}\nabla f(x^k) \rangle \\
&= f^* + \frac{1}{2\alpha}\left\langle \alpha \nabla f(x^k), 2\left(x^k - x^* - \frac{\alpha}{2}\nabla f(x^k)\right)\right\rangle
\end{aligned}
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Let $a = x^k - x^*$ and $b = x^k - x^* - \alpha \nabla f(x^k)$. Then $a + b = \alpha \nabla f(x^k)$ and $a - b = 2\left(x^k - x^* - \frac{\alpha}{2}\nabla f(x^k)\right)$.

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

(3)

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Convergence analysis

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

Convergence analysis

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

$$
kf(x^k) \leq \sum_{i=0}^{k-1} f(x^{i+1})
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Convergence analysis

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Convergence analysis

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$$
kf(x^k) \leq \sum_{i=0}^{k-1} f(x^{i+1})
$$

- Now putting it to Уравнение 3:

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

Convergence analysis

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$$

$$
f(x^k) - f^* \leq \frac{\|x^0 - x^*\|_2^2}{2\alpha k}
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$$

$$
f(x^k) - f^* \leq \frac{\|x^0 - x^*\|_2^2}{2\alpha k} \leq \frac{L\|x^0 - x^*\|_2^2}{2k}
$$

Summary

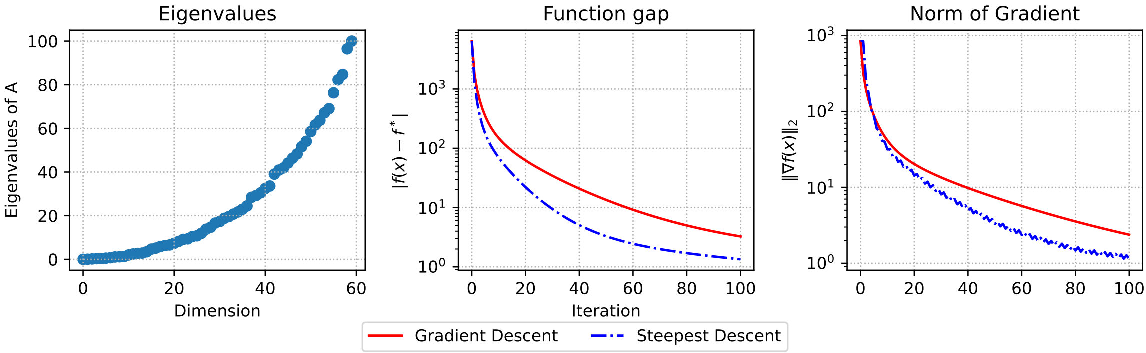
Gradient Descent: $$\min_{x \in \mathbb{R}^n} f(x) \qquad x^{k+1} = x^k - \alpha^k \nabla f(x^k)$$

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

Numerical experiments

$$f(x) = \frac{1}{2}x^T A x - b^T x \to \min_{x \in \mathbb{R}^n}$$

Convex quadratics. n=60, random matrix.



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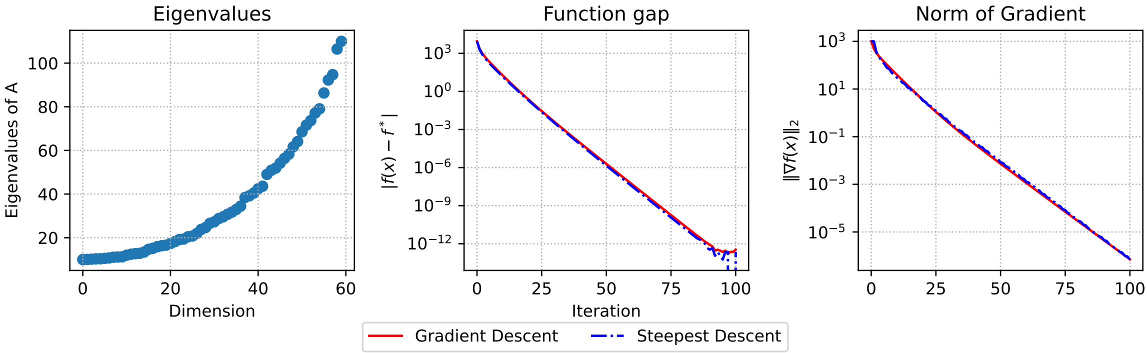
$$f(x) = \frac{1}{2}x^T A x - b^T x \to \min_{x \in \mathbb{R}^n}$$

Strongly convex quadratics. n=60, random matrix.



