

Mathematics of Data: From Theory to Computation

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Lecture 7: Introduction to proximal-operators. Conditional gradient methods.

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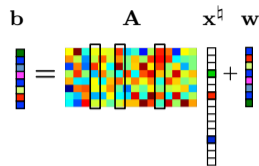
Outline

- ▶ Composite minimization
- ▶ Proximal gradient methods
- ▶ Introduction to Frank-Wolfe method

Recall sparse regression in generalized linear models (GLMs)

Problem (Sparse regression in GLM)

Our goal is to estimate $\mathbf{x}^{\natural} \in \mathbb{R}^p$ given $\{b_i\}_{i=1}^n$ and $\{\mathbf{a}_i\}_{i=1}^n$, knowing that the likelihood function at y_i given \mathbf{a}_i and \mathbf{x}^{\natural} is given by $L(\langle \mathbf{a}_i, \mathbf{x}^{\natural} \rangle, b_i)$, and that \mathbf{x}^{\natural} is *sparse*.



Optimization formulation

$$\min_{\mathbf{x} \in \mathbb{R}^p} \left\{ \underbrace{-\sum_{i=1}^n \log L(\langle \mathbf{a}_i, \mathbf{x}^{\natural} \rangle, b_i)}_{f(\mathbf{x})} + \underbrace{\rho_n \|\mathbf{x}\|_1}_{g(\mathbf{x})} \right\}$$

where $\rho_n > 0$ is a parameter which controls the strength of sparsity regularization.

Theorem (cf. [13] for details)

Under some technical conditions, there exists $\{\rho_i\}_{i=1}^{\infty}$ such that with high probability, the following holds

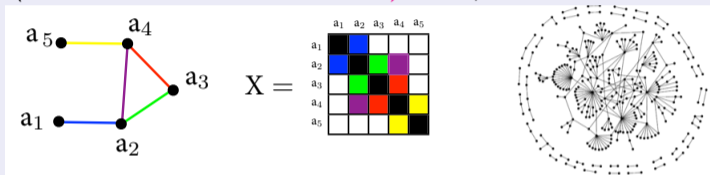
$$\|\mathbf{x}^{\star} - \mathbf{x}^{\natural}\|_2^2 = \mathcal{O}\left(\frac{s \log p}{n}\right), \quad \text{supp } \mathbf{x}^{\star} = \text{supp } \mathbf{x}^{\natural}.$$

$$\text{Recall ML: } \|\mathbf{x}_{ML} - \mathbf{x}^{\natural}\|_2^2 = \mathcal{O}\left(\frac{p}{n}\right).$$

Sparse inverse covariance estimation

Problem (Graphical model selection)

Given a data set $\mathcal{D} := \{\mathbf{x}_1, \dots, \mathbf{x}_n\}$, where \mathbf{x}_i is a Gaussian random variable. Let Σ be the covariance matrix corresponding to the graphical model of the Gaussian Markov random field. Our goal is to learn a sparse precision matrix \mathbf{X} (i.e., the inverse covariance matrix Σ^{-1}) that captures the Markov random field structure.



Optimization formulation [16]

$$\min_{\mathbf{X} \succ 0} \left\{ \underbrace{\text{tr}(\Sigma \mathbf{X}) - \log \det(\mathbf{X})}_{f(\mathbf{x})} + \underbrace{\rho_n \|\text{vec}(\mathbf{X})\|_1}_{g(\mathbf{x})} \right\}, \quad (1)$$

where $\mathbf{X} \succ 0$ means that \mathbf{X} is symmetric and positive definite and $\rho_n > 0$ is a regularization parameter and vec is the vectorization operator. Let \mathbf{X}^* be the minimizer of (1), under some technical conditions, there exists a ρ_n such that $\|\mathbf{X}^* - \Sigma^{-1}\|_2^2 = \mathcal{O}(\min \frac{1}{n} \{d^2 \log p, (s+p) \log p\})$ where d is the maximum node degree.

Composite **convex** minimization

Problem (Composite **convex** minimization)

$$F^* := \min_{\mathbf{x} \in \mathbb{R}^p} \{F(\mathbf{x}) := f(\mathbf{x}) + g(\mathbf{x})\} \quad (2)$$

- ▶ f and g are both *proper, closed, and convex*.
- ▶ $\text{dom}(F) := \text{dom}(f) \cap \text{dom}(g) \neq \emptyset$ and $-\infty < F^* < +\infty$.
- ▶ The solution set $\mathcal{S}^* := \{\mathbf{x}^* \in \text{dom}(F) : F(\mathbf{x}^*) = F^*\}$ is nonempty.

Remarks:

- Without loss of generality, f is smooth and g is non-smooth in the sequel.
- By Moreau-Rockafellar Theorem, we have $\partial F = \partial(f + g) = \partial f + \partial g = \nabla f + \partial g$.
- Subgradient method attains a $\mathcal{O}\left(\frac{1}{\sqrt{T}}\right)$ rate.
- Without g , accelerated gradient method attains a $\mathcal{O}\left(\frac{1}{T^2}\right)$ rate.

Composite **convex** minimization

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Can we design algorithms that achieve a faster convergence rate for composite convex minimization?

Designing algorithms for finding a solution \mathbf{x}^*

Quadratic *majorizer* for f

When f has L -Lipschitz continuous gradient, we have, $\forall \mathbf{x}, \mathbf{y} \in \mathbb{R}^p$

$$f(\mathbf{x}) \leq f(\mathbf{y}) + \nabla f(\mathbf{y})^T (\mathbf{x} - \mathbf{y}) + \frac{L}{2} \|\mathbf{x} - \mathbf{y}\|_2^2$$

Designing algorithms for finding a solution \mathbf{x}^*

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Quadratic majorizer for $f + g$

When f has L -Lipschitz continuous gradient, we have, $\forall \mathbf{x}, \mathbf{y} \in \mathbb{R}^p$

$$f(\mathbf{x}) + g(\mathbf{x}) \leq f(\mathbf{y}) + \nabla f(\mathbf{y})^T (\mathbf{x} - \mathbf{y}) + \frac{L}{2} \|\mathbf{x} - \mathbf{y}\|_2^2 + g(\mathbf{x}) := P_L(\mathbf{x}, \mathbf{y})$$

Designing algorithms for finding a solution \mathbf{x}^*

Quadratic majorizer for f

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Quadratic majorizer for $f + g$

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Majorization-minimization for $f + g$

$$\begin{aligned} \mathbf{x}^{k+1} &= \arg \min_{\mathbf{x} \in \mathbb{R}^p} P_L(\mathbf{x}, \mathbf{x}^k) \\ &= \arg \min_{\mathbf{x} \in \mathbb{R}^p} \left\{ g(\mathbf{x}) + \frac{L}{2} \left\| \mathbf{x} - \left(\mathbf{x}^k - \frac{1}{L} \nabla f(\mathbf{x}^k) \right) \right\|^2 \right\} \end{aligned}$$

A short detour: Proximal-point operators

Definition (Proximal operator [18])

Let $g \in \mathcal{F}(\mathbb{R}^p)$, $\mathbf{x} \in \mathbb{R}^p$ and $\lambda > 0$. The proximal operator (or prox-operator) of g is defined as:

$$\text{prox}_{\lambda g}(\mathbf{y}) \equiv \arg \min_{\mathbf{x} \in \mathbb{R}^p} \left\{ g(\mathbf{x}) + \frac{1}{2\lambda} \|\mathbf{y} - \mathbf{x}\|_2^2 \right\}. \quad (3)$$

A short detour: Proximal-point operators

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Remarks:

- The *proximal operator* of $\frac{1}{L}g$ evaluated at $\left(\mathbf{x}^k - \frac{1}{L}\nabla f(\mathbf{x}^k)\right)$ is given by

$$\text{prox}_{\frac{1}{L}g} \left(\mathbf{x}^k - \frac{1}{L}\nabla f(\mathbf{x}^k) \right) = \arg \min_{\mathbf{x} \in \mathbb{R}^p} \left\{ g(\mathbf{x}) + \frac{L}{2} \left\| \mathbf{x} - \left(\mathbf{x}^k - \frac{1}{L}\nabla f(\mathbf{x}^k) \right) \right\|_2^2 \right\}.$$

- This prox-operator minimizes the majorizing bound:

$$f(\mathbf{x}) + g(\mathbf{x}) \leq f(\mathbf{x}^k) + \nabla f(\mathbf{x}^k)^T (\mathbf{x} - \mathbf{x}^k) + \frac{L}{2} \|\mathbf{x} - \mathbf{x}^k\|_2^2 + g(\mathbf{x})$$

- Rule of thumb: Replace gradient steps with proximal gradient steps!

Tractable prox-operators

Processing non-smooth terms in (2)

- ▶ We handle the nonsmooth term g in (2) using its proximal operator.
- ▶ **However**, computing proximal operator prox_g of a general convex function g

$$\text{prox}_g(\mathbf{y}) \equiv \arg \min_{\mathbf{x} \in \mathbb{R}^p} \left\{ g(\mathbf{x}) + \frac{1}{2} \|\mathbf{y} - \mathbf{x}\|_2^2 \right\}.$$

can be **computationally demanding**.

Definition (Tractable proximity)

- ▶ Given $g \in \mathcal{F}(\mathbb{R}^p)$. We say that g is **proximally tractable** if prox_g defined by (3) can be computed **efficiently**.
- ▶ "**efficiently**" = {closed form solution, low-cost computation, polynomial time}.

Tractable prox-operators

Example

- ▶ For separable functions, the prox-operator can be efficient. When $g(\mathbf{x}) := \|\mathbf{x}\|_1 = \sum_{i=1}^p |\mathbf{x}_i|$, we have

$$\text{prox}_{\lambda g}(\mathbf{x}) = \text{sign}(\mathbf{x}) \otimes \max\{|\mathbf{x}| - \lambda, 0\}.$$

- ▶ Sometimes, we can compute the prox-operator via basic algebra. When $g(\mathbf{x}) := \frac{1}{2} \|\mathbf{A}\mathbf{x} - \mathbf{b}\|_2^2$, we have

$$\text{prox}_{\lambda g}(\mathbf{x}) = (\mathbb{I} + \lambda \mathbf{A}^T \mathbf{A})^{-1} (\mathbf{x} + \lambda \mathbf{A}^T \mathbf{b}).$$

- ▶ For the indicator functions of simple sets, e.g., $g(\mathbf{x}) := \delta_{\mathcal{X}}(\mathbf{x})$, the prox-operator is the projection operator

$$\text{prox}_{\lambda g}(\mathbf{x}) := \pi_{\mathcal{X}}(\mathbf{x}),$$

where $\pi_{\mathcal{X}}(\mathbf{x})$ denotes the projection of \mathbf{x} onto \mathcal{X} . For instance, when $\mathcal{X} = \{\mathbf{x} : \|\mathbf{x}\|_1 \leq \lambda\}$, the projection can be obtained efficiently.

Computational efficiency - Example

Proximal operator of quadratic function

The **proximal operator** of a quadratic function $g(\mathbf{x}) := \frac{1}{2}\|\mathbf{Ax} - \mathbf{b}\|_2^2$ is defined as

$$\text{prox}_{\lambda g}(\mathbf{x}) := \arg \min_{\mathbf{y} \in \mathbb{R}^p} \left\{ \frac{1}{2}\|\mathbf{Ay} - \mathbf{b}\|_2^2 + \frac{1}{2\lambda}\|\mathbf{y} - \mathbf{x}\|_2^2 \right\}. \quad (4)$$

How do we compute $\text{prox}_{\lambda g}(\mathbf{x})$?

