

Proximal Gradient Method.

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Методы Оптимизации в Машинном Обучении. ФКН ВШЭ

Subgradient method

Non-smooth problems

ℓ_1 induces sparsity

ℓ_2 regularization. $\|Xw - y\|_2^2 \rightarrow \min_{\|w\|_2 \leq 1}$



ℓ_1 regularization. $\|Xw - y\|_2^2 \rightarrow \min_{\|w\|_1 \leq 1}$



@fminxyz

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$$x_{k+1} = x_k - \alpha_k g_k, \quad g_k \in \partial f(x_k)$$

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convex (non-smooth)

$$f(x_k) - f^* \sim \mathcal{O}\left(\frac{1}{\sqrt{k}}\right)$$
$$k_\varepsilon \sim \mathcal{O}\left(\frac{1}{\varepsilon^2}\right)$$

strongly convex (non-smooth)

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

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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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$$\begin{aligned}\frac{x_{k+1} - x_k}{\alpha} &= -\nabla f(x_{k+1}) \\ \frac{x_{k+1} - x_k}{\alpha} + \nabla f(x_{k+1}) &= 0\end{aligned}$$

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! Proximal operator

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Proximal operator visualization

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



Рисунок 1: Source

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

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From projections to proximity

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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

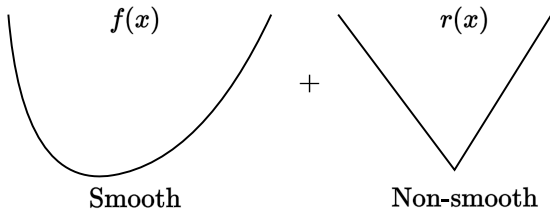
Regularized / Composite Objectives

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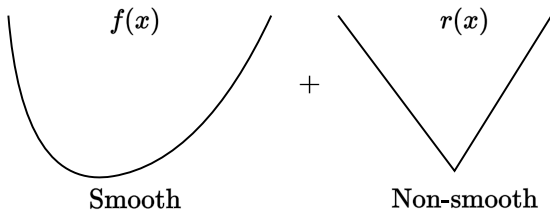
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- **Lasso, L1-LS, compressed sensing**

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

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

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



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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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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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Proximal operators examples

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

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

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

$$\text{prox}_r(x_k - \alpha \nabla f(x_k)) = \text{proj}_r(x_k - \alpha \nabla f(x_k))$$

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Let $r : \mathbb{R}^n \rightarrow \mathbb{R} \cup \{+\infty\}$ be a convex function for which prox_r is defined. If there exists such an $\hat{x} \in \mathbb{R}^n$ that $r(\hat{x}) < +\infty$. Then, the proximal operator is uniquely defined (i.e., it always returns a single unique value).

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It is strongly convex, meaning it has exactly one unique minimum (the existence of \hat{x} is necessary for $r(\tilde{x}) + \frac{1}{2}\|x - \tilde{x}\|_2^2$ to take a finite value somewhere).

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Let $r : \mathbb{R}^n \rightarrow \mathbb{R} \cup \{+\infty\}$ be a convex function for which prox_r is defined. Then, for any $x, y \in \mathbb{R}^n$, the following three conditions are equivalent:

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1. Let's establish the equivalence between the first and second conditions. The first condition can be rewritten as

$$y = \arg \min_{\tilde{x} \in \mathbb{R}^d} \left(r(\tilde{x}) + \frac{1}{2} \|x - \tilde{x}\|^2 \right).$$

From the optimality condition for the convex function r , this is equivalent to:

$$0 \in \partial \left(r(\tilde{x}) + \frac{1}{2} \|x - \tilde{x}\|^2 \right) \Big|_{\tilde{x}=y} = \partial r(y) + y - x.$$

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2. From the definition of the subdifferential, for any subgradient $g \in \partial f(y)$ and for any $z \in \mathbb{R}^d$:

$$\langle g, z - y \rangle \leq r(z) - r(y).$$

In particular, this holds true for $g = x - y$. Conversely, it is also clear: for $g = x - y$, the above relationship holds, which means $g \in \partial r(y)$.

