Proximal gradient method

Daniil Merkulov
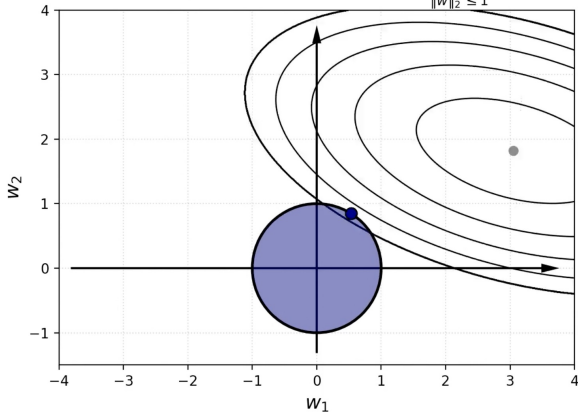
Optimization methods. MIPT

Subgradient method

Non-smooth problems

ℓ_1 induces sparsity

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

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

@fminxyz

$f \to \min_{x,y,z}$ Subgradient method

3

Subgradient method

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

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convex (non-smooth)	strongly convex (non-smooth)
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Assume that f is G-Lipschitz and convex, then Subgradient method converges as:

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

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

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- One can use Mirror Descent (a generalization of the subgradient method to a possibly non-Euclidian distance) with the same convergence rate to better fit the geometry of the problem.
- However, we can achieve standard gradient descent rate $\mathcal{O}\left(\frac{1}{k}\right)$ (and even accelerated version $\mathcal{O}\left(\frac{1}{k^2}\right)$) if we will exploit the structure of the problem.

Proximal operator

Proximal mapping intuition

Consider Gradient Flow ODE:

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

Explicit Euler discretization:

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Leads to ordinary Gradient Descent method

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! Proximal operator

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

Proximal operator visualization

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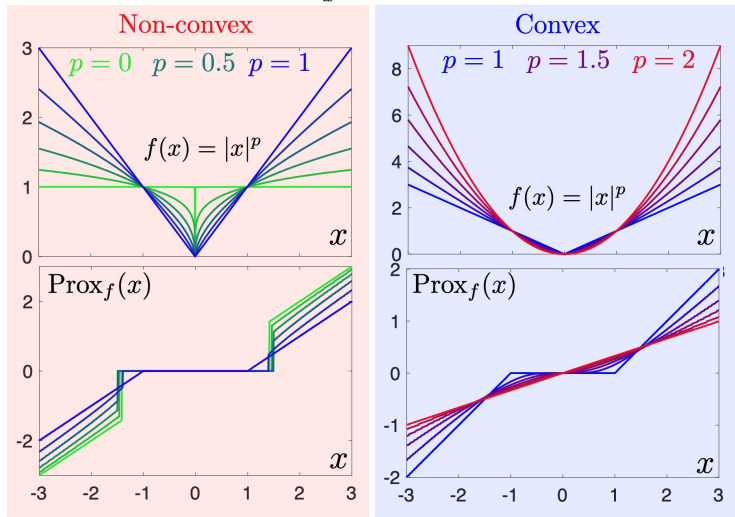

Figure 1: Source

Proximal mapping intuition

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$$x_{k+1} = x_k - \left[\nabla^2 f(x_k) + \frac{1}{\alpha} I \right]^{-1} \nabla f(x_k)$$

From projections to proximity

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

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

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**

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

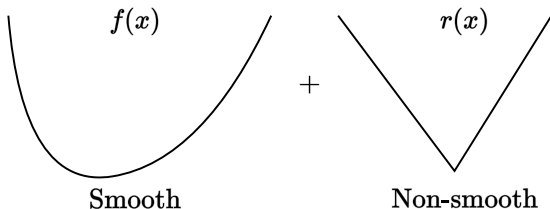$f(x)$ $+$ $r(x)$

Smooth   Non-smooth

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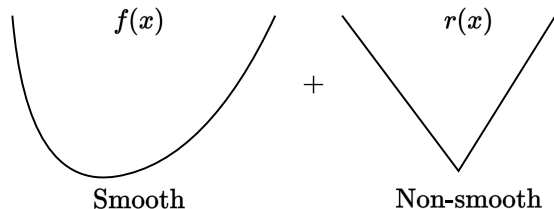$$\min_{x \in \mathbb{R}^n} \varphi(x) = f(x) + r(x)$$