The derivation: ○ The **optimality condition** implies that the solution of (4) should satisfy the following:

$$\mathbf{A}^T(\mathbf{Ay} - \mathbf{b}) + \lambda^{-1}(\mathbf{y} - \mathbf{x}) = 0.$$

○ Setting $\mathbf{y} = \text{prox}_{\lambda g}(\mathbf{x})$, we obtain

$$\text{prox}_{\lambda g}(\mathbf{x}) = (\mathbb{I} + \lambda\mathbf{A}^T\mathbf{A})^{-1} (\mathbf{x} + \lambda\mathbf{A}^T\mathbf{b})$$

Remarks:

- The Woodbury matrix identity can be useful: $(\mathbb{I} + \lambda\mathbf{A}^T\mathbf{A})^{-1} = \mathbb{I} - \mathbf{A}^T(\lambda^{-1}\mathbb{I} + \mathbf{A}\mathbf{A}^T)^{-1}\mathbf{A}$.
- When $\mathbf{A}^T\mathbf{A}$ is efficiently **diagonalizable**, i.e., $\mathbf{A}^T\mathbf{A} := \mathbf{U}\mathbf{\Lambda}\mathbf{U}^T$, such that
 - ▶ \mathbf{U} is a unitary matrix, i.e., $\mathbf{U}\mathbf{U}^T = \mathbf{U}^T\mathbf{U} = \mathbb{I}$, and $\mathbf{\Lambda}$ is a diagonal matrix.
 - ▶ $\text{prox}_{\lambda g}(\mathbf{x}) = \mathbf{U}(\mathbb{I} + \lambda\mathbf{\Lambda})^{-1}\mathbf{U}^T(\mathbf{x} + \lambda\mathbf{A}\mathbf{b})$.

A non-exhaustive list of proximal tractability functions

Name	Function	Proximal operator	Complexity
ℓ_1 -norm	$f(\mathbf{x}) := \ \mathbf{x}\ _1$	$\text{prox}_{\lambda f}(\mathbf{x}) = \text{sign}(\mathbf{x}) \otimes [\mathbf{x} - \lambda]_+$	$\mathcal{O}(p)$
ℓ_2 -norm	$f(\mathbf{x}) := \ \mathbf{x}\ _2$	$\text{prox}_{\lambda f}(\mathbf{x}) = [1 - \frac{\lambda}{\ \mathbf{x}\ _2}]_+ \mathbf{x}$	$\mathcal{O}(p)$
Support function	$f(\mathbf{x}) := \max_{\mathbf{y} \in \mathcal{C}} \mathbf{x}^T \mathbf{y}$	$\text{prox}_{\lambda f}(\mathbf{x}) = \mathbf{x} - \lambda \pi_{\mathcal{C}}(\mathbf{x})$	
Box indicator	$f(\mathbf{x}) := \delta_{[\mathbf{a}, \mathbf{b}]}(\mathbf{x})$	$\text{prox}_{\lambda f}(\mathbf{x}) = \pi_{[\mathbf{a}, \mathbf{b}]}(\mathbf{x})$	$\mathcal{O}(p)$
Positive semidefinite cone indicator	$f(\mathbf{X}) := \delta_{\mathbb{S}_+^p}(\mathbf{X})$	$\text{prox}_{\lambda f}(\mathbf{X}) = \mathbf{U}[\Sigma]_+ \mathbf{U}^T$, where $\mathbf{X} = \mathbf{U}\Sigma\mathbf{U}^T$	$\mathcal{O}(p^3)$
Hyperplane indicator	$f(\mathbf{x}) := \delta_{\mathcal{X}}(\mathbf{x})$, $\mathcal{X} := \{\mathbf{x} : \mathbf{a}^T \mathbf{x} = b\}$	$\text{prox}_{\lambda f}(\mathbf{x}) = \pi_{\mathcal{X}}(\mathbf{x}) = \mathbf{x} + \left(\frac{b - \mathbf{a}^T \mathbf{x}}{\ \mathbf{a}\ _2}\right) \mathbf{a}$	$\mathcal{O}(p)$
Simplex indicator	$f(\mathbf{x}) = \delta_{\mathcal{X}}(\mathbf{x})$, $\mathcal{X} := \{\mathbf{x} : \mathbf{x} \geq 0, \mathbf{1}^T \mathbf{x} = 1\}$	$\text{prox}_{\lambda f}(\mathbf{x}) = (\mathbf{x} - \nu \mathbf{1})$ for some $\nu \in \mathbb{R}$, which can be efficiently calculated	$\tilde{\mathcal{O}}(p)$
Convex quadratic	$f(\mathbf{x}) := \frac{1}{2} \mathbf{x}^T \mathbf{Q} \mathbf{x} + \mathbf{q}^T \mathbf{x}$	$\text{prox}_{\lambda f}(\mathbf{x}) = (\lambda \mathbf{I} + \mathbf{Q})^{-1} \mathbf{x}$	$\mathcal{O}(p \log p) \rightarrow \mathcal{O}(p^3)$
Square ℓ_2 -norm	$f(\mathbf{x}) := \frac{1}{2} \ \mathbf{x}\ _2^2$	$\text{prox}_{\lambda f}(\mathbf{x}) = \frac{1}{1+\lambda} \mathbf{x}$	$\mathcal{O}(p)$
log-function	$f(x) := -\log(x)$	$\text{prox}_{\lambda f}(x) = \frac{1}{2} (\sqrt{x^2 + 4\lambda} + x)$	$\mathcal{O}(1)$
log det-function	$f(\mathbf{X}) := -\log \det(\mathbf{X})$	$\text{prox}_{\lambda f}(\mathbf{X})$ is the log-function prox applied to the individual eigenvalues of \mathbf{X}	$\mathcal{O}(p^3)$

Remarks:

- Here: $[\mathbf{x}]_+ := \max\{0, \mathbf{x}\}$ and $\delta_{\mathcal{X}}$ is the indicator function of the convex set \mathcal{X} .
- sign is the sign function, \mathbb{S}_+^p is the cone of symmetric positive semidefinite matrices.
- For more functions, see [5, 15].

Solution methods

Composite convex minimization

$$F^* := \min_{\mathbf{x} \in \mathbb{R}^p} \left\{ F(\mathbf{x}) := f(\mathbf{x}) + g(\mathbf{x}) \right\}. \quad (5)$$

Choice of numerical solution methods

◦ **Solve (5)** = Find $\mathbf{x}^k \in \mathbb{R}^p$ such that

$$F(\mathbf{x}^k) - F^* \leq \varepsilon$$

for a given tolerance $\varepsilon > 0$.

◦ **Oracles:** We can use one of the following configurations (**oracles**):

1. $\partial f(\cdot)$ and $\partial g(\cdot)$ at any point $\mathbf{x} \in \mathbb{R}^p$.
2. $\nabla f(\cdot)$ and $\text{prox}_{\lambda g}(\cdot)$ at any point $\mathbf{x} \in \mathbb{R}^p$.
3. $\text{prox}_{\lambda f}$ and $\text{prox}_{\lambda g}(\cdot)$ at any point $\mathbf{x} \in \mathbb{R}^p$.
4. $\nabla f(\cdot)$, inverse of $\nabla^2 f(\cdot)$ and $\text{prox}_{\lambda g}(\cdot)$ at any point $\mathbf{x} \in \mathbb{R}^p$.

Remark: Using different oracle leads to different types of algorithms.

Proximal-gradient algorithm

Basic proximal-gradient scheme (ISTA)

1. Choose $\mathbf{x}^0 \in \text{dom}(F)$ arbitrarily as a starting point.
2. For $k = 0, 1, \dots$, generate a sequence $\{\mathbf{x}^k\}_{k \geq 0}$ as:

$$\mathbf{x}^{k+1} := \text{prox}_{\alpha g} \left(\mathbf{x}^k - \alpha \nabla f(\mathbf{x}^k) \right),$$

where $\alpha := \frac{1}{L}$.

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where $\alpha := \frac{1}{L}$.

Theorem (Convergence of ISTA [2])

Let $\{\mathbf{x}^k\}$ be generated by ISTA. Then:

$$F(\mathbf{x}^k) - F^* \leq \frac{L_f \|\mathbf{x}^0 - \mathbf{x}^*\|_2^2}{2(k+1)}$$

The worst-case complexity to reach $F(\mathbf{x}^k) - F^* \leq \varepsilon$ of (ISTA) is $\mathcal{O}\left(\frac{L_f R_0^2}{\varepsilon}\right)$, where $R_0 := \max_{\mathbf{x}^* \in \mathcal{S}^*} \|\mathbf{x}^0 - \mathbf{x}^*\|_2$.

- o **Oracles:** $\text{prox}_{\alpha g}(\cdot)$ and $\nabla f(\cdot)$.
- o Compared to the subgradient gradient method, the rate improves at the cost of prox-computation.

Fast proximal-gradient algorithm

Fast proximal-gradient scheme (FISTA)

1. Choose $\mathbf{x}^0 \in \text{dom}(F)$ arbitrarily as a starting point.
2. Set $\mathbf{y}^0 := \mathbf{x}^0$ and $t_0 := 1$, $\alpha := L^{-1}$.
3. For $k = 0, 1, \dots$, generate two sequences $\{\mathbf{x}^k\}_{k \geq 0}$ and $\{\mathbf{y}^k\}_{k \geq 0}$ as:

$$\begin{cases} \mathbf{x}^{k+1} & := \text{prox}_{\alpha g}(\mathbf{y}^k - \alpha \nabla f(\mathbf{y}^k)), \\ t_{k+1} & := \frac{1}{2}(1 + \sqrt{4t_k^2 + 1}), \\ \mathbf{y}^{k+1} & := \mathbf{x}^{k+1} + \frac{t_k - 1}{t_{k+1}}(\mathbf{x}^{k+1} - \mathbf{x}^k). \end{cases}$$

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Theorem (Convergence of FISTA [2])

Let $\{\mathbf{x}^k\}$ be generated by FISTA. Then:

$$F(\mathbf{x}^k) - F^* \leq \frac{2L_f \|\mathbf{x}^0 - \mathbf{x}^*\|_2^2}{(k+1)^2}$$

The worst-case complexity to reach $F(\mathbf{x}^k) - F^* \leq \varepsilon$ of (FISTA) is $\mathcal{O}\left(R_0 \sqrt{\frac{L_f}{\varepsilon}}\right)$, $R_0 := \max_{\mathbf{x}^* \in \mathcal{S}^*} \|\mathbf{x}^0 - \mathbf{x}^*\|_2$.

Fast proximal-gradient algorithm

Fast proximal-gradient scheme (FISTA)

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Remark: From $\mathcal{O}\left(\frac{L_f R_0^2}{\epsilon}\right)$ to $\mathcal{O}\left(R_0 \sqrt{\frac{L_f}{\epsilon}}\right)$ iterations at almost no additional cost!