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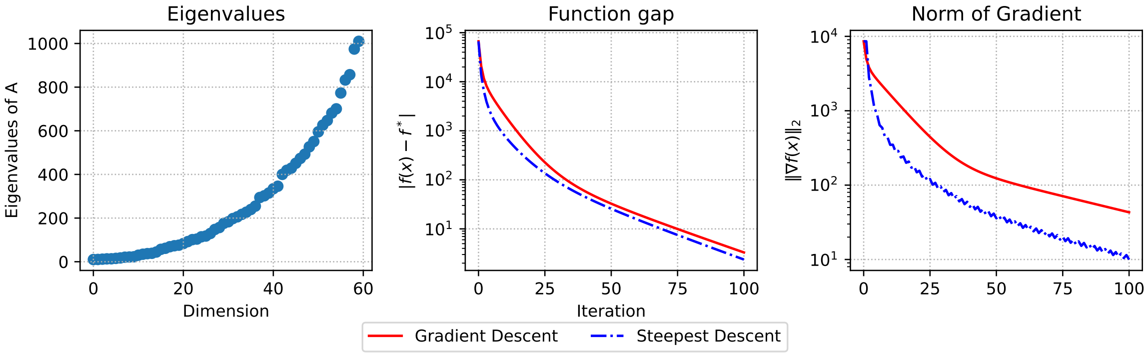
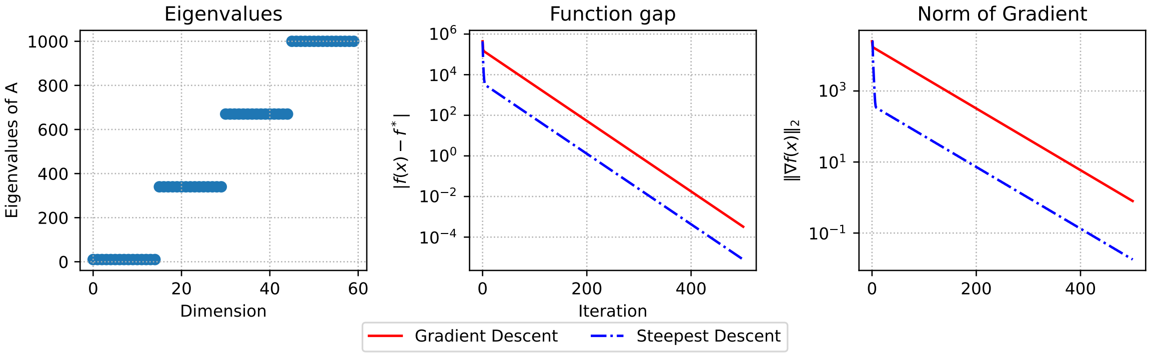


Numerical experiments

$$
f(x) = \frac{1}{2}x^T A x - b^T x \to \min_{x \in \mathbb{R}^n}
$$

Strongly convex quadratics. n=60, clustered matrix.



Numerical experiments

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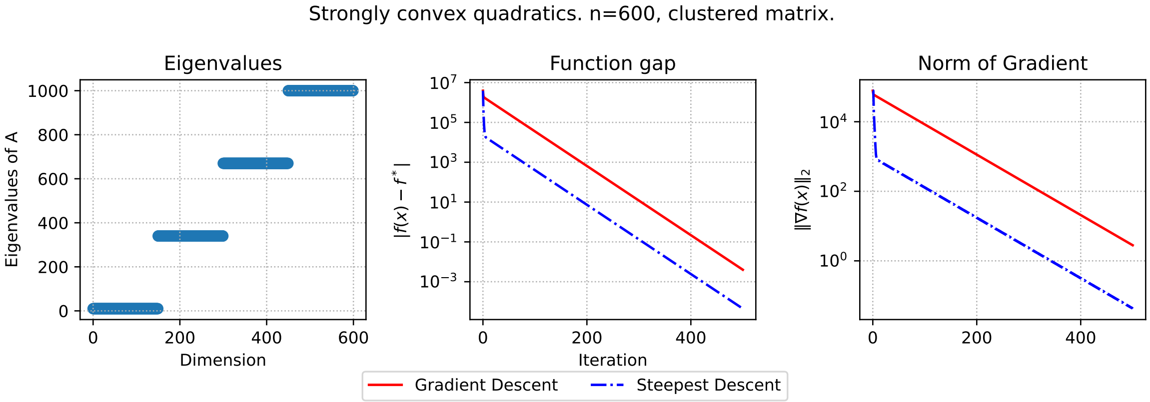
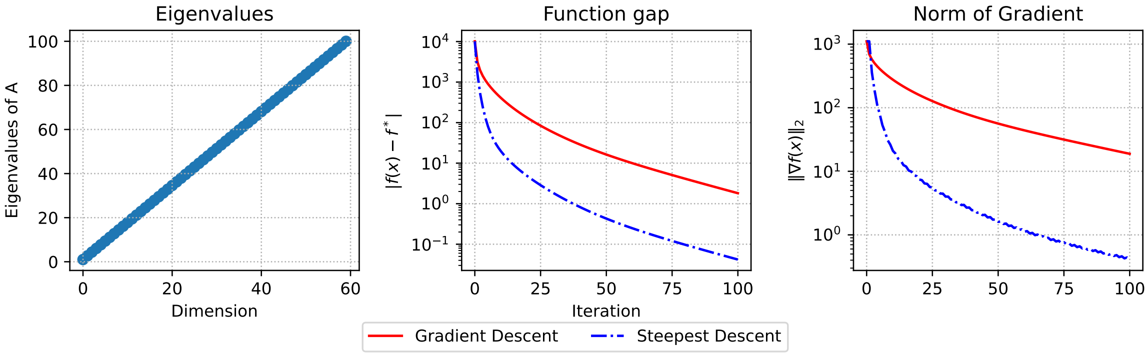
f(x) = \frac{1}{2}x^T A x - b^T x \to \min_{x \in \mathbb{R}^n}
$$



