Gradient Descent. Non-smooth case. Linear Least squares with l_1-regularization.

Daniil Merkulov

Optimization methods. MIPT

Previously

- Gradient Descent. Convergence for strongly convex quadratic function. Optimal hyperparameters.

$$\alpha = \frac{2}{\mu + L} \quad \varkappa = \frac{L}{\mu} \geq 1 \quad \rho = \frac{\varkappa - 1}{\varkappa + 1}$$

$$\|x_k - x^*\| \leq \rho^k \|x_0 - x^*\|$$

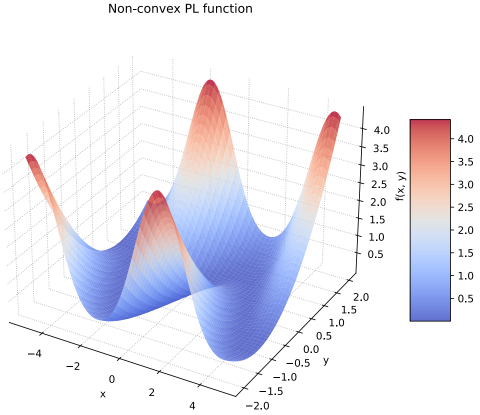

Figure 1: PL function

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- Gradient Descent. Smooth convex case convergence.

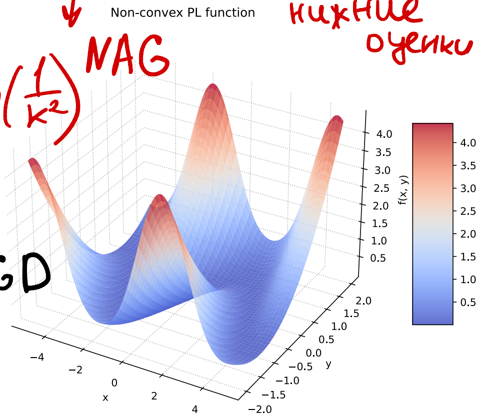
$$f(x_k) - f^* \leq \frac{L\|x_0 - x^*\|^2}{2k}.$$

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

лучше, что возможн.

нижние оценки

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



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- Gradient Descent. Smooth PL case convergence.

$$f(x_k) - f^* \leq \left(1 - \frac{\mu}{L}\right)^k (f(x_0) - f^*).$$

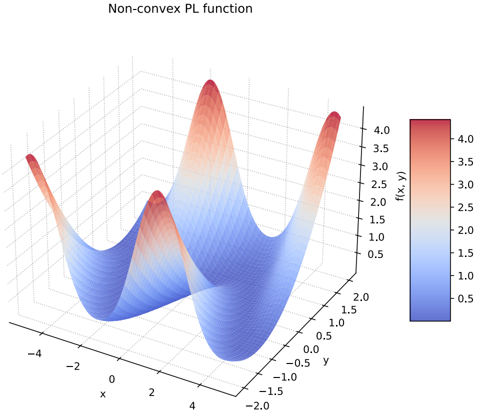

Figure 1: PL function

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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$$\begin{aligned}
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f(x) - f(x^*) &\leq \nabla f(x)^T(x - x^*) - \frac{\mu}{2}\|x^* - x\|_2^2 = \\
&= \left(\nabla f(x)^T - \frac{\mu}{2}(x^* - x)\right)^T (x - x^*) =
\end{aligned}$$

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

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

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

$a - b$ $\qquad$ $a + b$

Let $a = \frac{1}{\sqrt{\mu}}\nabla f(x)$ and
$b = \sqrt{\mu}(x - x^*) - \frac{1}{\sqrt{\mu}}\nabla f(x)$
Then $a + b = \sqrt{\mu}(x - x^*)$ and
$a - b = \frac{2}{\sqrt{\mu}}\nabla f(x) - \sqrt{\mu}(x - x^*)$

$\|x^* - x\|^2 = (x^* - x)^T (x^* - x)$

$a^2 - b^2$

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

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

which is exactly PL-condition. It means, that we already have linear convergence proof for any strongly convex function.

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

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

which is exactly PL-condition. It means, that we already have linear convergence proof for any strongly convex function.