Proximal operator properties

i Theorem

The operator $\text{prox}_r(x)$ is firmly nonexpansive (FNE)

$$\|\text{prox}_r(x) - \text{prox}_r(y)\|_2^2 \leq \langle \text{prox}_r(x) - \text{prox}_r(y), x - y \rangle$$

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1. Let $u = \text{prox}_r(x)$, and $v = \text{prox}_r(y)$. Then, from the previous property:

$$\langle x - u, z_1 - u \rangle \leq r(z_1) - r(u)$$

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4. The last point comes from simple Cauchy-Bunyakovsky-Schwarz for the last inequality.

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3. Finally,

$$x^* = \text{prox}_{\alpha r}(x^* - \alpha \nabla f(x^*)) = \text{prox}_{r,\alpha}(x^* - \alpha \nabla f(x^*))$$

Theoretical tools for convergence analysis



i Theorem

Let $f : \mathbb{R}^n \rightarrow \mathbb{R}$ be an L -smooth convex function. Then, for any $x, y \in \mathbb{R}^n$, the following inequality holds:

$$f(x) + \langle \nabla f(x), y - x \rangle + \frac{1}{2L} \|\nabla f(x) - \nabla f(y)\|_2^2 \leq f(y) \text{ or, equivalently,}$$
$$\|\nabla f(y) - \nabla f(x)\|_2^2 = \|\nabla f(x) - \nabla f(y)\|_2^2 \leq 2L (f(x) - f(y) - \langle \nabla f(y), x - y \rangle)$$

Proof

1. To prove this, we'll consider another function $\varphi(y) = f(y) - \langle \nabla f(x), y \rangle$. It is obviously a convex function (as a sum of convex functions). And it is easy to verify, that it is an L -smooth function by definition, since $\nabla \varphi(y) = \nabla f(y) - \nabla f(x)$ and $\|\nabla \varphi(y_1) - \nabla \varphi(y_2)\| = \|\nabla f(y_1) - \nabla f(y_2)\| \leq L\|y_1 - y_2\|$.



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Convergence tools

3. From the first order optimality conditions for the convex function $\nabla\varphi(y) = \nabla f(y) - \nabla f(x) = 0$. We can conclude, that for any x , the minimum of the function $\varphi(y)$ is at the point $y = x$. Therefore:

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switch x and y $\|\nabla f(x) - \nabla f(y)\|_2^2 \leq 2L(f(x) - f(y) - \langle\nabla f(y), x - y\rangle)$

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$$\varphi(x) \leq \varphi\left(y - \frac{1}{L}\nabla\varphi(y)\right) \leq \varphi(y) - \frac{1}{2L}\|\nabla\varphi(y)\|_2^2$$

4. Now, substitute $\varphi(y) = f(y) - \langle\nabla f(x), y\rangle$:

$$f(x) - \langle\nabla f(x), x\rangle \leq f(y) - \langle\nabla f(x), y\rangle - \frac{1}{2L}\|\nabla f(y) - \nabla f(x)\|_2^2$$

$$f(x) + \langle\nabla f(x), y - x\rangle + \frac{1}{2L}\|\nabla f(x) - \nabla f(y)\|_2^2 \leq f(y)$$

$$\|\nabla f(y) - \nabla f(x)\|_2^2 \leq 2L(f(y) - f(x) - \langle\nabla f(x), y - x\rangle)$$

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The lemma has been proved. From the first view it does not make a lot of geometrical sense, but we will use it as a convenient tool to bound the difference between gradients.



i Theorem

Let $f : \mathbb{R}^n \rightarrow \mathbb{R}$ be continuously differentiable on \mathbb{R}^n . Then, the function f is μ -strongly convex if and only if for any $x, y \in \mathbb{R}^d$ the following holds:

$$\text{Strongly convex case } \mu > 0 \quad \langle \nabla f(x) - \nabla f(y), x - y \rangle \geq \mu \|x - y\|^2$$

$$\text{Convex case } \mu = 0 \quad \langle \nabla f(x) - \nabla f(y), x - y \rangle \geq 0$$

Proof

1. We will only give the proof for the strongly convex case, the convex one follows from it with setting $\mu = 0$. We start from necessity. For the strongly convex function

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

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

$$\text{sum} \quad \langle \nabla f(x) - \nabla f(y), x - y \rangle \geq \mu \|x - y\|^2$$

Convergence tools

2. For the sufficiency we assume, that $\langle \nabla f(x) - \nabla f(y), x - y \rangle \geq \mu \|x - y\|^2$. Using Newton-Leibniz theorem $f(x) = f(y) + \int_0^1 \langle \nabla f(y + t(x - y)), x - y \rangle dt$:

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$$f(x) - f(y) - \langle \nabla f(y), x - y \rangle = \int_0^1 \langle \nabla f(y + t(x - y)), x - y \rangle dt - \langle \nabla f(y), x - y \rangle$$

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$$\langle \nabla f(y), x - y \rangle = \int_0^1 \langle \nabla f(y), x - y \rangle dt \quad \quad = \int_0^1 \langle \nabla f(y + t(x - y)) - \nabla f(y), (x - y) \rangle dt$$

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$$\begin{aligned} &= \int_0^1 \langle \nabla f(y + t(x - y)) - \nabla f(y), (x - y) \rangle dt \\ &= \int_0^1 t^{-1} \langle \nabla f(y + t(x - y)) - \nabla f(y), t(x - y) \rangle dt \end{aligned}$$

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Thus, we have a strong convexity criterion satisfied

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$$\text{switch } x \text{ and } y \quad - \langle \nabla f(x), x - y \rangle \leq - \left(f(x) - f(y) + \frac{\mu}{2} \|x - y\|_2^2 \right)$$

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 ∇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)

Convergence

Proof

1. Let's introduce the **gradient mapping**, denoted as $G_\alpha(x)$, acts as a “gradient-like object”:

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

$$x_{k+1} = x_k - \alpha G_\alpha(x_k).$$

where $G_\alpha(x)$ is:

$$G_\alpha(x) = \frac{1}{\alpha} (x - \text{prox}_{\alpha r}(x - \alpha \nabla f(x)))$$

Observe that $G_\alpha(x) = 0$ if and only if x is optimal. Therefore, G_α is analogous to ∇f . If x is locally optimal, then $G_\alpha(x) = 0$ even for nonconvex f . This demonstrates that the proximal gradient method effectively combines gradient descent on f with the proximal operator of r , allowing it to handle non-differentiable components effectively.

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$$r(x) \geq r(x_{k+1}) + \langle g, x - x_{k+1} \rangle, \quad g \in \partial r(x_{k+1})$$

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substitute specific subgradient

$$r(x) \geq r(x_{k+1}) + \langle G_\alpha(x_k) - \nabla f(x), x - x_{k+1} \rangle$$

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- Using $\varphi(x) = f(x) + r(x)$ we can now prove extremely useful inequality, which will allow us to demonstrate monotonic decrease of the iteration:



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7. Now it is easy to verify, that when $x = x_k$ we have monotonic decrease for the proximal gradient algorithm:

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 \varphi(x_{k+1}) &\leq \varphi(x^*) + \langle G_\alpha(x_k), x_k - x^* \rangle - \frac{\alpha}{2} \|G_\alpha(x_k)\|_2^2 \\
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 &\leq \frac{1}{2\alpha} [2\langle \alpha G_\alpha(x_k), x_k - x^* \rangle - \|\alpha G_\alpha(x_k)\|_2^2 - \|x_k - x^*\|_2^2 + \|x_k - x^*\|_2^2] \\
 &\leq \frac{1}{2\alpha} [-\|x_k - x^* - \alpha G_\alpha(x_k)\|_2^2 + \|x_k - x^*\|_2^2] \\
 &\leq \frac{1}{2\alpha} [\|x_k - x^*\|_2^2 - \|x_{k+1} - x^*\|_2^2]
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Which is a standard $\frac{L\|x_0 - x^*\|_2^2}{2k}$ with $\alpha = \frac{1}{L}$, or, $\mathcal{O}\left(\frac{1}{k}\right)$ rate for smooth convex problems with Gradient Descent!

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 μ -strongly convex, differentiable, $\text{dom}(f) = \mathbb{R}^n$, and ∇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

$$\|x_k - x^*\|_2^2 \leq (1 - \alpha\mu)^k \|x_0 - x^*\|_2^2$$

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

Proof

1. Considering the distance to the solution and using the stationary point lemm:

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$$\|x_{k+1} - x^*\|_2^2 = \|\text{prox}_{\alpha f}(x_k - \alpha \nabla f(x_k)) - x^*\|_2^2$$

