Proximal gradient method

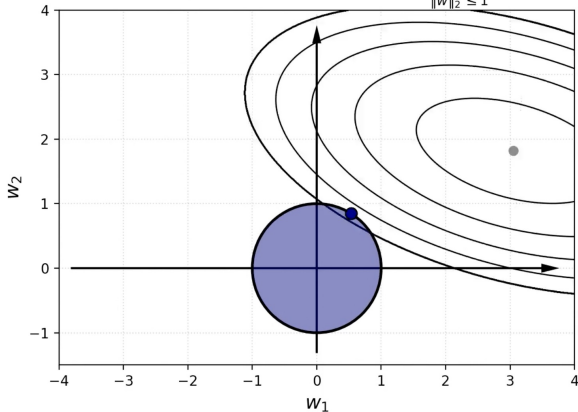## Daniil Merkulov

Optimization for ML. Faculty of Computer Science. HSE University
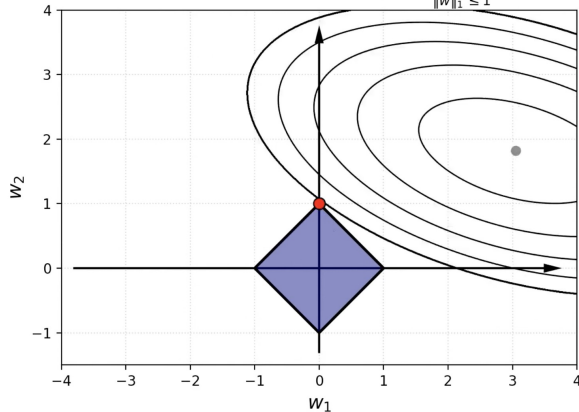
Non-smooth problems

ℓ_1 induces sparsity

Left plot title: ℓ_2 regularization. $\|Xw - y\|_2^2 \to \min_{\|w\|_2 \le 1}$

Right plot title: ℓ_1 regularization. $\|Xw - y\|_2^2 \to \min_{\|w\|_1 \le 1}$

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

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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 possiby 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 mapping intuition

Consider Gradient Flow ODE:

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

Explicit Euler discretization:

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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

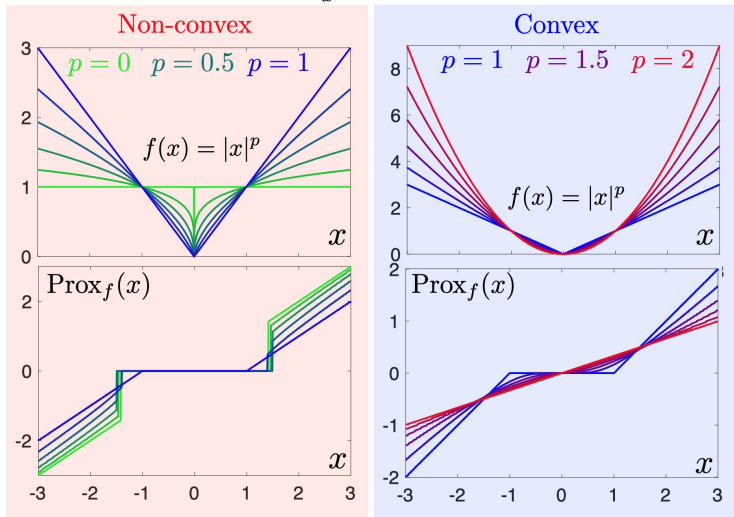$$\text{Prox}_f(x) = \underset{x'}{\text{argmin}} \; \frac{1}{2}\|x - x'\|^2 + f(x')$$

Figure 1: Source

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

- **Newton from proximal method.** Now let's consider proximal mapping of a second order Taylor approximation of the function $f_{x_k}^{II}(x)$:

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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!

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

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**

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

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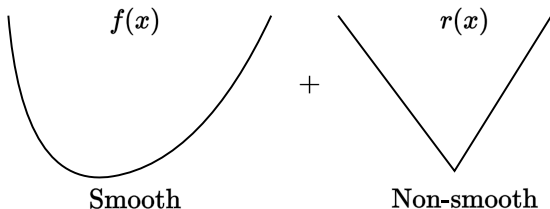
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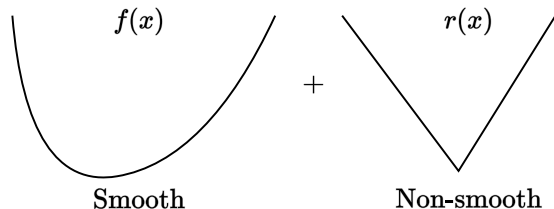$$\min_{x \in \mathbb{R}^n} \varphi(x) = f(x) + r(x)$$

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

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

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

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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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).

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Question: What can be said about this 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

> **i Theorem**
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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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1. Optimality conditions:

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2. Recall from the previous lemma:

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3. Finally,

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

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

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

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

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

Convergence tools

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

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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)

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:

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

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

22

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

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

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

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!

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, $\mathsf{dom}(f) = \mathbb{R}^n$, 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!

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

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

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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.

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- Convergence rate theoretically optimal

Example: 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**:

Example: ISTA

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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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$$x_{k+1} = \text{prox}_{\lambda\alpha\|\cdot\|_1}\left(x_k - \alpha\nabla f(x_k)\right),$$

  where $\text{prox}_{\lambda\alpha\|\cdot\|_1}(v)$ applies soft thresholding to each component of v.

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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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  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.