Complexity per iteration

- ▶ **One** gradient $\nabla f(\mathbf{y}^k)$ and **one** prox-operator of g ;
- ▶ 8 arithmetic operations for t_{k+1} and γ_{k+1} ;
- ▶ 2 more vector additions, and **one** scalar-vector multiplication.

The **cost per iteration** is **almost the same** as in **gradient scheme** if proximal operator of g is efficient.

Example 1: ℓ_1 -regularized least squares

Problem (ℓ_1 -regularized least squares)

Given $\mathbf{A} \in \mathbb{R}^{n \times p}$ and $\mathbf{b} \in \mathbb{R}^n$, solve:

$$F^* := \min_{\mathbf{x} \in \mathbb{R}^p} \left\{ F(\mathbf{x}) := \frac{1}{2} \|\mathbf{A}\mathbf{x} - \mathbf{b}\|_2^2 + \lambda \|\mathbf{x}\|_1 \right\}, \quad (6)$$

where $\lambda > 0$ is a regularization parameter.

Complexity per iterations

- ▶ Evaluating $\nabla f(\mathbf{x}^k) = \mathbf{A}^T(\mathbf{A}\mathbf{x}^k - \mathbf{b})$ requires one $\mathbf{A}\mathbf{x}$ and one $\mathbf{A}^T\mathbf{y}$.
- ▶ One soft-thresholding operator $\text{prox}_{\lambda g}(\mathbf{x}) = \text{sign}(\mathbf{x}) \otimes \max\{|\mathbf{x}| - \lambda, 0\}$.
- ▶ **Optional:** Evaluating $L = \|\mathbf{A}^T\mathbf{A}\|$ (spectral norm) - via **power iterations**

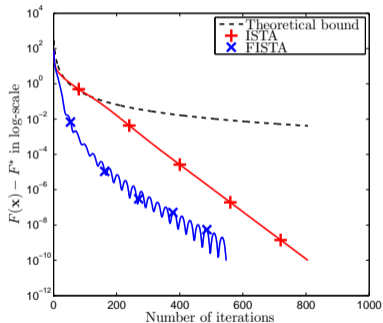
Synthetic data generation

- ▶ $\mathbf{A} := \text{randn}(n, p)$ - standard Gaussian $\mathcal{N}(0, \mathbb{I})$.
- ▶ \mathbf{x}^* is a k -sparse vector generated randomly.
- ▶ $\mathbf{b} := \mathbf{A}\mathbf{x}^* + \mathcal{N}(0, 10^{-3})$.

Example 1: Theoretical bounds vs practical performance

Theoretical bounds

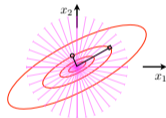
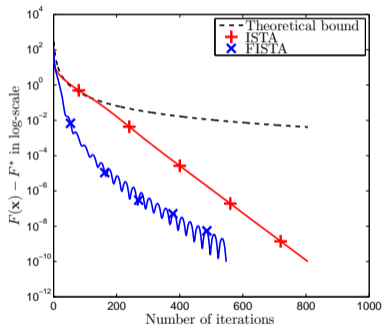
We have the following guarantees for **FISTA** $:= \frac{2L_f R_0^2}{(k+2)^2}$ and for **ISTA** $:= \frac{L_f R_0^2}{2(k+2)}$. In the figure below, ISTA's practical behavior outperforms the theoretical bound for FISTA.



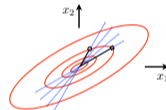
Example 1: Theoretical bounds vs practical performance

Theoretical bounds

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descent directions

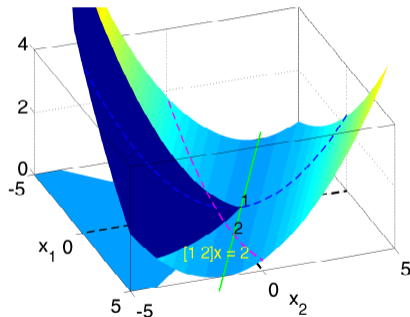
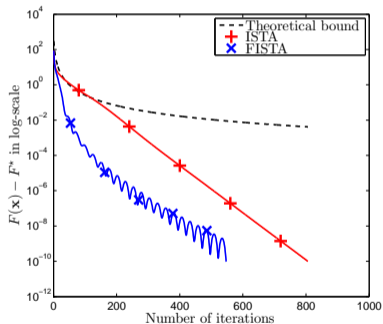


restricted descent directions

Example 1: Theoretical bounds vs practical performance

Theoretical bounds

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Remarks:

- ℓ_1 -regularized least squares formulation has **restricted strong convexity**.
- The proximal-gradient method can automatically exploit this structure.

Example 2: Sparse logistic regression

Problem (Sparse logistic regression)

Given $\mathbf{A} \in \mathbb{R}^{n \times p}$ and $\mathbf{b} \in \{-1, +1\}^n$, solve:

$$F^* := \min_{\mathbf{x}, \beta} \left\{ F(\mathbf{x}) := \frac{1}{n} \sum_{j=1}^n \log(1 + \exp(-\mathbf{b}_j(\mathbf{a}_j^T \mathbf{x} + \beta))) + \rho \|\mathbf{x}\|_1 \right\}.$$

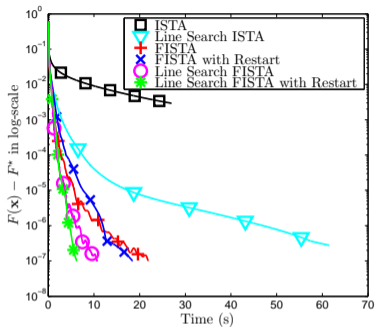
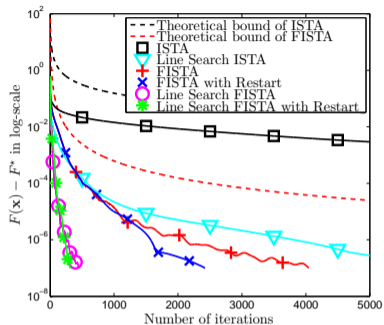
Real data

- ▶ Real data: w8a with $n = 49'749$ data points, $p = 300$ features
- ▶ Available at <http://www.csie.ntu.edu.tw/~cjlin/libsvmtools/datasets/binary.html>.

Parameters

- ▶ $\rho = 10^{-4}$.
- ▶ Number of iterations 5000, tolerance 10^{-7} .
- ▶ Ground truth: Solve problem up to 10^{-9} accuracy by TFOCS to get a high accuracy approximation of \mathbf{x}^* and F^* .

Example 2: Sparse logistic regression - numerical results



	ISTA	LS-ISTA	FISTA	FISTA-R	LS-FISTA	LS-FISTA-R
Number of iterations	5000	5000	4046	2423	447	317
CPU time (s)	26.975	61.506	21.859	18.444	10.683	6.228
Solution error ($\times 10^{-7}$)	29370	2.774	1.000	0.998	0.961	0.985

When f is **strongly convex**: Algorithms

Proximal-gradient scheme (ISTA $_{\mu}$)

1. Given $\mathbf{x}^0 \in \mathbb{R}^p$ as a starting point.
2. For $k = 0, 1, \dots$, generate a sequence $\{\mathbf{x}^k\}_{k \geq 0}$ as:

$$\mathbf{x}^{k+1} := \text{prox}_{\alpha_k g} \left(\mathbf{x}^k - \alpha_k \nabla f(\mathbf{x}^k) \right),$$

where $\alpha_k := \frac{2}{L_f + \mu}$ is the optimal step-size.

Fast proximal-gradient scheme (FISTA $_{\mu}$)

1. Given $\mathbf{x}^0 \in \mathbb{R}^p$ as a starting point. Set $\mathbf{y}^0 := \mathbf{x}^0$.
2. For $k = 0, 1, \dots$, generate sequences $\{\mathbf{x}^k\}_{k \geq 0}$ and $\{\mathbf{y}^k\}_{k \geq 0}$ as:

$$\begin{cases} \mathbf{x}^{k+1} := \text{prox}_{\alpha_k g} \left(\mathbf{y}^k - \alpha_k \nabla f(\mathbf{y}^k) \right), \\ \mathbf{y}^{k+1} := \mathbf{x}^{k+1} + \left(\frac{\sqrt{c_f - 1}}{\sqrt{c_f + 1}} \right) (\mathbf{x}^{k+1} - \mathbf{x}^k), \end{cases}$$

where $c_f := \frac{L_f}{\mu}$ and $\alpha_k := L_f^{-1}$ is the optimal step-size.

When f is **strongly convex**: Convergence

Assumption

f is **strongly convex** with parameter $\mu > 0$, i.e., $f \in \mathcal{F}_{L,\mu}^{1,1}(\mathbb{R}^p)$.

Condition number: $c_f := \frac{L_f}{\mu} \geq 0$.

Theorem (**ISTA** _{μ} [14])

$$F(\mathbf{x}^k) - F^* \leq \frac{L_f}{2} \left(\frac{c_f - 1}{c_f + 1} \right)^{2k} \|\mathbf{x}^0 - \mathbf{x}^*\|_2^2.$$

Convergence rate: **Linear** with contraction factor: $\omega := \left(\frac{c_f - 1}{c_f + 1} \right)^2 = \left(\frac{L_f - \mu}{L_f + \mu} \right)^2$.

Theorem (**FISTA** _{μ} [14])

$$F(\mathbf{x}^k) - F^* \leq \frac{L_f + \mu}{2} \left(1 - \sqrt{\frac{\mu}{L_f}} \right)^k \|\mathbf{x}^0 - \mathbf{x}^*\|_2^2.$$

Convergence rate: **Linear** with contraction factor: $\omega_f = \frac{\sqrt{L_f} - \sqrt{\mu}}{\sqrt{L_f}} < \omega$.

Summary of the worst-case complexities

Comparison

Complexity	Proximal-gradient scheme	Fast proximal-gradient scheme
Complexity [$\mu = 0$]	$\mathcal{O}\left(R_0^2 \frac{L_f}{\varepsilon}\right)$	$\mathcal{O}\left(R_0 \sqrt{\frac{L_f}{\varepsilon}}\right)$
Per iteration	1-gradient, 1-prox, 1- sv , 1- $v+$	1-gradient, 1-prox, 2- sv , 3- $v+$
Complexity [$\mu > 0$]	$\mathcal{O}\left(\kappa \log(\varepsilon^{-1})\right)$	$\mathcal{O}\left(\sqrt{\kappa} \log(\varepsilon^{-1})\right)$
Per iteration	1-gradient, 1-prox, 1- sv , 1- $v+$	1-gradient, 1-prox, 1- sv , 2- $v+$

Here: sv = scalar-vector multiplication, $v+$ = vector addition.

$R_0 := \max_{\mathbf{x}^* \in \mathcal{S}^*} \|\mathbf{x}^0 - \mathbf{x}^*\|$ and $\kappa = \frac{L_f}{\mu_f}$ is the condition number.

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- ▶ computing $\nabla f(\mathbf{x})$ is much costlier than computing prox_g

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Need alternatives when

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Software

TFOCS is a good software package to learn about first order methods.