Proof

1. Considering the distance to the solution and using the stationary point lemm:

$$\begin{aligned}\|x_{k+1} - x^*\|_2^2 &= \|\text{prox}_{\alpha f}(x_k - \alpha \nabla f(x_k)) - x^*\|_2^2 \\ \text{stationary point lemm} &= \|\text{prox}_{\alpha f}(x_k - \alpha \nabla f(x_k)) - \text{prox}_{\alpha f}(x^* - \alpha \nabla f(x^*))\|_2^2\end{aligned}$$

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$$\begin{aligned} \|x_{k+1} - x^*\|_2^2 &= \|\text{prox}_{\alpha f}(x_k - \alpha \nabla f(x_k)) - x^*\|_2^2 \\ \text{stationary point lemm} &= \|\text{prox}_{\alpha f}(x_k - \alpha \nabla f(x_k)) - \text{prox}_{\alpha f}(x^* - \alpha \nabla f(x^*))\|_2^2 \\ \text{nonexpansiveness} &\leq \|x_k - \alpha \nabla f(x_k) - x^* + \alpha \nabla f(x^*)\|_2^2 \end{aligned}$$

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4. Due to convexity of f : $f(x_k) - f(x^*) - \langle \nabla f(x^*), x_k - x^* \rangle \geq 0$. Therefore, if we use $\alpha \leq \frac{1}{L}$:

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

which is exactly linear convergence of the method with up to $1 - \frac{\mu}{L}$ convergence rate.

Accelerated Proximal Gradient – *convex* objective

i Accelerated Proximal Gradient Method

Let $f : \mathbb{R}^n \rightarrow \mathbb{R}$ be **convex** and L -**smooth**, $r : \mathbb{R}^n \rightarrow \mathbb{R} \cup \{+\infty\}$ be proper, closed and convex, $\varphi(x) = f(x) + r(x)$ admit a minimiser x^* , and suppose $\text{prox}_{\alpha r}$ is easy to evaluate for $\alpha > 0$. With any $x_0 \in \text{dom } r$ define the sequence

$$\begin{aligned}t_0 &= 1, & y_0 &= x_0, \\x_k &= \text{prox}_{\frac{1}{L}r}(y_{k-1} - \frac{1}{L}\nabla f(y_{k-1})), \\t_k &= \frac{1 + \sqrt{1 + 4t_{k-1}^2}}{2}, \\y_k &= x_k + \frac{t_{k-1} - 1}{t_k}(x_k - x_{k-1}), & k &\geq 1.\end{aligned}$$

Then for every $k \geq 1$

$$\boxed{\varphi(x_k) - \varphi(x^*) \leq \frac{2L \|x_0 - x^*\|_2^2}{(k+1)^2}}$$

Accelerated Proximal Gradient – μ -strongly convex objective

i Accelerated Proximal Gradient Method

Assume in addition that f is μ -strongly convex ($\mu > 0$).

Set the step $\alpha = \frac{1}{L}$ and the fixed momentum parameter

$$\beta = \frac{\sqrt{L/\mu} - 1}{\sqrt{L/\mu} + 1}.$$

Generate the iterates for $k \geq 0$ (take $x_{-1} = x_0$):

$$\begin{aligned} y_k &= x_k + \beta(x_k - x_{k-1}), \\ x_{k+1} &= \text{prox}_{\alpha r}(y_k - \alpha \nabla f(y_k)). \end{aligned}$$

Then for every $k \geq 0$

$$\varphi(x_k) - \varphi(x^*) \leq \left(1 - \sqrt{\frac{\mu}{L}}\right)^k \left(\varphi(x_0) - \varphi(x^*) + \frac{\mu}{2} \|x_0 - x^*\|_2^2\right)$$

Numerical experiments

Quadratic case

$$f(x) = \frac{1}{2m} \|Ax - b\|_2^2 + \lambda \|x\|_1 \rightarrow \min_{x \in \mathbb{R}^n}, \quad A \in \mathbb{R}^{m \times n}, \quad \lambda \left(\frac{1}{m} A^T A \right) \in [\mu; L].$$

Linear Least Squares with ℓ_1 Regularization (LASSO).
m=1000, n=100, $\lambda=0$, $\mu=0$, L=10. Optimal sparsity: 0.0e+00