Non-smooth optimization

$\|x\|_p \leq t$

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

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

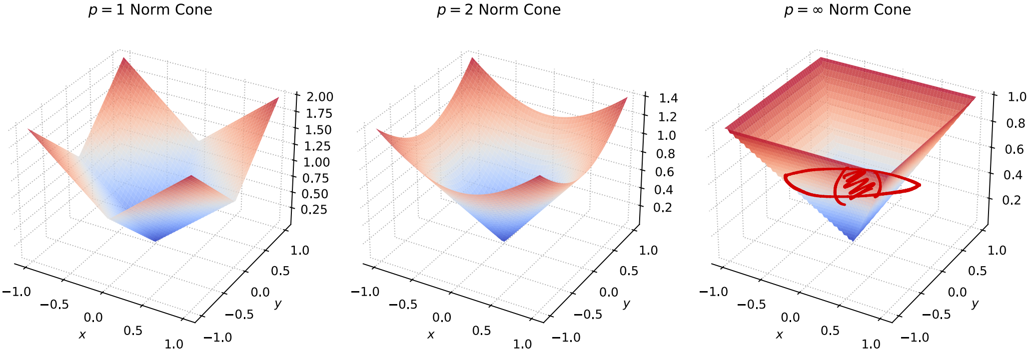

Figure 2: Norm cones for different p - norms are non-smooth

Non-smooth optimization

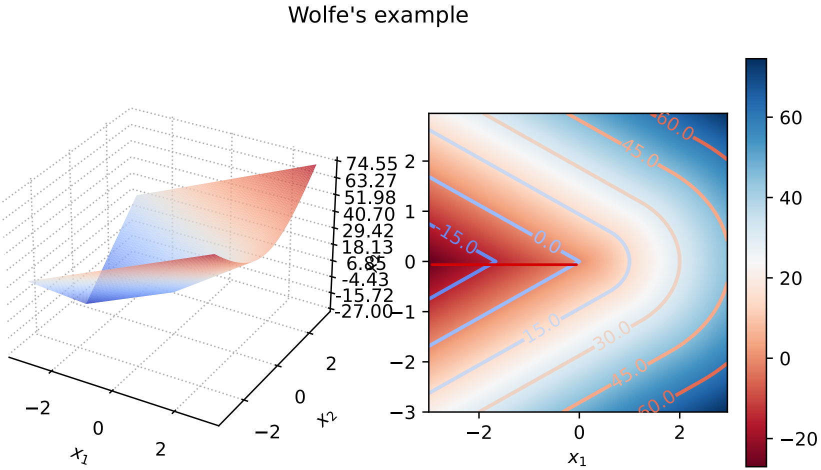

Figure 3: Wolfe's example. Open in Colab

Algorithm

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

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

Algorithm

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

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

$$g^T(x - x_0) \leq f(x) - f(x_0)$$

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:

$$x_{k+1} = x_k - \alpha_k g_k, \qquad \text{(SD)}$$

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 bound

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

$$\|x_{k+1} - x^*\|^2 = \|x_k - x^* - \alpha_k g_k\|^2 =$$

Convergence bound

$$
\begin{aligned}
\|x_{k+1} - x^*\|^2 &= \|x_k - x^* - \alpha_k g_k\|^2 = \\
&= \|x_k - x^*\|^2 + \alpha_k^2 \|g_k\|^2 - 2\alpha_k \langle g_k, x_k - x^* \rangle
\end{aligned}
$$

Convergence bound

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2\alpha_k \langle g_k, x_k - x^* \rangle &= \|x_k - x^*\|^2 + \alpha_k^2 \|g_k\|^2 - \|x_{k+1} - x^*\|^2
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Let us sum the obtained equality for $k = 0, \ldots, T-1$:

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&\leq \|x_0 - x^*\|^2 + \sum_{k=0}^{T-1} \alpha_k^2 \|g_k\|^2
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&\leq \|x_0 - x^*\|^2 + \sum_{k=0}^{T-1} \alpha_k^2 \|g_k^2\| \\
&\leq R^2 + G^2 \sum_{k=0}^{T-1} \alpha_k^2
\end{aligned}
$$

$$\|g_k\|^2 \leq G^2 \quad \forall k$$

$$\max_k \|g_k\| = G$$

$$\|x_0 - x^*\| = R$$

Convergence bound

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- Let's write down how close we came to the optimum $x^* = \text{arg} \min\limits_{x \in \mathbb{R}^n} f(x) = \text{arg} f^*$ on the last iteration:

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Let us sum the obtained equality for $k = 0, \ldots, T-1$:

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$$
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Convergence bound

$$\|x_{k+1} - x^*\|^2 = \|x_k - x^* - \alpha_k g_k\|^2 =$$
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$$\leq \|x_0 - x^*\|^2 + \sum_{k=0}^{T-1} \alpha_k^2 \|g_k^2\|$$
$$\leq R^2 + G^2 \sum_{k=0}^{T-1} \alpha_k^2$$

- Let's write down how close we came to the optimum $x^* = \text{arg} \min\limits_{x \in \mathbb{R}^n} f(x) = \text{arg} f^*$ on the last iteration:
- For a subgradient: $\langle g_k, x_k - x^* \rangle \leq f(x_k) - f(x^*) = f(x_k) - f^*$.
- We additionaly assume, that $\|g_k\|^2 \leq G^2$
- We use the notation $R = \|x_0 - x^*\|_2$

Convergence bound

Assuming $\boxed{\alpha_k = \alpha}$ (constant stepsize), we have:

$$\sum_{k=0}^{T-1} \langle g_k, x_k - x^* \rangle \leq \frac{R^2}{2\alpha} + \frac{\alpha}{2} G^2 T$$

Convergence bound

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$$\sum_{k=0}^{T-1} \langle g_k, x_k - x^* \rangle \leq \frac{R^2}{2\alpha} + \frac{\alpha}{2} G^2 T$$

$$\frac{R^2}{2\alpha^*} = \frac{\alpha^* G^2 T}{2}$$

Minimizing the right-hand side by α gives $\boxed{\alpha^* = \frac{R}{G}\sqrt{\frac{1}{T}}}$ and

$$\sum_{k=0}^{T-1} \langle g_k, x_k - x^* \rangle \leq GR\sqrt{T}.$$

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$$\sum_{k=0}^{T-1} \langle g_k, x_k - x^* \rangle \leq GR\sqrt{T}.$$

$$f(\overline{x}) - f^* = f\left(\frac{1}{T}\sum_{k=0}^{T-1} x_k\right) - f^* \leq \frac{1}{T}\left(\sum_{k=0}^{T-1}(f(x_k) - f^*)\right)$$

Введём $\overline{x} = \frac{1}{T}\sum_{k=0}^{T-1} x_k$

$f(\overline{x}) - f^* =$

$= f$

$\leq \frac{1}{T}\sum_{k=0}^{T-1} f(x_k)$

нер-во Йенсена

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$$\sum_{k=0}^{T-1} \langle g_k, x_k - x^* \rangle \leq \frac{R^2}{2\alpha} + \frac{\alpha}{2} G^2 T$$

Minimizing the right-hand side by α gives $\alpha^* = \dfrac{R}{G}\sqrt{\dfrac{1}{T}}$ and

$\sum\limits_{k=0}^{T-1} \langle g_k, x_k - x^* \rangle \leq GR\sqrt{T}$.

$$f(\overline{x}) - f^* = f\left(\frac{1}{T} \sum_{k=0}^{T-1} x_k \right) - f^* \leq \frac{1}{T} \left(\sum_{k=0}^{T-1} (f(x_k) - f^*) \right)$$

$$\leq \frac{1}{T} \left(\sum_{k=0}^{T-1} \langle g_k, x_k - x^* \rangle \right)$$

по опр. субградиента.

Convergence bound

Assuming $\alpha_k = \alpha$ (constant stepsize), we have:

$$\sum_{k=0}^{T-1} \langle g_k, x_k - x^* \rangle \leq \frac{R^2}{2\alpha} + \frac{\alpha}{2} G^2 T$$

Minimizing the right-hand side by α gives $\alpha^* = \frac{R}{G}\sqrt{\frac{1}{T}}$ and

$\sum\limits_{k=0}^{T-1} \langle g_k, x_k - x^* \rangle \leq GR\sqrt{T}$.

$$\begin{aligned} f(\overline{x}) - f^* = f\left(\frac{1}{T} \sum_{k=0}^{T-1} x_k \right) - f^* &\leq \frac{1}{T} \left(\sum_{k=0}^{T-1} (f(x_k) - f^*) \right) \\ &\leq \frac{1}{T} \left(\sum_{k=0}^{T-1} \langle g_k, x_k - x^* \rangle \right) \\ &\leq GR \frac{1}{\sqrt{T}} \end{aligned}$$

Convergence bound

Assuming $\alpha_k = \alpha$ (constant stepsize), we have:

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&\leq GR \frac{1}{\sqrt{T}}
\end{aligned}
$$