<http://cvxr.com/tfocs/>

Composite minimization: **Non-convex** case

Problem (Unconstrained composite minimization)

$$F^* := \min_{\mathbf{x} \in \mathbb{R}^p} \{F(\mathbf{x}) := f(\mathbf{x}) + g(\mathbf{x})\}$$

(CM)

- ▶ $g: \mathbb{R}^p \rightarrow \mathbb{R} \cup \{\infty\}$ is **proper, closed, convex**, and (possibly) **nonsmooth**.
- ▶ $f: \mathbb{R}^p \rightarrow \mathbb{R}$ is **proper and closed**, $\text{dom}(f)$ is **convex**, and f is **L_f -smooth**.
- ▶ $\text{dom}(F) := \text{dom}(f) \cap \text{dom}(g) \neq \emptyset$ and $-\infty < F^* < +\infty$.
- ▶ The solution set $\mathcal{S}^* := \{\mathbf{x}^* \in \text{dom}(F) : F(\mathbf{x}^*) = F^*\}$ is **nonempty**.

A different quantification of convergence: Gradient mapping

Definition (Gradient mapping)

Let prox_g denote the proximal operator of g and $\lambda > 0$ some real constant. Then, the gradient mapping operator is defined as

$$\mathcal{G}_\lambda(\mathbf{x}) := \frac{1}{\lambda} \left(\mathbf{x} - \text{prox}_{\lambda g}(\mathbf{x} - \lambda \nabla f(\mathbf{x})) \right).$$

Properties [1]

- ▶ $\|\mathcal{G}_\lambda(\mathbf{x})\| = 0 \iff \mathbf{x}$ is a stationary point.
- ▶ Lipschitz continuity: $\|\mathcal{G}_{\frac{1}{L}}(\mathbf{x}) - \mathcal{G}_{\frac{1}{L}}(\mathbf{y})\| \leq (2L + L_f)\|\mathbf{x} - \mathbf{y}\|$

Why do we care about gradient mapping?

- ▶ It is the generalization of the gradient of f , $\nabla f(\mathbf{x})$
- ▶ Recall prox-gradient update: $\mathbf{x}^{t+1} = \text{prox}_{\lambda g}(\mathbf{x}^t - \lambda \nabla f(\mathbf{x}^t))$, which is equivalent to $\mathbf{x}^{t+1} = \mathbf{x}^t - \lambda \mathcal{G}_\lambda(\mathbf{x}^t)$.
- ▶ In fact, when $\text{prox}_g = \mathbb{I}$, then, $\mathcal{G}_\lambda(\mathbf{x}) = \frac{1}{\lambda} (\mathbf{x} - (\mathbf{x} - \lambda \nabla f(\mathbf{x}))) = \nabla f(\mathbf{x})$.

Sufficient Decrease property for proximal-gradient

Assumption

- ▶ f is L_f -smooth.
- ▶ g is proper, closed, convex, and (possibly) nonsmooth. g is proximally tractable.

$$\mathbf{x}^{k+1} := \text{prox}_{\frac{1}{L}g} \left(\mathbf{x}^k - \frac{1}{L} \nabla f(\mathbf{x}^k) \right)$$

Lemma (Sufficient decrease [1])

For any $\mathbf{x} \in \text{int}(\text{dom}(f))$ and $L \in (\frac{L_f}{2}, \infty)$, it holds that

$$F(\mathbf{x}^{k+1}) \leq F(\mathbf{x}^k) - \frac{L - \frac{L_f}{2}}{L^2} \left\| \mathcal{G}_{\frac{1}{L}}(\mathbf{x}^k) \right\|_2^2, \quad (7)$$

Corollary

$$F(\mathbf{x}^{k+1}) \leq F(\mathbf{x}^k) - \frac{1}{2L_f} \left\| \mathcal{G}_{\frac{1}{L_f}}(\mathbf{x}^k) \right\|_2^2, \quad \text{for } L = L_f$$

Non-convex case: Convergence

Basic proximal-gradient scheme

1. Choose $\mathbf{x}^0 \in \text{dom}(F)$ arbitrarily as a starting point.
2. For $k = 0, 1, \dots$, generate a sequence $\{\mathbf{x}^k\}_{k \geq 0}$ as:

$$\mathbf{x}^{k+1} := \text{prox}_{\alpha g} \left(\mathbf{x}^k - \alpha \nabla f(\mathbf{x}^k) \right),$$

$$\text{where } \alpha := \left(0, \frac{2}{L_f} \right).$$

Theorem (Convergence of proximal-gradient method: Non-convex [1])

Let $\{\mathbf{x}^k\}$ be generated by proximal-gradient scheme above. Then, we have

$$\min_{i=0,1,\dots,k} \|\mathcal{G}_\alpha(\mathbf{x}^i)\|_2^2 \leq \frac{F(\mathbf{x}^0) - F(\mathbf{x}^*)}{M(k+1)}, \quad \text{where } M := \alpha^2 \left(\frac{1}{\alpha} - \frac{L_f}{2} \right)$$

- ▶ When $\alpha = \frac{1}{L_f}$, $M = \frac{1}{2L_f}$.
- ▶ The worst-case complexity to reach $\min_{i=0,1,\dots,k} \|\mathcal{G}_\alpha(\mathbf{x}^i)\|_2^2 \leq \varepsilon$ is $\mathcal{O}\left(\frac{1}{\varepsilon}\right)$.

Stochastic **convex** composite minimization

Problem (Mathematical formulation)

Consider the following composite convex minimization problem:

$$F^* = \min_{\mathbf{x} \in \mathbb{R}^p} \left\{ F(\mathbf{x}) := \mathbb{E}_\theta[F(\mathbf{x}, \theta)] := \mathbb{E}_\theta[f(\mathbf{x}, \theta) + g(\mathbf{x}, \theta)] \right\}$$

- ▶ θ is a random vector whose probability distribution is supported on set Θ .
- ▶ The solution set $\mathcal{S}^* := \{\mathbf{x}^* \in \text{dom}(F) : F(\mathbf{x}^*) = F^*\}$ is nonempty.
- ▶ **Oracles:** (sub)gradient of $f(\cdot, \theta)$, $\nabla f(\mathbf{x}, \theta)$, and stochastic prox operator of $g(\cdot, \theta)$, $\text{prox}_{g(\cdot, \theta)}(\mathbf{x})$.

Remark

- In this setting, we replace $\nabla f(\cdot)$ with its stochastic estimates.
- It is possible to replace $\text{prox}_g(\cdot)$ with its stochastic estimate (advanced material).

Stochastic proximal gradient method

Stochastic proximal gradient method (SPG)

1. Choose $\mathbf{x}^0 \in \mathbb{R}^p$ and $(\alpha_k)_{k \in \mathbb{N}} \in]0, +\infty[^{\mathbb{N}}$.
2. For $k = 0, 1, \dots$ perform:

$$\mathbf{x}^{k+1} = \text{prox}_{\alpha_k g(\cdot, \theta)}(\mathbf{x}^k - \alpha_k G(\mathbf{x}^k, \theta_k)).$$

Definitions:

- $\text{prox}_{\alpha g(\cdot, \theta)} := \arg \min_{\mathbf{y} \in \mathbb{R}^p} \left\{ g(\mathbf{y}, \theta) + \frac{1}{2\alpha} \|\mathbf{y} - \mathbf{x}\|^2 \right\}$
- $\{\theta_k\}_{k=0,1,\dots}$: sequence of independent random variables.
- $G(\mathbf{x}^k, \theta_k) \in \partial f(\mathbf{x}^k, \theta_k)$: an unbiased estimate of the deterministic (sub)gradient:

$$\mathbb{E}[G(\mathbf{x}^k, \theta_k)] \in \partial f(\mathbf{x}^k).$$

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$$\mathbb{E}[G(\mathbf{x}^k, \theta_k)] \in \partial f(\mathbf{x}^k).$$

Remark

Cost of computing $G(\mathbf{x}^k, \theta_k)$ is usually much cheaper than $\nabla f(\mathbf{x}^k)$.

Convergence analysis

Assumptions for the problem setting

- ▶ $f(\cdot, \theta)$ and $g(\cdot, \theta)$ are convex functions in the first argument, g is proximally-tractable.
- ▶ (Sub)gradients of F satisfy stochastic bounded gradient condition: $\exists C \geq 0, B \geq 0$ such that

$$\mathbb{E}_\theta[\|\partial F(\mathbf{x}, \theta)\|^2] \leq B^2 + C(F(\mathbf{x}) - F(\mathbf{x}^*)).$$

- ▶ $\mathbb{E}[\|\mathbf{x}^t - \mathbf{x}^*\|^2] \leq R^2$ for all $t \geq 0$.

Implications of the assumptions

- ▶ None of the above assumptions enforce that f is smooth.
- ▶ Stochastic bounded gradient condition holds with $C = 0$ when both $f(\cdot, \theta)$ and $g(\cdot, \theta)$ are Lipschitz continuous.
- ▶ The same condition holds when $f(\cdot, \theta)$ is L_f -smooth and $g(\cdot, \theta)$ is Lipschitz continuous.
- ▶ **However, for the upcoming theorem, we will take $C > 0$, which rules out the case when both functions are only Lipschitz continuous.**

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- ▶ $\mathbb{E}[\|\mathbf{x}^t - \mathbf{x}^*\|^2] \leq R^2$ for all $t \geq 0$.

Theorem (Ergodic convergence [12])

- ▶ Assume the above assumptions hold with $C > 0$.
- ▶ Let the sequence $\{\mathbf{x}^k\}_{k \geq 0}$ be generated by SPG.
- ▶ Set $\alpha_k = \frac{1}{C\sqrt{k}}$.

Conclusion:

- ▶ Define $\bar{\mathbf{x}}^k = \frac{1}{k} \sum_{i=0}^{k-1} \mathbf{x}^i$, then

$$\mathbb{E}[F(\bar{\mathbf{x}}^k) - F(\mathbf{x}^*)] \leq \frac{1}{\sqrt{k}} \left(R^2 C + \frac{B^2}{C} \right), \quad \forall k \geq 1.$$

Revisiting a special composite structure

A basic constrained problem setting

$$f^* := \min_{\mathbf{x} \in \mathbb{R}^p} \left\{ f(\mathbf{x}) + \delta_{\mathcal{X}}(\mathbf{x}) \right\} := \min_{\mathbf{x} \in \mathbb{R}^p} \left\{ f(\mathbf{x}) : \mathbf{x} \in \mathcal{X} \right\}, \quad (8)$$

Assumptions

- ▶ \mathcal{X} is nonempty, convex and compact (closed and bounded) where $\delta_{\mathcal{X}}$ is its indicator function.
- ▶ $f \in \mathcal{F}_L^{1,1}(\mathbb{R}^p)$ (i.e., convex with Lipschitz gradient).

Recall proximal gradient algorithm

Basic proximal-gradient scheme (ISTA)

1. Choose $\mathbf{x}^0 \in \text{dom}(F)$ arbitrarily as a starting point.
2. For $k = 0, 1, \dots$, generate a sequence $\{\mathbf{x}^k\}_{k \geq 0}$ as:

$$\mathbf{x}^{k+1} := \text{prox}_{\alpha g} \left(\mathbf{x}^k - \alpha \nabla f(\mathbf{x}^k) \right)$$

where $\alpha := \frac{1}{L}$.

- ▶ Prox-operator of indicator of \mathcal{X} is projection onto $\mathcal{X} \implies$ ensures feasibility

How else can we ensure feasibility?