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

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

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

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

$f(x)$ $+$ $r(x)$

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Which leads to the proximal gradient method:

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

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

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x^* &\in \alpha \nabla f(x^*) + (I + \alpha \partial r)(x^*) \\
x^* - \alpha \nabla f(x^*) &\in (I + \alpha \partial r)(x^*) \\
x^* &= (I + \alpha \partial r)^{-1}(x^* - \alpha \nabla f(x^*)) \\
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> **i** Another form of proximal operator
>
> $$\mathsf{prox}_{f,\alpha}(x_k) = \mathsf{prox}_{\alpha f}(x_k) = \arg \min_{x \in \mathbb{R}^n} \left[\alpha f(x) + \frac{1}{2} \|x - x_k\|_2^2 \right] \qquad \mathsf{prox}_f(x_k) = \arg \min_{x \in \mathbb{R}^n} \left[f(x) + \frac{1}{2} \|x - x_k\|_2^2 \right]$$

Proximal operators examples

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

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

  which is also known as soft-thresholding operator.

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$$\mathsf{prox}_r(x) = \frac{x}{1 + \lambda}.$$

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

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

Proximal operator properties

ⓘ Theorem

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

Proof:

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The proximal operator returns the minimum of some optimization problem.

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Question: What can be said about this problem?

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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Proof

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

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> The operator $\text{prox}_r(x)$ is firmly nonexpansive (FNE)
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> $$\|\text{prox}_r(x) - \text{prox}_r(y)\|_2^2 \leq \langle \text{prox}_r(x) - \text{prox}_r(y), x - y \rangle$$
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> and nonexpansive:
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Proof

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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2. Substitute $z_1 = v$ and $z_2 = u$. Summing up, we get:

$$\langle x - u, v - u \rangle + \langle y - v, u - v \rangle \leq 0,$$
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4. The last point comes from simple Cauchy-Bunyakovsky-Schwarz for the last inequality.

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Proof

1. Optimality conditions:

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3. Finally,

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

Theoretical tools for convergence analysis

Convergence tools

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> Let $f : \mathbb{R}^n \to \mathbb{R}$ be an L-smooth convex function. Then, for any $x, y \in \mathbb{R}^n$, the following inequality holds:
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> $$f(x) + \langle \nabla f(x), y - x \rangle + \frac{1}{2L} \|\nabla f(x) - \nabla f(y)\|_2^2 \leq f(y) \text{ or, equivalently,}$$
> $$\|\nabla f(y) - \nabla f(x)\|_2^2 = \|\nabla f(x) - \nabla f(y)\|_2^2 \leq 2L \left(f(x) - f(y) - \langle \nabla f(y), x - y \rangle \right)$$

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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$$x := y, y := y - \frac{1}{L}\nabla \varphi(y) \quad \varphi\left(y - \frac{1}{L}\nabla \varphi(y)\right) \le \varphi(y) + \left\langle \nabla \varphi(y), -\frac{1}{L}\nabla \varphi(y) \right\rangle + \frac{1}{2L}\|\nabla \varphi(y)\|_2^2$$

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

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:

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

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

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

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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.

Convergence tools

> **ℹ Theorem**
>
> Let $f : \mathbb{R}^n \to \mathbb{R}$ 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

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

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

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

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

Convergence tools

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

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Thus, we have a strong convexity criterion satisfied

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Proximal Gradient Method. Convex case

Convergence

> **ℹ Theorem**
>
> Consider the proximal gradient method
>
> $$x_{k+1} = \text{prox}_{\alpha r} \left(x_k - \alpha \nabla f(x_k) \right)$$
>
> For the criterion $\varphi(x) = f(x) + r(x)$, we assume:
> - f is convex, differentiable, $\text{dom}(f) = \mathbb{R}^n$, and ∇f is Lipschitz continuous with constant $L > 0$.
> - r is convex, and $\text{prox}_{\alpha r}(x_k) = \arg \min\limits_{x \in \mathbb{R}^n} \left[\alpha r(x) + \frac{1}{2} \|x - x_k\|_2^2 \right]$ can be evaluated.
>
> Proximal gradient descent with fixed step size $\alpha = 1/L$ satisfies
>
> $$\varphi(x_k) - \varphi^* \leq \frac{L\|x_0 - x^*\|^2}{2k},$$