$f(x) \geq f(x_k) + \langle g_k, x - x_k \rangle$

$f(x_k) - f(x) \leq \langle g_k, x_k - x$

$|x|$

jnp.sign =

$$= \begin{cases} 1, & x > 0 \\ 0, & x = 0 \\ -1, & x < 0 \end{cases}$$

Convergence bound

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Important notes:

- Obtaining bounds not for x_T but for the arithmetic mean over iterations $\overline{x}$ is a typical trick in obtaining estimates for methods where there is convexity but no monotonic decreasing at each iteration. There is no guarantee of success at each iteration, but there is a guarantee of success on average

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Important notes:

- Obtaining bounds not for x_T but for the arithmetic mean over iterations $\overline{x}$ is a typical trick in obtaining estimates for methods where there is convexity but no monotonic decreasing at each iteration. There is no guarantee of success at each iteration, but there is a guarantee of success on average
- To choose the optimal step, we need to know (assume) the number of iterations in advance. Possible solution: initialize T with a small value, after reaching this number of iterations double T and restart the algorithm. A more intelligent way: adaptive selection of stepsize.

Steepest subgradient descent convergence bound

$$\|x_{k+1} - x^*\|^2 = \|x_k - x^* - \alpha_k g_k\|^2 =$$

Steepest subgradient descent convergence bound

$$
\begin{aligned}
\|x_{k+1} - x^*\|^2 = \|x_k - x^* - \alpha_k g_k\|^2 = \\
= \|x_k - x^*\|^2 + \alpha_k^2 \|g_k\|^2 - 2\alpha_k \langle g_k, x_k - x^* \rangle \stackrel{\circ}{=}
\end{aligned}
$$

Steepest subgradient descent convergence bound

$\not\alpha \langle \alpha_k \|g_k\|^2 = \not\alpha \langle \quad \rangle$

$$
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\|x_{k+1} - x^*\|^2 &= \|x_k - x^* - \alpha_k g_k\|^2 = \\
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&\circeq \|x_k - x^*\|^2 - \frac{\langle g_k, x_k - x^* \rangle^2}{\|g_k\|^2}
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&\doteq \|x_k - x^*\|^2 - \frac{\langle g_k, x_k - x^* \rangle^2}{\|g_k\|^2} \\
\langle g_k, x_k - x^* \rangle^2 &= \left(\|x_k - x^*\|^2 - \|x_{k+1} - x^*\|^2 \right) \|g_k\|^2 \leq \left(\|x_k - x^*\|^2 - \|x_{k+1} - x^*\|^2 \right) G^2
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\sum_{k=0}^{T-1} \langle g_k, x_k - x^* \rangle^2 &\leq \sum_{k=0}^{T-1} \left(\|x_k - x^*\|^2 - \|x_{k+1} - x^*\|^2 \right) G^2 \leq \left(\|x_0 - x^*\|^2 - \|x_T - x^*\|^2 \right) G^2
\end{aligned}
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$$\sum_{k=0}^{T-1} \langle g_k, x_k - x^* \rangle^2 \le \sum_{k=0}^{T-1} \left(\|x_k - x^*\|^2 - \|x_{k+1} - x^*\|^2\right) G^2 \le \left(\|x_0 - x^*\|^2 - \|x_T - x^*\|^2\right) G^2$$

$$\frac{1}{T}\left(\sum_{k=0}^{T-1} \langle g_k, x_k - x^* \rangle\right)^2 \le \sum_{k=0}^{T-1} \langle g_k, x_k - x^* \rangle^2 \le R^2 G^2 \qquad \sum_{k=0}^{T-1} \langle g_k, x_k - x^* \rangle \le GR\sqrt{T}$$

