Proximal gradient method

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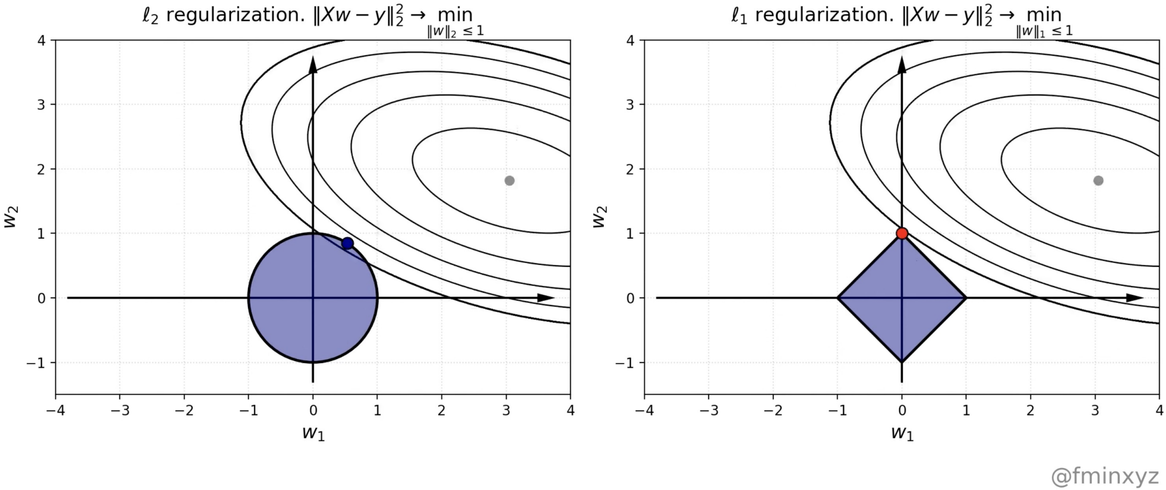
Non-smooth problems

ℓ_1 induces sparsity



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

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Theorem

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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- Subgradient method is optimal for the problems above.
- 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

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

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

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

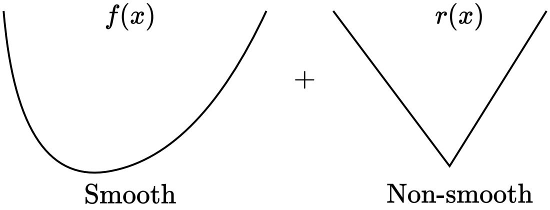
Regularized / Composite Objectives

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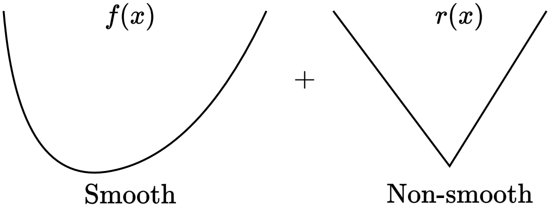
- **L1-Logistic regression, sparse LR**

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



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

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Another form of proximal operator

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

Proximal operators examples

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

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[\text{prox}_r(x)]_i = [|x_i| - \lambda]_+ \cdot \text{sign}(x_i),
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which is also known as soft-thresholding operator.

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

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

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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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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Let $r : \mathbb{R}^n \to \mathbb{R} \cup \{+\infty\}$ 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:

- $\text{prox}_r(x) = y$,

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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:

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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

Theorem

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

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

and nonexpansive:

$$\|\text{prox}_r(x) - \text{prox}_r(y)\|_2 \leq \|x - y\|_2$$

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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$$\|u - v\|_2^2 \leq \langle x - y, u - v \rangle$$

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

Proximal operator properties

Theorem

Let $f : \mathbb{R}^n \to \mathbb{R} \cup \{+\infty\}$ and $r : \mathbb{R}^n \to \mathbb{R} \cup \{+\infty\}$ be convex functions. Additionally, assume that f is continuously differentiable and L-smooth, and for r, prox_r is defined. Then, x^* is a solution to the composite optimization problem if and only if, for any $\alpha > 0$, it satisfies:

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

Proof

1. Optimality conditions:

Proximal operator properties

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2. Recall from the previous lemma:

$$\text{prox}_r(x) = y \Leftrightarrow x - y \in \partial r(y)$$

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2. Recall from the previous lemma:

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3. Finally,

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

Convergence tools

Theorem

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:

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

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

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

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)
\end{aligned}$$

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 $\varphi(y) = f(y) - \langle \nabla f(x), y\rangle$:

$$\begin{aligned}
& f(x) - \langle \nabla f(x), x\rangle \leq f(y) - \langle \nabla f(x), y\rangle - \frac{1}{2L}\|\nabla f(y) - \nabla f(x)\|_2^2 \\
& f(x) + \langle \nabla f(x), y - x\rangle + \frac{1}{2L}\|\nabla f(x) - \nabla f(y)\|_2^2 \leq f(y) \\
& \|\nabla f(y) - \nabla f(x)\|_2^2 \leq 2L\left(f(y) - f(x) - \langle \nabla f(x), y - x\rangle\right) \\
\text{switch x and y} \quad & \|\nabla f(x) - \nabla f(y)\|_2^2 \leq 2L\left(f(x) - f(y) - \langle \nabla f(y), x - y\rangle\right)
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\end{aligned}$$

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

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:

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

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

$$
\begin{aligned}
& f(y) \geq f(x) + \langle \nabla f(x), y - x \rangle + \frac{\mu}{2} \|x - y\|_2^2 \\
& f(x) \geq f(y) + \langle \nabla f(y), x - y \rangle + \frac{\mu}{2} \|x - y\|_2^2 \\
\text{sum} \quad & \langle \nabla f(x) - \nabla f(y), x - y \rangle \geq \mu \|x - y\|^2
\end{aligned}
$$

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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Thus, we have a strong convexity criterion satisfied

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

Convergence

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 $\text{prox}_{\alpha r}(x_k) = \text{arg}\min\limits_{x \in \mathbb{R}^n} \left[\alpha r(x) + \frac{1}{2}\|x - x_k\|_2^2\right]$ 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":

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

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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2. We will use smoothness and convexity of f for some arbitrary point x:

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\text{smoothness} \quad 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\|_2^2
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&\leq f(x) + \langle \nabla f(x_k), x_{k+1} - x \rangle + \frac{\alpha^2 L}{2}\|G_\alpha(x_k)\|_2^2
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$$x_{k+1} = \text{prox}_{\alpha r}\left(x_k - \alpha \nabla f(x_k)\right) \qquad \Leftrightarrow \qquad x_k - \alpha \nabla f(x_k) - x_{k+1} \in \partial \alpha r(x_{k+1})$$

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$$
f(x_{k+1}) + r(x_{k+1}) \leq f(x) + r(x) - \langle G_\alpha(x_k), x - x_k + \alpha G_\alpha(x_k) \rangle + \frac{\alpha^2 L}{2} \|G_\alpha(x_k)\|_2^2
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$$\varphi(x_{k+1}) \leq \varphi(x) + \langle G_\alpha(x_k), x_k - x \rangle + \frac{\alpha}{2} \left(\alpha L - 2\right) \|G_\alpha(x_k)\|_2^2$$

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$\alpha \leq \frac{1}{L} \Rightarrow \frac{\alpha}{2} (\alpha L - 2) \leq -\frac{\alpha}{2}$

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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:

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

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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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\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 \\
\varphi(x_{k+1}) - \varphi(x^*) &\leq \langle G_\alpha(x_k), x_k - x^* \rangle - \frac{\alpha}{2}\|G_\alpha(x_k)\|_2^2 \\
&\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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9. Now we write the bound above for all iterations $i \in 0, k-1$ and sum them:

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

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10. Since $\varphi(x_k)$ is a decreasing sequence, it follows that:

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&\leq \frac{1}{2\alpha} \|x_0 - x^*\|_2^2
\end{aligned}
$$

10. Since $\varphi(x_k)$ is a decreasing sequence, it follows that:

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

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

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

$$
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Convergence

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 μ-strongly convex, differentiable, $\text{dom}(f) = \mathbb{R}^n$, and ∇f is Lipschitz continuous with constant $L > 0$.
- r is convex, and $\text{prox}_{\alpha r}(x_k) = \text{arg}\min\limits_{x\in\mathbb{R}^n} \left[\alpha r(x) + \frac{1}{2}\|x - x_k\|_2^2\right]$ can be evaluated.

Proximal gradient descent with fixed step size $\alpha \leq 1/L$ 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

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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} \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
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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 Method

Accelerated Proximal Method

Let $x_0 = y_0 \in \mathrm{dom}(r)$. For $k \geq 1$:

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x_k &= \mathrm{prox}_{\alpha_k h}(y_{k-1} - \alpha_k \nabla f(y_{k-1})) \\
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- Uses extra "memory" for interpolation
- Same computational cost as ordinary prox-grad
- Convergence rate theoretically optimal

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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- **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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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.
- **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.
- **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.