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

$f \to \min\limits_{x,y,z}$ Proximal Gradient Method. Convex case

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Convergence
Proof

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

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

where $G_\alpha(x)$ is:

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

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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$$\text{Since } x_{k+1} - x_k = -\alpha G_\alpha(x_k) \qquad \Rightarrow \qquad \alpha G_\alpha(x_k) - \alpha \nabla f(x_k) \in \partial \alpha r(x_{k+1})$$

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$f \to \min\limits_{x,y,z}$ Proximal Gradient Method. Convex case

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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:

$$\varphi(x_{k+1}) \leq \varphi(x_k) - \frac{\alpha}{2} \|G_\alpha(x_k)\|_2^2$$

Convergence

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$f \to \min\limits_{x,y,z}$ Proximal Gradient Method. Convex case

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Convergence

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$$\leq \frac{1}{2\alpha} \left[2\langle \alpha G_\alpha(x_k), x_k - x^* \rangle - \|\alpha G_\alpha(x_k)\|_2^2 \right]$$

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Convergence

9. Now we write the bound above for all iterations $i \in 0, k-1$ and sum them:

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!

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$$\sum_{i=0}^{k-1} \varphi(x_k) = k\varphi(x_k) \leq \sum_{i=0}^{k-1} \varphi(x_{i+1})$$

$$\varphi(x_k) \leq \frac{1}{k} \sum_{i=0}^{k-1} \varphi(x_{i+1})$$

$$\varphi(x_k) - \varphi(x^*) \leq \frac{1}{k} \sum_{i=0}^{k-1} [\varphi(x_{i+1}) - \varphi(x^*)] \leq \frac{\|x_0 - x^*\|_2^2}{2\alpha k}$$

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
>
> $$x_{k+1} = \mathsf{prox}_{\alpha r} \left(x_k - \alpha \nabla f(x_k) \right)$$
>
> For the criterion $\varphi(x) = f(x) + r(x)$, we assume:
> - f is μ-strongly convex, differentiable, $\mathrm{dom}(f) = \mathbb{R}^n$, and ∇f is Lipschitz continuous with constant $L > 0$.
> - r is convex, and $\mathsf{prox}_{\alpha r}(x_k) = \arg \min_{x \in \mathbb{R}^n} \left[\alpha r(x) + \frac{1}{2}\|x - x_k\|_2^2 \right]$ can be evaluated.
>
> Proximal gradient descent with fixed step size $\alpha \leq 1/L$ 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!

Convergence

Proof

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

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$f \to \min\limits_{x,y,z}$ Proximal Gradient Method. Strongly convex case

33

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$$\text{nonexpansiveness} \leq \|x_k - \alpha \nabla f(x_k) - x^* + \alpha \nabla f(x^*)\|_2^2$$

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2. Now we use smoothness from the convergence tools and strong convexity:

$$\text{smoothness} \quad \|\nabla f(x_k) - \nabla f(x^*)\|_2^2 \leq 2L \left(f(x_k) - f(x^*) - \langle \nabla f(x^*), x_k - x^* \rangle \right)$$

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$$\text{strong convexity} \quad -\langle\nabla f(x_k) - \nabla f(x^*), x_k - x^*\rangle \leq -\left(f(x_k) - f(x^*) + \frac{\mu}{2}\|x_k - x^*\|_2^2\right) - \langle\nabla f(x^*), x_k - x^*\rangle$$

$f \to \min\limits_{x,y,z}$ Proximal Gradient Method. Strongly convex case

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$$+ \alpha^2 2L \left(f(x_k) - f(x^*) - \langle \nabla f(x^*), x_k - x^* \rangle \right)$$
$$\le (1 - \alpha\mu)\|x_k - x^*\|^2 + 2\alpha(\alpha L - 1) \left(f(x_k) - f(x^*) - \langle \nabla f(x^*), x_k - x^* \rangle \right)$$

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

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

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

Accelerated Proximal Method

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> Let $x_0 = y_0 \in \mathsf{dom}(r)$. For $k \geq 1$:
>
> $$x_k = \mathsf{prox}_{\alpha_k h}(y_{k-1} - \alpha_k \nabla f(y_{k-1}))$$
> $$y_k = x_k + \frac{k-1}{k+2}(x_k - x_{k-1})$$
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Framework due to: Nesterov (1983, 2004); also Beck, Teboulle (2009). Simplified analysis: Tseng (2008).