Numerical experiments

$$
f(x) = \frac{1}{2}x^T A x - b^T x \to \min_{x \in \mathbb{R}^n}
$$

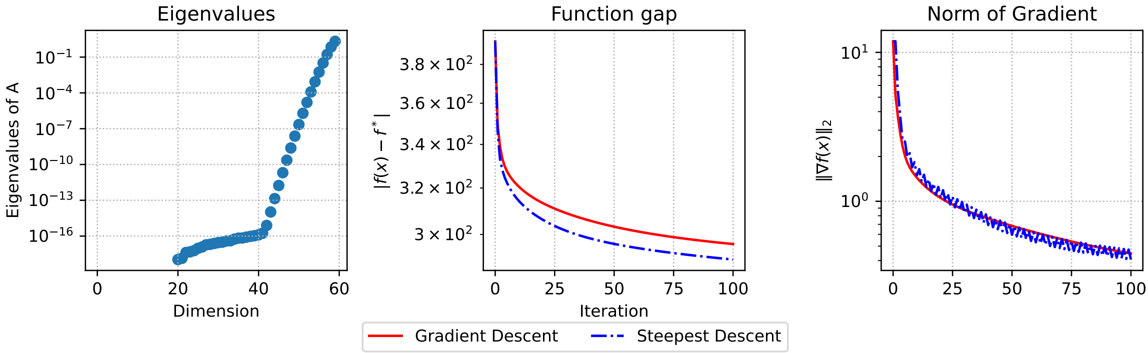
Strongly convex quadratics. n=60, uniform spectrum matrix.



Numerical experiments

$$
f(x) = \frac{1}{2}x^T A x - b^T x \to \min_{x \in \mathbb{R}^n}
$$

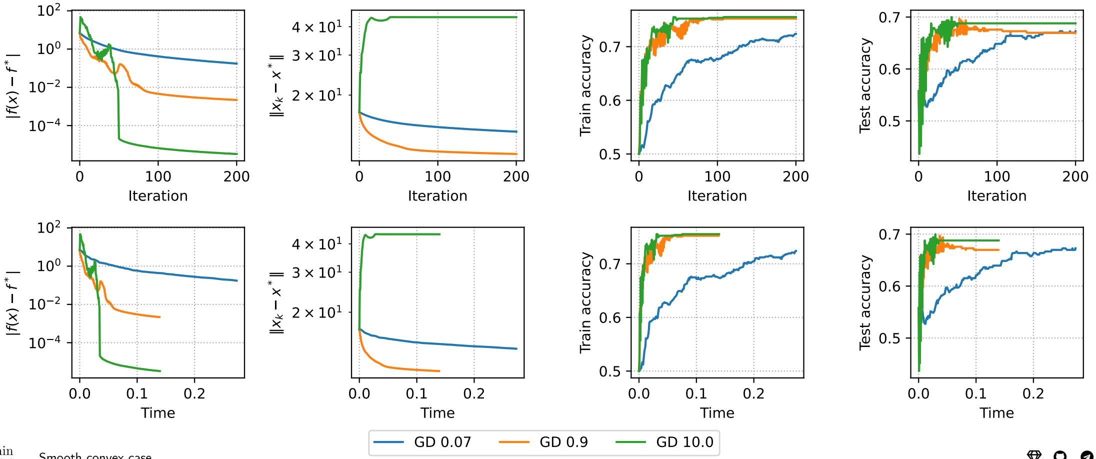
Strongly convex quadratics. n=60, Hilbert matrix.