Frank-Wolfe's approach - I

$$f^* := \min_{\mathbf{x} \in \mathbb{R}^p} \left\{ f(\mathbf{x}) : \mathbf{x} \in \mathcal{X} \right\},$$

Conditional gradient method (CGM, see [10] for review)

A plausible strategy which dates back to 1956 [6]. At iteration k :

1. Consider the linear approximation of f at \mathbf{x}^k

$$\phi_k(\mathbf{x}) := f(\mathbf{x}^k) + \nabla f(\mathbf{x}^k)^T (\mathbf{x} - \mathbf{x}^k)$$

2. Minimize this approximation within constraint set

$$\hat{\mathbf{x}}^k \in \min_{\mathbf{x} \in \mathcal{X}} \phi_k(\mathbf{x}) = \min_{\mathbf{x} \in \mathcal{X}} \nabla f(\mathbf{x}^k)^T \mathbf{x}$$

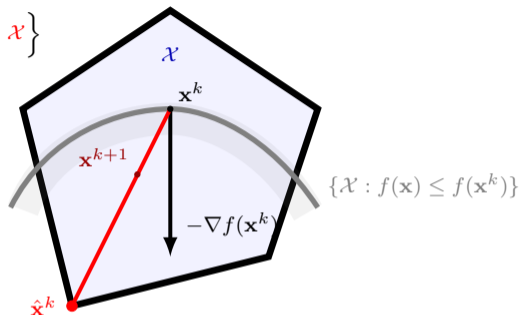
3. Take a step towards $\hat{\mathbf{x}}^k$ with step-size $\alpha_k \in [0, 1]$

$$\mathbf{x}^{k+1} = \mathbf{x}^k + \alpha_k (\hat{\mathbf{x}}^k - \mathbf{x}^k)$$

- \mathbf{x}^{k+1} is feasible since it is convex combination of two other feasible points.

Frank-Wolfe's approach - II

$$f^* := \min_{\mathbf{x} \in \mathbb{R}^p} \left\{ f(\mathbf{x}) : \mathbf{x} \in \mathcal{X} \right\}$$



Conditional gradient method (CGM)

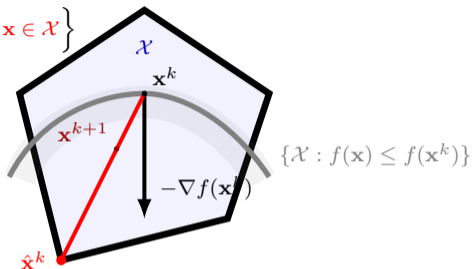
1. Choose $\mathbf{x}^0 \in \mathcal{X}$.
2. For $k = 0, 1, \dots$ perform:

$$\begin{cases} \hat{\mathbf{x}}^k & := \arg \min_{\mathbf{x} \in \mathcal{X}} \nabla f(\mathbf{x}^k)^T \mathbf{x} \\ \mathbf{x}^{k+1} & := (1 - \alpha_k) \mathbf{x}^k + \alpha \hat{\mathbf{x}}^k, \end{cases}$$

where $\alpha_k := \frac{2}{k+2}$.

On the linear minimization oracle

$$f^* := \min_{\mathbf{x} \in \mathbb{R}^p} \left\{ f(\mathbf{x}) : \mathbf{x} \in \mathcal{X} \right\}$$



Definition (Linear minimization oracle)

Let \mathcal{X} be a convex, closed and bounded set. Then, the linear minimization oracle of \mathcal{X} ($\text{lmo}_{\mathcal{X}}$) returns a vector $\hat{\mathbf{x}}$ such that

$$\text{lmo}_{\mathcal{X}}(\mathbf{x}) := \hat{\mathbf{x}} \in \arg \min_{\mathbf{y} \in \mathcal{X}} \mathbf{x}^T \mathbf{y} \quad (9)$$

- ▶ $\text{lmo}_{\mathcal{X}}$ returns an extreme point of \mathcal{X} .
- ▶ $\text{lmo}_{\mathcal{X}}$ is arguably cheaper than projection.
- ▶ $\text{lmo}_{\mathcal{X}}$ is not single valued, note \in in the definition.

Convergence guarantees of CGM

Problem setting

$$f^* := \min_{\mathbf{x} \in \mathbb{R}^p} \left\{ f(\mathbf{x}) : \mathbf{x} \in \mathcal{X} \right\},$$

Assumptions

- ▶ \mathcal{X} is nonempty, **convex**, closed and **bounded**.
- ▶ $f \in \mathcal{F}_L^{1,1}(\mathbb{R}^p)$ (i.e., convex with Lipschitz gradient).

Theorem

Under **assumptions** listed above, CGM with step size $\alpha_k = \frac{2}{k+2}$ satisfies

$$f(\mathbf{x}^k) - f(\mathbf{x}^*) \leq \frac{4LD_{\mathcal{X}}^2}{k+1} \quad (10)$$

where $D_{\mathcal{X}} := \max_{\mathbf{x}, \mathbf{y} \in \mathcal{X}} \|\mathbf{x} - \mathbf{y}\|_2$ is diameter of constraint set.

*Convergence guarantees of CGM: A faster rate

Problem setting

$$f^* := \min_{\mathbf{x} \in \mathbb{R}^p} \left\{ f(\mathbf{x}) : \mathbf{x} \in \mathcal{X} \right\},$$

Assumptions

- ▶ \mathcal{X} is nonempty, α -strongly convex, closed and bounded.
- ▶ $f \in \mathcal{F}_{L,\mu}^{1,1}(\mathbb{R}^p)$ (i.e., strongly convex with Lipschitz gradient).

Definition (α -strongly convex set) [7]

A convex set $\mathcal{X} \in \mathbb{R}^{p \times p}$ is α -strongly convex with respect to $\|\cdot\|$ if for any $\mathbf{x}, \mathbf{y} \in \mathcal{X}$, any $\alpha \in [0, 1]$ and any vector $\mathbf{z} \in \mathbb{R}^{p \times p}$ such that $\|\mathbf{z}\| = 1$, it holds that

$$\alpha \mathbf{x} + (1 - \alpha) \mathbf{y} + \alpha(1 - \alpha) \frac{\alpha}{2} \|\mathbf{x} - \mathbf{y}\|^2 \mathbf{z} \in \mathcal{X}$$

That is, for any $\mathbf{x}, \mathbf{y} \in \mathcal{X}$, the ball centered at $\alpha \mathbf{x} + (1 - \alpha) \mathbf{y}$ with radius $\alpha(1 - \alpha) \frac{\alpha}{2} \|\mathbf{x} - \mathbf{y}\|^2$ is contained in \mathcal{X} .

*CGM for strongly convex objective + strongly convex set

Conditional gradient method - CGM2

1. Choose $\mathbf{x}^0 \in \mathcal{X}$.
2. For $k = 0, 1, \dots$ perform:

$$\begin{cases} \hat{\mathbf{x}}^k & := \arg \min_{\mathbf{x} \in \mathcal{X}} \nabla f(\mathbf{x}^k)^T \mathbf{x} \\ \alpha_k & := \arg \min_{\alpha \in [0,1]} \alpha \langle \hat{\mathbf{x}}^k - \mathbf{x}^k, \nabla f(\mathbf{x}^k) \rangle + \alpha^2 \frac{L}{2} \|\hat{\mathbf{x}}^k - \mathbf{x}^k\|^2 \\ \mathbf{x}^{k+1} & := (1 - \alpha_k) \mathbf{x}^k + \alpha_k \hat{\mathbf{x}}^k, \end{cases}$$

Theorem ([7])

Under *assumptions* listed previously, CGM2 satisfies

$$f(\mathbf{x}^k) - f(\mathbf{x}^*) = \mathcal{O}\left(\frac{1}{k^2}\right).$$

(11)

Example: lmo of nuclear-norm ball

Consider $\delta_{\mathcal{X}}$, the indicator of nuclear-norm ball $\mathcal{X} := \{\mathbf{X} : \mathbf{X} \in \mathbb{R}^{p \times p}, \|\mathbf{X}\|_* \leq \alpha\}$

lmo of nuclear-norm ball

$$\text{lmo}_{\mathcal{X}}(\mathbf{X}) := \hat{\mathbf{X}} \in \arg \min_{\mathbf{Y} \in \mathcal{X}} \langle \mathbf{Y}, \mathbf{X} \rangle$$

This can be computed as follows:

- ▶ Compute top singular vectors of $\mathbf{X} \implies (\mathbf{u}_1, \sigma_1, \mathbf{v}_1) = \text{svds}(\mathbf{X}, 1)$.
- ▶ Form the rank-1 output $\implies \hat{\mathbf{X}} = \alpha \mathbf{u}_1 \mathbf{v}_1^T$

We can efficiently approximate top singular vectors by power method!

Proximal gradient vs. Frank-Wolfe

Definitions:

- ▶ Here: sv = scalar-vector multiplication, $v+$ = vector addition.
- ▶ $R_0 := \max_{\mathbf{x}^* \in \mathcal{S}^*} \|\mathbf{x}^0 - \mathbf{x}^*\|$ is the maximum initial distance.
- ▶ $D_{\mathcal{X}} := \max_{\mathbf{x}, \mathbf{y} \in \mathcal{X}} \|\mathbf{x} - \mathbf{y}\|_2$ is diameter of constraint set \mathcal{X} .

Algorithm	Proximal-gradient scheme	Frank-Wolfe method
Rate	$\mathcal{O}\left(\frac{L_f R_0^2}{k}\right)$	$\mathcal{O}\left(\frac{L_f D_{\mathcal{X}}^2}{k}\right)$
Complexity	$\mathcal{O}\left(R_0^2 \frac{L_f}{\epsilon}\right)$	$\mathcal{O}\left(D_{\mathcal{X}}^2 \frac{L_f}{\epsilon}\right)$
Per iteration	1-gradient, 1-prox, 1- sv , 1- $v+$	1-gradient, 1-lmo, 2- sv , 1- $v+$

How do prox operator and lmo compare in practice?

An example with matrices

Problem Definition

$$\min_{\mathbf{X} \in \mathbb{R}^{p \times p}} f(\mathbf{X}) + g(\mathbf{X})$$

- ▶ Define $g(\mathbf{X}) = \delta_{\mathcal{X}}(\mathbf{X})$, where $\mathcal{X} := \{\mathbf{X} : \mathbf{X} \in \mathbb{R}^{p \times p}, \|\mathbf{X}\|_* \leq \alpha\}$ is nuclear norm ball.
- ▶ This problem is equivalent to:

$$\min_{\mathbf{X} \in \mathcal{X}} f(\mathbf{X})$$

Observations

- ▶ $\text{prox}_g = \pi_{\mathcal{X}}$. Projection requires full SVD, $\mathcal{O}(p^3)$.
- ▶ Imo computes (approximately) top singular vectors, roughly in $\approx \mathcal{O}(p^2)$ with Lanczos algorithm.

Example: Phase retrieval

Phase retrieval

Aim: Recover signal $\mathbf{x}^\natural \in \mathbb{C}^p$ from the measurements $\mathbf{b} \in \mathbb{R}^n$:

$$b_i = |\langle \mathbf{a}_i, \mathbf{x}^\natural \rangle|^2 + \omega_i.$$

($\mathbf{a}_i \in \mathbb{C}^p$ are known measurement vectors, ω_i models noise).

- Non-linear measurements \rightarrow **non-convex** maximum likelihood estimators.