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- Uses extra "memory" for interpolation
- Same computational cost as ordinary prox-grad
- Convergence rate theoretically optimal

Numerical experiments

Quadratic case

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

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

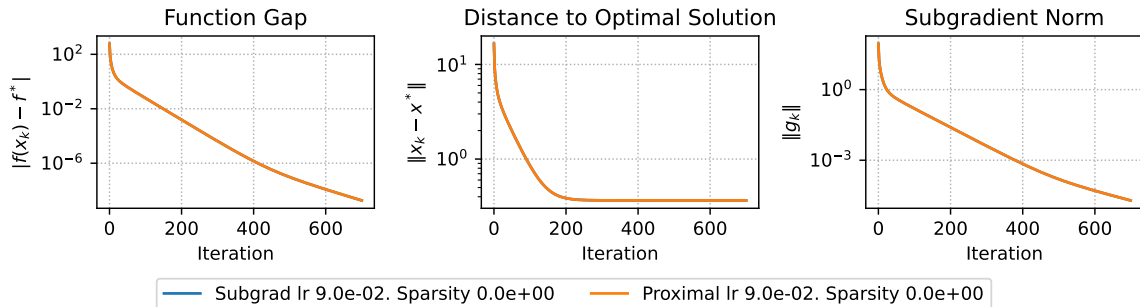Figure 2: Smooth convex case. Sublinear convergence, no convergence in domain, no difference between subgradient and proximal methods

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Linear Least Squares with ℓ_1 Regularization (LASSO).
m=1000, n=100, λ=1, μ=0, L=10. Optimal sparsity: 2.3e-01

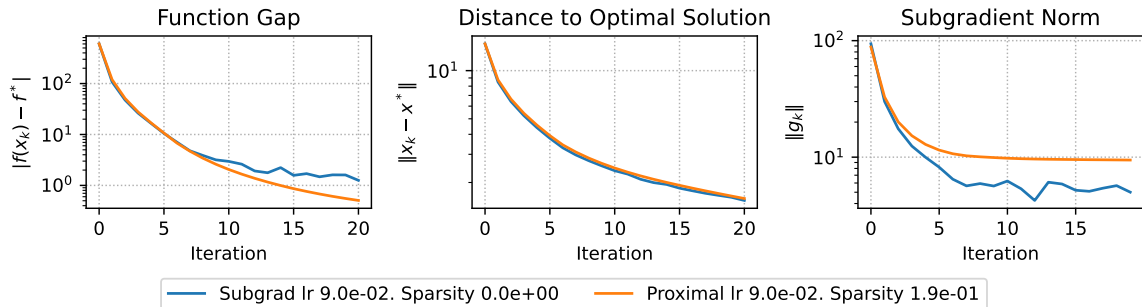Subgrad lr 9.0e-02. Sparsity 0.0e+00 — Proximal lr 9.0e-02. Sparsity 1.9e-01

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

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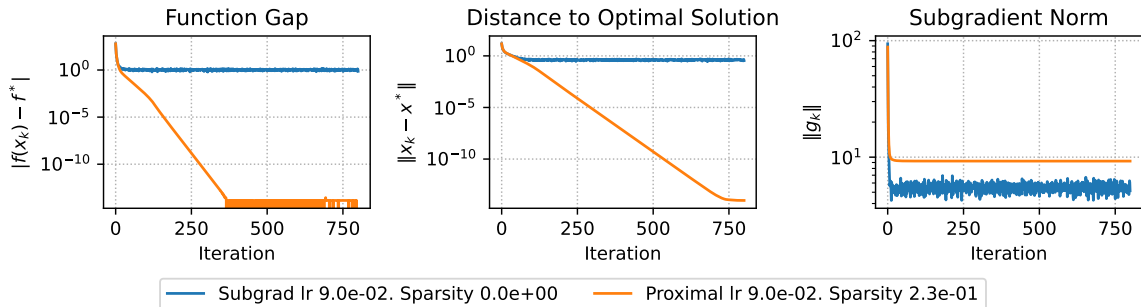m=1000, n=100, λ=1, μ=0, L=10. Optimal sparsity: 2.3e-01