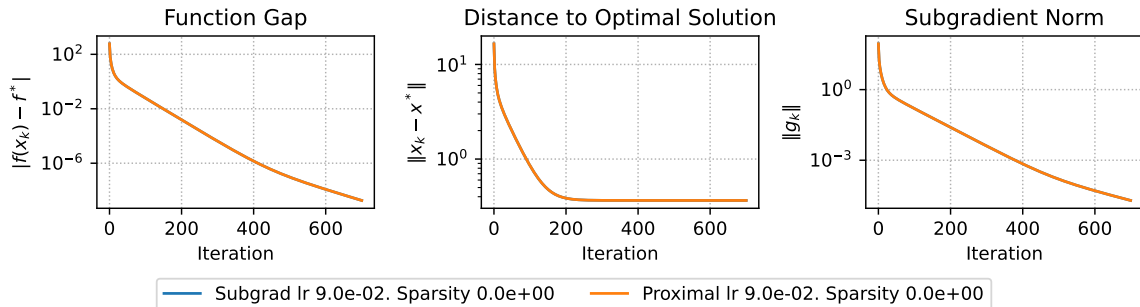


Рисунок 2: Smooth convex case. Sublinear convergence, no convergence in domain, no difference between subgradient and proximal methods

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 $m=1000$, $n=100$, $\lambda=1$, $\mu=0$, $L=10$. Optimal sparsity: $2.3e-01$

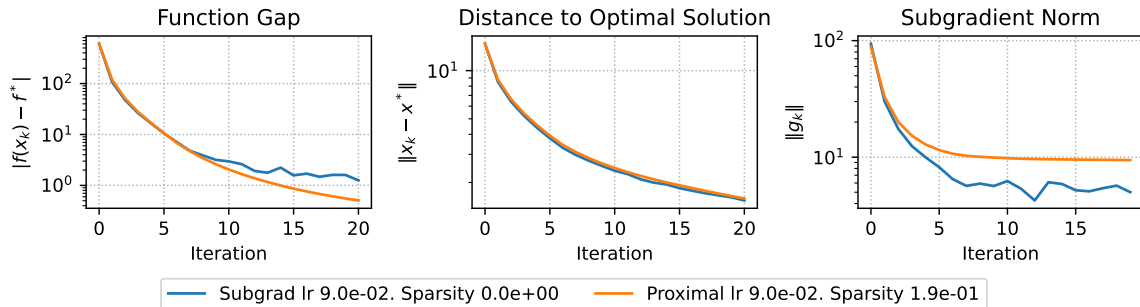


Рисунок 3: Non-smooth convex case. Sublinear convergence. At the beginning, the subgradient method and proximal method are close.

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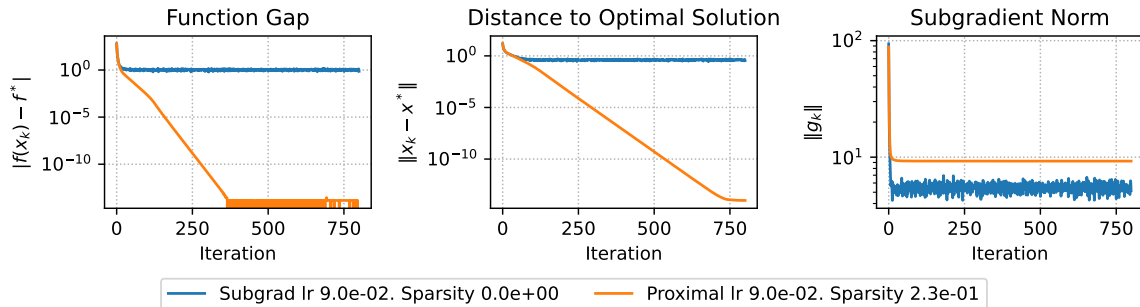
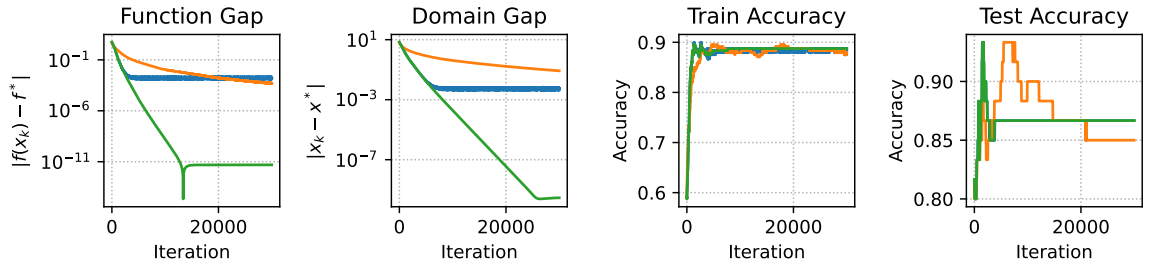


Рисунок 4: Non-smooth convex case. If we take more iterations, the proximal method converges with the constant learning rate, which is not the case for the subgradient method. The difference is tremendous, while the iteration complexity is the same.