PhaseLift [4]

Phase retrieval can be solved as a convex matrix completion problem, following a combination of

- ▶ semidefinite relaxation ($\mathbf{x}^\natural \mathbf{x}^{\natural H} = \mathbf{X}^\natural$)
- ▶ convex relaxation ($\text{rank} \rightarrow \|\cdot\|_*$)

albeit in terms of the lifted variable $\mathbf{X} \in \mathbb{C}^{p \times p}$.

Example: Phase retrieval - II

Problem formulation

We solve the following PhaseLift variant:

$$f^* := \min_{\mathbf{X} \in \mathbb{C}^{P \times P}} \left\{ \frac{1}{2} \|\mathcal{A}(\mathbf{X}) - \mathbf{b}\|_2^2 : \|\mathbf{X}\|_* \leq \kappa, \mathbf{X} \geq 0 \right\}. \quad (12)$$

Experimental setup [19]

Coded diffraction pattern measurements, $\mathbf{b} = [\mathbf{b}_1, \dots, \mathbf{b}_L]$ with $L = 20$ different masks

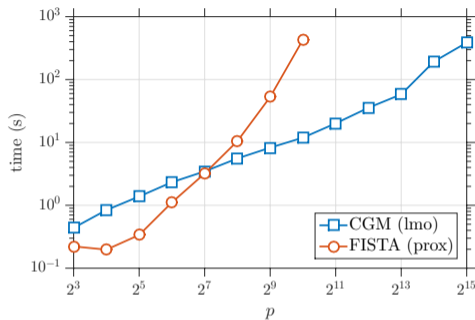
$$\mathbf{b}_\ell = |\text{fft}(\mathbf{d}_\ell^H \odot \mathbf{x}^h)|^2$$

→ \odot denotes Hadamard product; $|\cdot|^2$ applies element-wise

→ \mathbf{d}_ℓ are randomly generated octonary masks (distributions as proposed in [4])

→ Parametric choices: $\lambda^0 = \mathbf{0}^n$; $\epsilon = 10^{-2}$; $\kappa = \text{mean}(\mathbf{b})$.

Example: Phase retrieval - III



Test with synthetic data: Prox vs sharp

→ Synthetic data: $\mathbf{x}^h = \text{randn}(p, 1) + i \cdot \text{randn}(p, 1)$.

→ Stopping criteria: $\frac{\|\mathbf{x}^h - \mathbf{x}^k\|_2}{\|\mathbf{x}^h\|_2} \leq 10^{-2}$.

→ Averaged over 10 Monte-Carlo iterations.

Note that the problem is $p \times p$ dimensional!

A basic constrained **non-convex** problem

Problem setting

$$f^* := \min_{\mathbf{x} \in \mathcal{X}} \left\{ f(\mathbf{x}) : \mathbf{x} \in \mathcal{X} \right\},$$

Assumptions

- ▶ \mathcal{X} is nonempty, **convex**, closed and **bounded**.
- ▶ f has L -Lipschitz continuous gradients, but it is **non-convex**.

Stationary point

Due to constraints, $\|\nabla f(\mathbf{x}^*)\| = 0$ may not hold!

Frank-Wolfe gap: Following measure, known as FW-gap, generalizes the definition of stationary point for constrained problems:

$$g_{FW}(\mathbf{x}) := \max_{\mathbf{y} \in \mathcal{X}} (\mathbf{x} - \mathbf{y})^T \nabla f(\mathbf{x})$$

- ▶ $g_{FW}(\mathbf{x}) \geq 0$ for all $\mathbf{x} \in \mathcal{X}$.
- ▶ $\mathbf{x} \in \mathcal{X}$ is a stationary point if and only if $g_{FW}(\mathbf{x}) = 0$.

CGM for non-convex problems

CGM for non-convex problems
<ol style="list-style-type: none">1. Choose $\mathbf{x}^0 \in \mathcal{X}$, $K > 0$ total number of iterations.2. For $k = 0, 1, \dots, K - 1$ perform: $\begin{cases} \hat{\mathbf{x}}^k & := \text{lmo}_{\mathcal{X}}(\nabla f(\mathbf{x}^k)) \\ \mathbf{x}^{k+1} & := (1 - \alpha_k)\mathbf{x}^k + \alpha_k \hat{\mathbf{x}}^k, \end{cases}$
where $\alpha_k := \frac{1}{\sqrt{K+1}}$.

Theorem

Denote $\bar{\mathbf{x}}$ chosen uniformly random from $\{\mathbf{x}^1, \mathbf{x}^2, \dots, \mathbf{x}^K\}$. Then, CGM satisfies

$$\min_{k=1,2,\dots,K} g_{FW}(\mathbf{x}^k) \leq \mathbb{E}[g_{FW}(\bar{\mathbf{x}})] \leq \frac{1}{\sqrt{K}} \left(f(\mathbf{x}^0) - f^* + \frac{LD^2}{2} \right).$$

* There exist stochastic CGM methods for non-convex problems. See [17] for details.

A basic constrained **stochastic** problem

Problem setting (Stochastic)

$$f^* := \min_{\mathbf{x} \in \mathcal{X}} \left\{ \mathbb{E}[f(\mathbf{x}, \theta)] : \mathbf{x} \in \mathcal{X} \right\}, \quad (13)$$

Assumptions

- ▶ θ is a random vector whose probability distribution is supported on set Θ
- ▶ \mathcal{X} is nonempty, **convex**, closed and **bounded**.
- ▶ $f(\cdot, \theta) \in \mathcal{F}_L^{1,1}(\mathbb{R}^p)$ for all θ (i.e., convex with Lipschitz gradient).

Example (Finite-sum model)

$$\mathbb{E}[f(\mathbf{x}, \theta)] = \frac{1}{n} \sum_{j=1}^n f_j(\mathbf{x})$$

- ▶ $j = \theta$ is drawn uniformly from $\Theta = \{1, 2, \dots, n\}$
- ▶ $f_j \in \mathcal{F}_L^{1,1}(\mathbb{R}^p)$ for all j (i.e., convex with Lipschitz gradient).

Stochastic conditional gradient method

Stochastic conditional gradient method (SFW)

1. Choose $\mathbf{x}^0 \in \mathcal{X}$.
2. For $k = 0, 1, \dots$ perform:

$$\begin{cases} \hat{\mathbf{x}}^k & := \operatorname{lmo}_{\mathcal{X}}(\tilde{\nabla} f(\mathbf{x}^k, \theta_k)) \\ \mathbf{x}^{k+1} & := (1 - \alpha_k)\mathbf{x}^k + \alpha_k \hat{\mathbf{x}}^k, \end{cases}$$

where $\alpha_k := \frac{2}{k+2}$, and $\tilde{\nabla} f$ is an unbiased estimator of ∇f .

Theorem [9]

Assume that the following variance condition holds

$$\mathbb{E} \|\nabla f(\mathbf{x}^k) - \tilde{\nabla} f(\mathbf{x}^k, \theta_k)\|^2 \leq \left(\frac{LD}{k+1}\right)^2. \quad (*)$$

Then, the iterates of SFW satisfies

$$\mathbb{E}[f(\mathbf{x}^k, \theta)] - f^* \leq \frac{4LD^2}{k+1}.$$

(*) \rightarrow SFW requires decreasing variance!

Stochastic conditional gradient method

Stochastic conditional gradient method (SFW)

1. Choose $\mathbf{x}^0 \in \mathcal{X}$.
2. For $k = 0, 1, \dots$ perform:

$$\begin{cases} \hat{\mathbf{x}}^k & := \operatorname{lmo}_{\mathcal{X}}(\tilde{\nabla} f(\mathbf{x}^k, \theta_k)) \\ \mathbf{x}^{k+1} & := (1 - \alpha_k)\mathbf{x}^k + \alpha_k \hat{\mathbf{x}}^k, \end{cases}$$

where $\alpha_k := \frac{2}{k+2}$, and $\tilde{\nabla} f$ is an unbiased estimator of ∇f .

Example (Finite-sum model)

$$\mathbb{E}[f(\mathbf{x}, \theta)] = \frac{1}{n} \sum_{j=1}^n f_j(\mathbf{x})$$

Assume f_j is G -Lipschitz continuous for all j . Suppose that \mathcal{S}_k is a random sampling (with replacement) from $\Theta = \{1, 2, \dots, n\}$. Then,

$$\tilde{\nabla} f(\mathbf{x}^k, \theta_k) := \frac{1}{|\mathcal{S}_k|} \sum_{j \in \mathcal{S}_k} f_j(\mathbf{x}^k) \quad \implies \quad \mathbb{E} \|\nabla f(\mathbf{x}) - \tilde{\nabla} f(\mathbf{x}, \theta_k)\|^2 \leq \frac{G^2}{|\mathcal{S}_k|}.$$

Hence, by choosing $|\mathcal{S}_k| = \left(\frac{G(k+1)}{LD}\right)^2$ we satisfy the variance condition for SFW.

Wrap up!

- Friday: Transition from variance reduction to deep learning...

*Expanding on prox operator and optimality condition

Notes

- ▶ By definition, $g(\mathbf{y}) + \frac{1}{2\lambda} \|\mathbf{y} - \mathbf{x}\|^2$ attains its minimum when $\mathbf{y} = \text{prox}_{\lambda g}(\mathbf{x})$.
 - ▶ One can see that $g(\mathbf{y}) + \frac{1}{2\lambda} \|\mathbf{y} - \mathbf{x}\|^2$ is **convex**, and prox operator computes its minimizer **over \mathbb{R}^P** .
 - ▶ As a result, **subdifferential** of $g(\mathbf{y}) + \frac{1}{2\lambda} \|\mathbf{y} - \mathbf{x}\|^2$ **at the minimizer** ($\mathbf{y} = \text{prox}_{\lambda g}(\mathbf{x})$) should **include 0**.
 - ▶ Hence, $0 \in \partial g(\text{prox}_{\lambda g}(\mathbf{x})) + \frac{1}{\lambda} (\text{prox}_{\lambda g}(\mathbf{x}) - \mathbf{x})$.

 - ▶ After rearranging the above inclusion we obtain: $\mathbf{x} \in \lambda \partial g(\text{prox}_{\lambda g}(\mathbf{x})) + \text{prox}_{\lambda g}(\mathbf{x})$
 - ▶ We can rewrite the RHS as a **single function**: $\lambda \partial g(\text{prox}_{\lambda g}(\mathbf{x})) + \text{prox}_{\lambda g}(\mathbf{x}) = (\lambda \partial g + \mathbb{I})(\text{prox}_{\lambda g}(\mathbf{x}))$
 - ▶ The inclusion becomes: $\mathbf{x} \in (\lambda \partial g + \mathbb{I})(\text{prox}_{\lambda g}(\mathbf{x}))$.

 - ▶ Finally, we compute the inverse of $(\lambda \partial g + \mathbb{I})(\cdot)$ to conclude: $\text{prox}_{\lambda g}(\mathbf{x}) = (\lambda \partial g + \mathbb{I})^{-1}(\mathbf{x})$.
-
- In the literature, $(\lambda \partial g + \mathbb{I})^{-1}$ is called the **resolvent of the subdifferential of g with parameter λ** .
 - This is just a technical term that stands for **proximal operator of λg** , as we have defined in this course.