Figure 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

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

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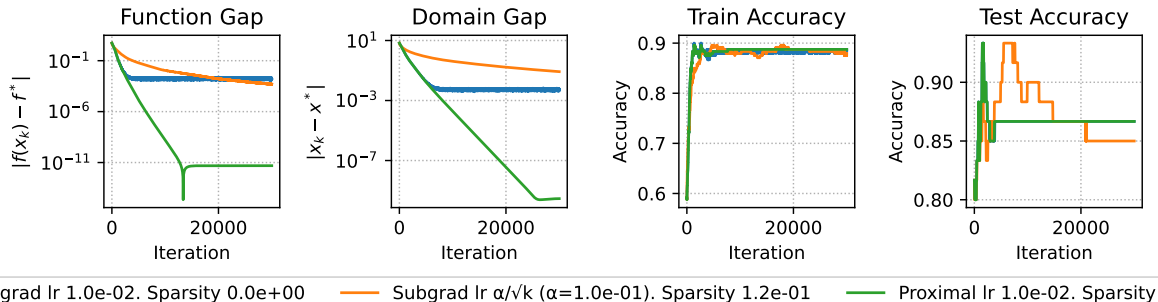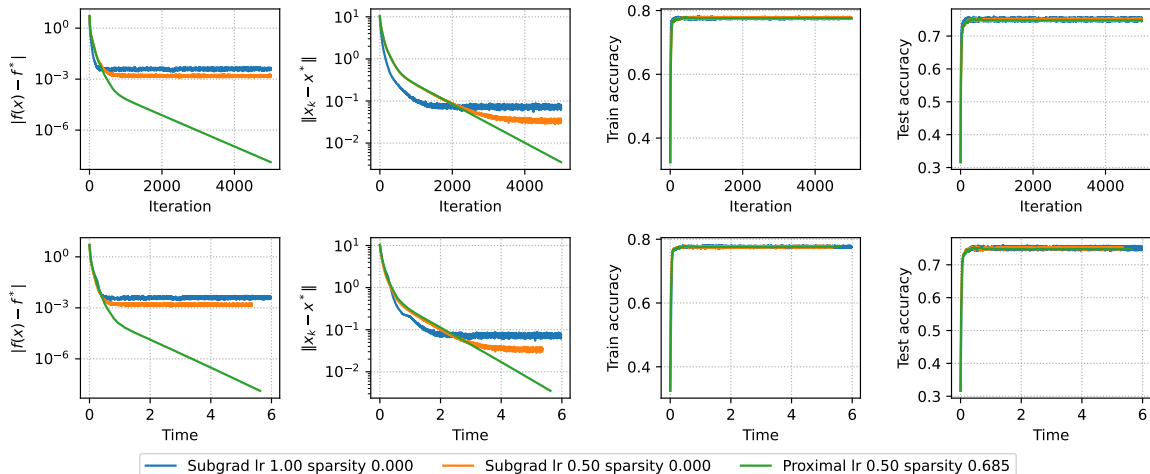m=300, n=50, λ=0.1. Optimal sparsity: 8.6e-01

Subgrad lr 1.0e-02. Sparsity 0.0e+00   Subgrad lr $\alpha/\sqrt{k}$ (α=1.0e-01). Sparsity 1.2e-01   Proximal lr 1.0e-02. Sparsity

Figure 5: Logistic regression with ℓ_1 regularization

Softmax multiclass regression

Convex multiclass regression. lam=0.01.

Subgrad lr 1.00 sparsity 0.000	Subgrad lr 0.50 sparsity 0.000
Proximal lr 0.50 sparsity 0.685	

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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- **Convergence**:
  - 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**:

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

where P_Ω projects onto the observed set Ω, and $\|\cdot\|_*$ denotes the nuclear norm.

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

  where P_Ω projects onto the observed set Ω, and $\|\cdot\|_*$ denotes the nuclear norm.

- **Proximal Operator**:
  - The proximal operator for the nuclear norm involves singular value decomposition (SVD) and soft-thresholding of the singular values.

- **Algorithm**:
  - Similar proximal gradient or accelerated proximal gradient methods can be applied, where the main computational effort lies in performing partial SVDs.

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