Binary logistic regression

$$f(x) = \frac{1}{m} \sum_{i=1}^m \log(1 + \exp(-b_i(A_i x))) + \lambda \|x\|_1 \rightarrow \min_{x \in \mathbb{R}^n}, \quad A_i \in \mathbb{R}^n, \quad b_i \in \{-1, 1\}$$

Binary Logistic Regression with ℓ_1 Regularization.
 $m=300$, $n=50$, $\lambda=0.1$. Optimal sparsity: $8.6e-01$



lbgrad lr 1.0e-02. Sparsity 0.0e+00

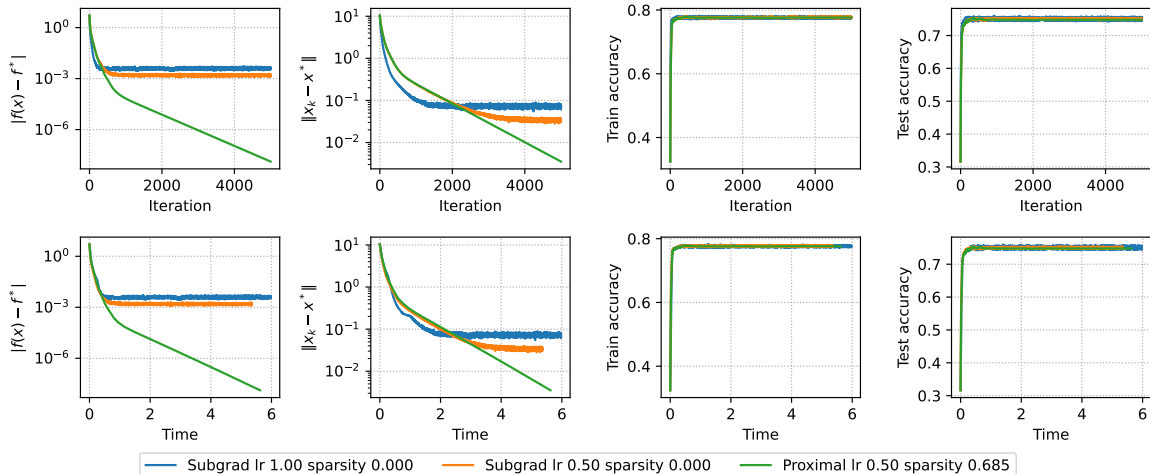
— Subgrad lr α/\sqrt{k} ($\alpha=1.0e-01$). Sparsity 1.2e-01

— Proximal lr 1.0e-02. Sparsity

Рисунок 5: Logistic regression with ℓ_1 regularization

Softmax multiclass regression

Convex multiclass regression. lam=0.01.



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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- **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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- 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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- **Algorithm:**

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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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- It seems that by putting $f = 0$, any nonsmooth problem can be solved using such a method. Question: is this true?

If we allow the proximal operator to be inexact (numerically), then it is true that we can solve any nonsmooth optimization problem. But this is not better from the point of view of theory than solving the problem by subgradient descent, because some auxiliary method (for example, the same subgradient descent) is used to solve the proximal subproblem.

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

Summary

- If we exploit the structure of the problem, we may beat the lower bounds for the unstructured problem.
- Proximal gradient method for a composite problem with an L -smooth convex function f and a convex proximal friendly function r has the same convergence as the gradient descent method for the function f . The smoothness/non-smoothness properties of r do not affect convergence.
- It seems that by putting $f = 0$, any nonsmooth problem can be solved using such a method. Question: is this true?

If we allow the proximal operator to be inexact (numerically), then it is true that we can solve any nonsmooth optimization problem. But this is not better from the point of view of theory than solving the problem by subgradient descent, because some auxiliary method (for example, the same subgradient descent) is used to solve the proximal subproblem.

- Proximal method is a general modern framework for many numerical methods. Further development includes accelerated, stochastic, primal-dual modifications and etc.
- Further reading: Proximal operator splitting, Douglas-Rachford splitting, Best approximation problem, Three operator splitting.