* A short detour: Basic properties of prox-operator

Property (Basic properties of prox-operator)

1. $\text{prox}_g(\mathbf{x})$ is *well-defined* and *single-valued* (i.e., the prox-operator (3) has a unique solution since $g(\cdot) + \frac{1}{2}\|\cdot - \mathbf{x}\|_2^2$ is strongly convex).

2. *Optimality condition*:

$$\mathbf{x} \in \text{prox}_g(\mathbf{x}) + \partial g(\text{prox}_g(\mathbf{x})), \quad \mathbf{x} \in \mathbb{R}^P.$$

3. \mathbf{x}^* is a *fixed point* of $\text{prox}_g(\cdot)$:

$$0 \in \partial g(\mathbf{x}^*) \Leftrightarrow \mathbf{x}^* = \text{prox}_g(\mathbf{x}^*).$$

4. *Nonexpansiveness*:

$$\|\text{prox}_g(\mathbf{x}) - \text{prox}_g(\tilde{\mathbf{x}})\|_2 \leq \|\mathbf{x} - \tilde{\mathbf{x}}\|_2, \quad \forall \mathbf{x}, \tilde{\mathbf{x}} \in \mathbb{R}^P.$$

Note: An operator is called *non-expansive* if it is L -Lipschitz continuous with $L = 1$.

*Adaptive Restart

It is possible to preserve $\mathcal{O}(\frac{1}{k^2})$ convergence guarantee !

One needs to slightly modify the algorithm as below.

Generalized fast proximal-gradient scheme

1. Choose $\mathbf{x}^0 = \mathbf{x}^{-1} \in \text{dom}(F)$ arbitrarily as a starting point.
2. Set $\theta_0 = \theta_{-1} = 1$, $\lambda := L_f^{-1}$
3. For $k = 0, 1, \dots$, generate two sequences $\{\mathbf{x}^k\}_{k \geq 0}$ and $\{\mathbf{y}^k\}_{k \geq 0}$ as:

$$\left\{ \begin{array}{l} \mathbf{y}^k := \mathbf{x}^k + \theta_k(\theta_{k-1}^{-1} - 1)(\mathbf{x}^k - \mathbf{x}^{k-1}) \\ \mathbf{x}^{k+1} := \text{prox}_{\lambda g}(\mathbf{y}^k - \lambda \nabla f(\mathbf{y}^k)), \\ \text{if restart test holds} \\ \theta_{k-1} = \theta_k = 1 \\ \mathbf{y}^k = \mathbf{x}^k \\ \mathbf{x}^{k+1} := \text{prox}_{\lambda g}(\mathbf{y}^k - \lambda \nabla f(\mathbf{y}^k)) \end{array} \right. \quad (14)$$

θ_k is chosen so that it satisfies

$$\theta_{k+1} = \frac{\sqrt{\theta_k^4 + 4\theta_k^2} - \theta_k^2}{2} < \frac{2}{k+3}$$

*Adaptive Restart: Guarantee

Theorem (Global complexity [8])

The sequence $\{\mathbf{x}^k\}_{k \geq 0}$ generated by the modified algorithm satisfies

$$F(\mathbf{x}^k) - F^* \leq \frac{2L_f}{(k+2)^2} \left(R_0^2 + \sum_{k_i \leq k} (\|\mathbf{x}^* - \mathbf{x}^{k_i}\|_2^2 - \|\mathbf{x}^* - \mathbf{z}^{k_i}\|_2^2) \right) \quad \forall k \geq 0. \quad (15)$$

where $R_0 := \min_{\mathbf{x}^* \in \mathcal{S}^*} \|\mathbf{x}^0 - \mathbf{x}^*\|$, $\mathbf{z}^k = \mathbf{x}^{k-1} + \theta_{k-1}^{-1}(\mathbf{x}^k - \mathbf{x}^{k-1})$ and $k_i, i = 1 \dots$ are the iterations for which the restart test holds.

Various restarts tests that might coincide with $\|\mathbf{x}^* - \mathbf{x}^{k_i}\|_2^2 \leq \|\mathbf{x}^* - \mathbf{z}^{k_i}\|_2^2$

- ▶ Exact non-monotonicity test: $F(\mathbf{x}^{k+1}) - F(\mathbf{x}^k) > 0$
- ▶ Non-monotonicity test: $\langle (L_F(\mathbf{y}^{k-1} - \mathbf{x}^k), \mathbf{x}^{k+1} - \frac{1}{2}(\mathbf{x}^k + \mathbf{y}^{k-1})) \rangle > 0$ (implies exact non-monotonicity and it is advantageous when function evaluations are expensive)
- ▶ Gradient-mapping based test: $\langle (L_f(\mathbf{y}^k - \mathbf{x}^{k+1}), \mathbf{x}^{k+1} - \mathbf{x}^k) \rangle > 0$

*Recall: Composite convex minimization

Problem (Unconstrained composite convex minimization)

$$F^* := \min_{\mathbf{x} \in \mathbb{R}^p} \{F(\mathbf{x}) := f(\mathbf{x}) + g(\mathbf{x})\}$$

- ▶ f and g are both *proper, closed, and convex*.
- ▶ $\text{dom}(F) := \text{dom}(f) \cap \text{dom}(g) \neq \emptyset$ and $-\infty < F^* < +\infty$.
- ▶ The solution set $\mathcal{S}^* := \{\mathbf{x}^* \in \text{dom}(F) : F(\mathbf{x}^*) = F^*\}$ is *nonempty*.

*Recall: Composite convex minimization guarantees

Proximal gradient method (ISTA) vs. fast proximal gradient method (FISTA)

Assumptions, step sizes and convergence rates

Proximal gradient method:

$$f \in \mathcal{F}_L^{1,1}, \quad \alpha = \frac{1}{L}$$

$$F(\mathbf{x}^k) - F(\mathbf{x}^*) \leq \epsilon, \quad \mathcal{O}\left(\frac{1}{\epsilon}\right).$$

Fast proximal gradient method:

$$f \in \mathcal{F}_L^{1,1}, \quad \alpha = \frac{1}{L}$$

$$F(\mathbf{x}^k) - F(\mathbf{x}^*) \leq \epsilon, \quad \mathcal{O}\left(\frac{1}{\sqrt{\epsilon}}\right).$$

*Recall: Composite convex minimization guarantees

Proximal gradient method (ISTA) vs. fast proximal gradient method (FISTA)

Assumptions, step sizes and convergence rates

Proximal gradient method:

$$f \in \mathcal{F}_L^{1,1}, \quad \alpha = \frac{1}{L}$$

$$F(\mathbf{x}^k) - F(\mathbf{x}^*) \leq \epsilon, \quad \mathcal{O}\left(\frac{1}{\epsilon}\right).$$

Fast proximal gradient method:

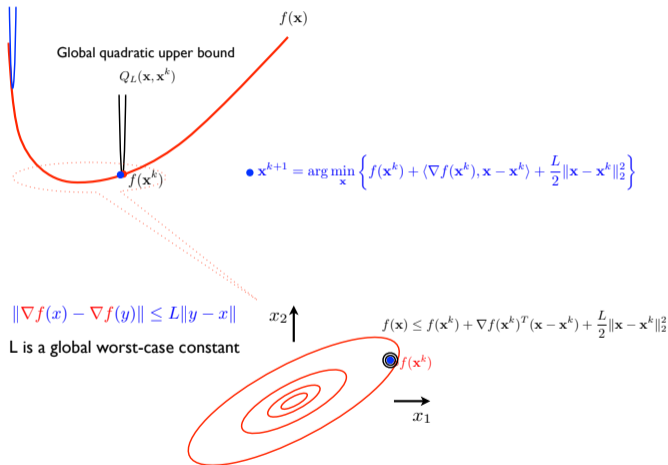
$$f \in \mathcal{F}_L^{1,1}, \quad \alpha = \frac{1}{L}$$

$$F(\mathbf{x}^k) - F(\mathbf{x}^*) \leq \epsilon, \quad \mathcal{O}\left(\frac{1}{\sqrt{\epsilon}}\right).$$

- We require α_k to be a function of L .
- It may not be possible to know exactly the Lipschitz constant. Line-search ?
- Adaptation to local geometry \rightarrow may lead to larger steps.

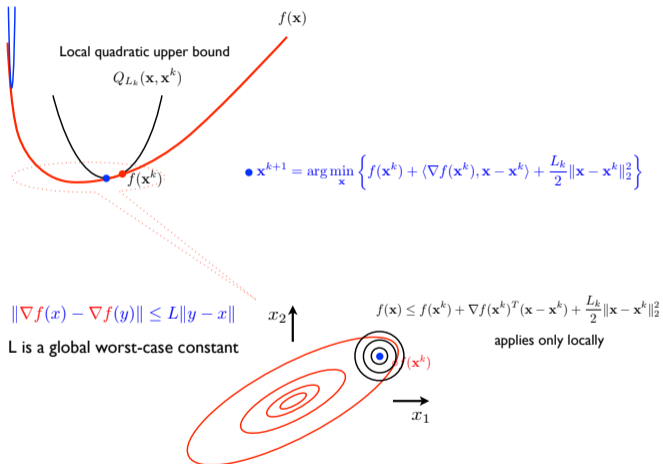
*How can we better adapt to the local geometry?

Non-adaptive:



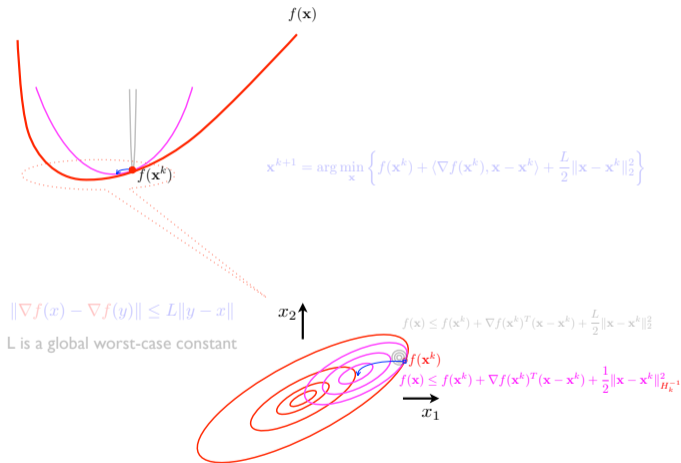
*How can we better adapt to the local geometry?

Line-search:



*How can we better adapt to the local geometry?

Variable metric:



*The idea of the proximal-Newton method

Assumptions A.2

Assume that $f \in \mathcal{F}_{L,\mu}^{2,1}(\mathbb{R}^p)$ and $g \in \mathcal{F}_{\text{prox}}(\mathbb{R}^p)$.