$$\frac{\left(\sum x_i\right)^2}{T} \le \sum x_i^2$$

$f(x) = x^2$ Иенсен

$$f\left(\frac{1}{T}\sum_i x_i\right) \le \frac{1}{T}\sum f_i$$

$$\left(\frac{1}{T}\sum x_i\right)^2 \le \frac{1}{T}\sum x_i^2$$

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\sum_{k=0}^{T-1} \langle g_k, x_k - x^* \rangle^2 &\leq \sum_{k=0}^{T-1} \left(\|x_k - x^*\|^2 - \|x_{k+1} - x^*\|^2\right) G^2 \leq \left(\|x_0 - x^*\|^2 - \|x_T - x^*\|^2\right) G^2 \\
\frac{1}{T}\left(\sum_{k=0}^{T-1} \langle g_k, x_k - x^* \rangle\right)^2 &\leq \sum_{k=0}^{T-1} \langle g_k, x_k - x^* \rangle^2 \leq R^2 G^2 \qquad \sum_{k=0}^{T-1} \langle g_k, x_k - x^* \rangle \leq GR\sqrt{T}
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\frac{1}{T} \left(\sum_{k=0}^{T-1} \langle g_k, x_k - x^* \rangle \right)^2 &\leq \sum_{k=0}^{T-1} \langle g_k, x_k - x^* \rangle^2 \leq R^2 G^2 \qquad \sum_{k=0}^{T-1} \langle g_k, x_k - x^* \rangle \leq GR\sqrt{T}
\end{aligned}
$$

Which leads to exactly the same bound of $\mathcal{O}\left(\frac{1}{\sqrt{T}}\right)$ on the primal gap. In fact, for this class of functions, you can't get a better result than $\frac{1}{\sqrt{T}}$.

Linear Least Squares with l_1-regularization

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

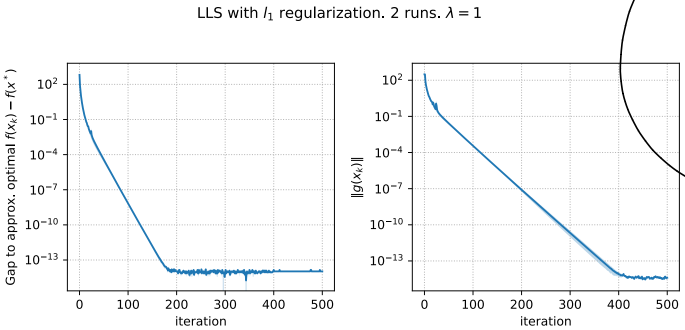
$$g_k = 2 \cdot \frac{1}{2} A^T (Ax_k - b) + \lambda \cdot \text{sign}(x_k)$$

Algorithm will be written as:

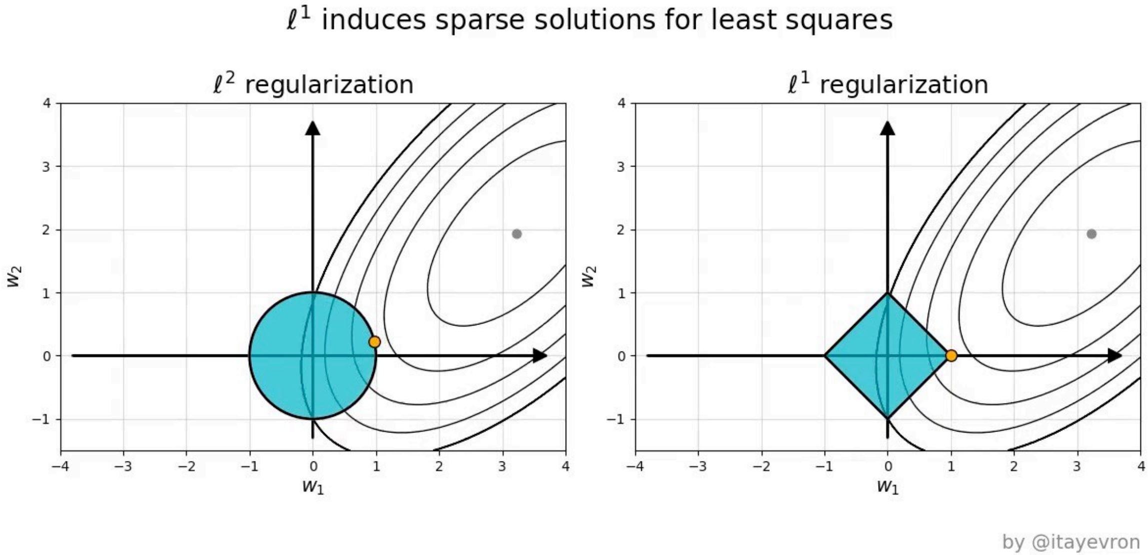
$$x_{k+1} = x_k - \alpha_k \left(A^\top (Ax_k - b) + \lambda \text{sign}(x_k) \right)$$

where signum function is taken element-wise.

$$\frac{1}{\sqrt{k}}$$



Great illustration of l_1-regularization



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 $\omega \in \mathbb{R}^n$ and $b \in \mathbb{R}$ such that

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