Numerical experiments

$$f(x) = \frac{\mu}{2}\|x\|_2^2 + \frac{1}{m}\sum_{i=1}^{m}\log(1+\exp(-y_i\langle a_i, x\rangle)) \to \min_{x\in\mathbb{R}^n}$$

Convex binary logistic regression. mu=0.



Numerical experiments

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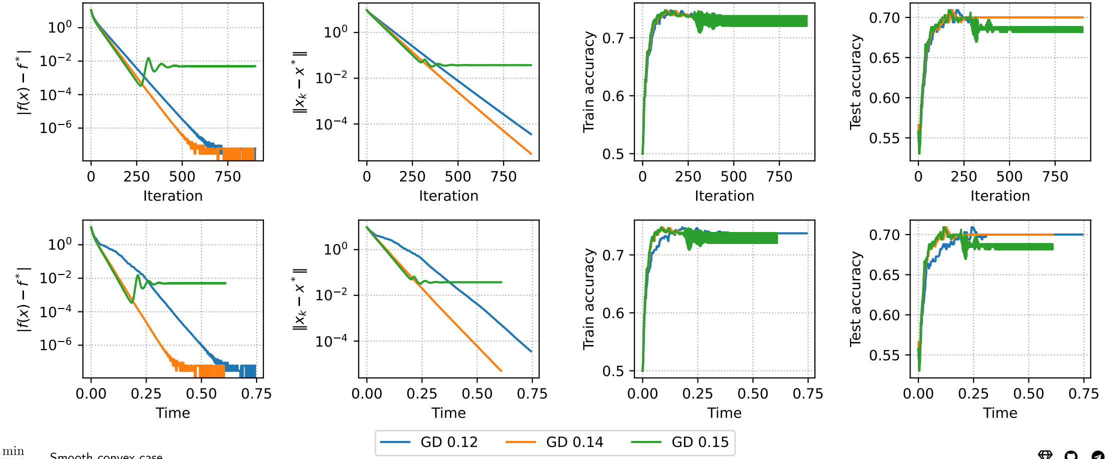
f(x) = \frac{\mu}{2}\|x\|_2^2 + \frac{1}{m}\sum_{i=1}^{m}\log(1+\exp(-y_i\langle a_i, x\rangle)) \to \min_{x\in\mathbb{R}^n}
$$

Strongly convex binary logistic regression. mu=0.1.



Numerical experiments

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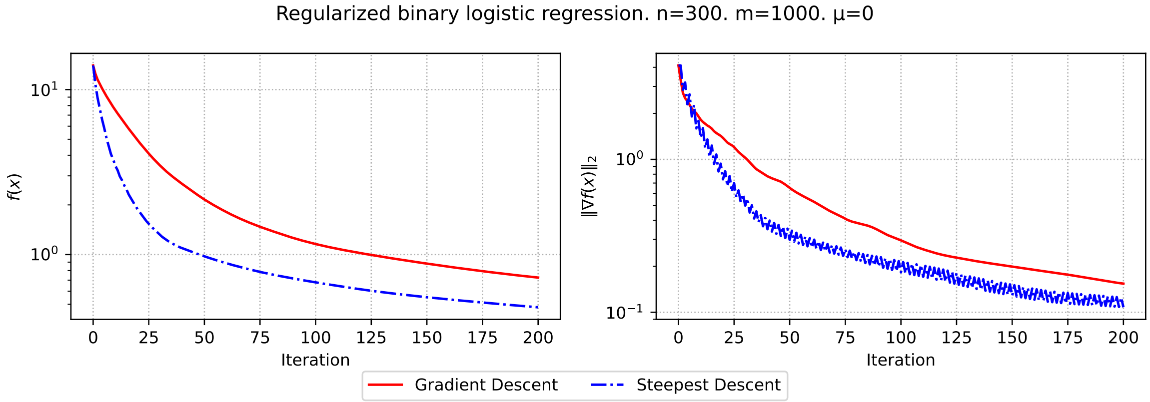
f(x) = \frac{\mu}{2}\|x\|_2^2 + \frac{1}{m}\sum_{i=1}^{m}\log(1+\exp(-y_i\langle a_i, x\rangle)) \to \min_{x\in\mathbb{R}^n}
$$



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