*Proximal-Newton update

- ▶ Similar to classical newton, proximal-newton suggests the following update scheme using second order Taylor series expansion near \mathbf{x}_k .

$$\mathbf{x}^{k+1} := \arg \min_{\mathbf{x} \in \mathbb{R}^p} \left\{ \underbrace{\frac{1}{2}(\mathbf{x} - \mathbf{x}^k)^T \nabla^2 f(\mathbf{x}^k)(\mathbf{x} - \mathbf{x}^k) + \nabla f(\mathbf{x}^k)^T (\mathbf{x} - \mathbf{x}^k)}_{\text{2nd-order Taylor expansion near } \mathbf{x}^k} + g(\mathbf{x}) \right\}. \quad (16)$$

*The proximal-Newton-type algorithm

Proximal-Newton algorithm (PNA)

1. Given $\mathbf{x}^0 \in \mathbb{R}^p$ as a starting point.
2. For $k = 0, 1, \dots$, perform the following steps:
 - 2.1. Evaluate an SDP matrix $\mathbf{H}_k \approx \nabla^2 f(\mathbf{x}^k)$ and $\nabla f(\mathbf{x}^k)$.
 - 2.2. Compute $\mathbf{d}^k := \text{prox}_{\mathbf{H}_k^{-1}g}(\mathbf{x}^k - \mathbf{H}_k^{-1}\nabla f(\mathbf{x}^k)) - \mathbf{x}^k$.
 - 2.3. Update $\mathbf{x}^{k+1} := \mathbf{x}^k + \alpha_k \mathbf{d}^k$.

*The proximal-Newton-type algorithm

Proximal-Newton algorithm (PNA)

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 - 2.3. Update $\mathbf{x}^{k+1} := \mathbf{x}^k + \alpha_k \mathbf{d}^k$.

Remark

- ▶ $\mathbf{H}_k \equiv \nabla^2 f(\mathbf{x}^k) \implies$ proximal-Newton algorithm.
- ▶ $\mathbf{H}_k \approx \nabla^2 f(\mathbf{x}^k) \implies$ proximal-quasi-Newton algorithm.
- ▶ A generalized prox-operator: $\text{prox}_{\mathbf{H}_k^{-1}g}(\mathbf{x}^k + \mathbf{H}_k^{-1}\nabla f(\mathbf{x}^k))$.

*Convergence analysis

Theorem (Global convergence [11])

Assume generalized-prox subproblem is solved *exactly* for the algorithm and there exists $\mu > 0$ such that $\mathbf{H}_k \succeq \mu \mathbf{I}$ for all $k \geq 0$. Then;

$\{\mathbf{x}^k\}_{k \geq 0}$ *globally converges* to a solution \mathbf{x}^* of (2).

*Convergence analysis

Theorem (Global convergence [11])

Assume generalized-prox subproblem is solved **exactly** for the algorithm and there exists $\mu > 0$ such that $\mathbf{H}_k \succeq \mu \mathbb{I}$ for all $k \geq 0$. Then;

$\{\mathbf{x}^k\}_{k \geq 0}$ **globally converges** to a solution \mathbf{x}^* of (2).

Theorem (Local convergence [11])

Assume generalized-prox subproblem is solved **exactly** for the algorithm there exists $0 < \mu \leq L_2 < +\infty$ such that $\mu \mathbb{I} \preceq \mathbf{H}_k \preceq L_2 \mathbb{I}$ for **all sufficiently large k** . Then;

- ▶ If $\mathbf{H}_k \equiv \nabla^2 f(\mathbf{x}^k)$, then $\alpha_k = 1$ for k **sufficiently large** (full-step).
- ▶ If $\mathbf{H}_k \equiv \nabla^2 f(\mathbf{x}^k)$, then $\{\mathbf{x}^k\}$ **locally converges** to \mathbf{x}^* at a **quadratic rate**.
- ▶ If \mathbf{H}_k satisfies the Dennis-Moré condition:

$$\lim_{k \rightarrow +\infty} \frac{\|(\mathbf{H}_k - \nabla^2 f(\mathbf{x}^*))(\mathbf{x}^{k+1} - \mathbf{x}^k)\|}{\|\mathbf{x}^{k+1} - \mathbf{x}^k\|} = 0, \quad (17)$$

then $\{\mathbf{x}^k\}$ **locally converges** to \mathbf{x}^* at a **super linear rate**.

*How to compute the approximation \mathbf{H}_k ?

How to update \mathbf{H}_k ?

Matrix \mathbf{H}_k can be updated by using **low-rank updates**.

- ▶ **BFGS update**: **maintain** the **Dennis-Moré condition** and $\mathbf{H}_k \succ 0$.

$$\mathbf{H}_{k+1} := \mathbf{H}_k + \frac{\mathbf{y}_k \mathbf{y}_k^T}{\mathbf{s}_k^T \mathbf{y}_k} - \frac{\mathbf{H}_k \mathbf{s}_k \mathbf{s}_k^T \mathbf{H}_k}{\mathbf{s}_k^T \mathbf{H}_k \mathbf{s}_k}, \quad \mathbf{H}_0 := \gamma \mathbb{I}, \quad (\gamma > 0).$$

where $\mathbf{y}_k := \nabla f(\mathbf{x}^{k+1}) - \nabla f(\mathbf{x}^k)$ and $\mathbf{s}_k := \mathbf{x}^{k+1} - \mathbf{x}^k$.

- ▶ **Diagonal+Rank-1 [3]**: computing PN direction \mathbf{d}^k is in **polynomial time**, but it **does not** maintain the Dennis-Moré condition:

$$\mathbf{H}_k := \mathbf{D}_k + \mathbf{u}_k \mathbf{u}_k^T, \quad \mathbf{u}_k := \frac{\mathbf{s}_k - \mathbf{H}_0 \mathbf{y}_k}{\sqrt{(\mathbf{s}_k - \mathbf{H}_0 \mathbf{y}_k)^T \mathbf{y}_k}},$$

where \mathbf{D}_k is a **positive diagonal matrix**.

*Pros and cons

Pros

- ▶ **Fast local convergence rate** (super-linear or quadratic)
- ▶ **Numerical robustness** under the inexactness/noise ([11]).
- ▶ Well-suited for problems with **many** data points but **few** parameters. For example,

$$F^* := \min_{\mathbf{x} \in \mathbb{R}^p} \left\{ \sum_{j=1}^n \ell_j(\mathbf{a}_j^T \mathbf{x} + b_j) + g(\mathbf{x}) \right\},$$

where ℓ_j is twice continuously differentiable and convex, $g \in \mathcal{F}_{\text{prox}}$, $p \ll n$.

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where ℓ_j is twice continuously differentiable and convex, $g \in \mathcal{F}_{\text{prox}}$, $p \ll n$.

Cons

- ▶ **Expensive iteration** compared to proximal-gradient methods.
- ▶ **Global convergence rate** may be **worse** than accelerated proximal-gradient methods.
- ▶ Requires a **good** initial point to get **fast local convergence**.
- ▶ Requires **strict conditions** for global/local convergence analysis.

*Example 1: Sparse logistic regression

Problem (Sparse logistic regression)

Given a sample vector $\mathbf{a} \in \mathbb{R}^p$ and a binary class label vector $\mathbf{b} \in \{-1, +1\}^n$. The conditional probability of a label b given \mathbf{a} is defined as:

$$\mathbb{P}(b|\mathbf{a}, \mathbf{x}, \mu) = \frac{1}{1 + e^{-b(\mathbf{x}^T \mathbf{a} + \mu)}},$$

where $\mathbf{x} \in \mathbb{R}^p$ is a weight vector, μ is called the intercept.

Goal: Find a sparse-weight vector \mathbf{x} via the maximum likelihood principle.

Optimization formulation

$$\min_{\mathbf{x} \in \mathbb{R}^p} \left\{ \underbrace{\frac{1}{n} \sum_{i=1}^n L(b_i(\mathbf{a}_i^T \mathbf{x} + \mu))}_{f(\mathbf{x})} + \underbrace{\rho \|\mathbf{x}\|_1}_{g(\mathbf{x})} \right\}, \quad (18)$$

where \mathbf{a}_i is the i -th row of data matrix \mathbf{A} in $\mathbb{R}^{n \times p}$, $\rho > 0$ is a regularization parameter, and ℓ is the logistic loss function $\ell(\tau) := \log(1 + e^{-\tau})$.

*Example: Sparse logistic regression

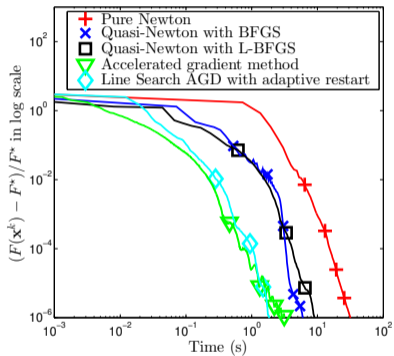
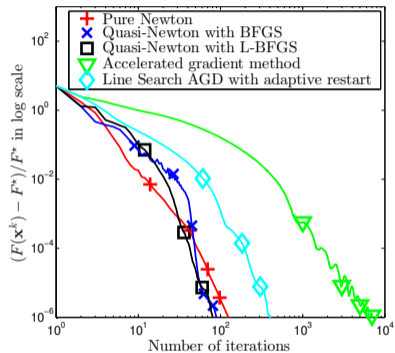
Real data

- ▶ Real data: w2a with $n = 3470$ data points, $p = 300$ features
- ▶ Available at <http://www.csie.ntu.edu.tw/~cjlin/libsvmtools/datasets/binary.html>.

Parameters

- ▶ Tolerance 10^{-6} .
- ▶ L-BFGS memory $m = 50$.
- ▶ Ground truth: Get a high accuracy approximation of \mathbf{x}^* and f^* by TFOCS with tolerance 10^{-12} .

*Example: Sparse logistic regression-Numerical results



*Example 2: ℓ_1 -regularized least squares

Problem (ℓ_1 -regularized least squares)

Given $\mathbf{A} \in \mathbb{R}^{n \times p}$ and $\mathbf{b} \in \mathbb{R}^n$, solve:

$$F^* := \min_{\mathbf{x} \in \mathbb{R}^p} \left\{ F(\mathbf{x}) := \frac{1}{2} \|\mathbf{Ax} - \mathbf{b}\|_2^2 + \rho \|\mathbf{x}\|_1 \right\},$$

where $\rho > 0$ is a regularization parameter.

Complexity per iterations

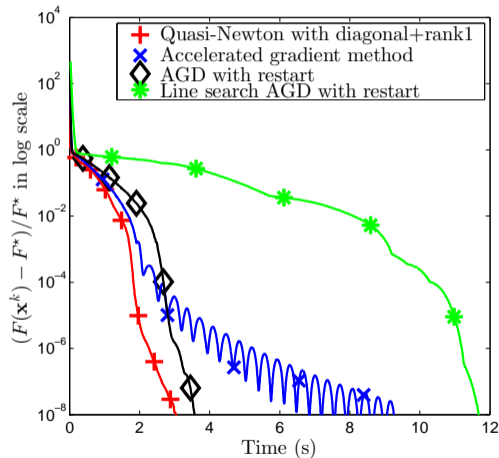
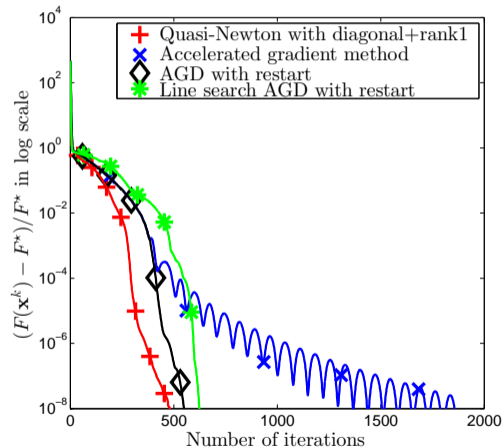
- ▶ Evaluating $\nabla f(\mathbf{x}^k) = \mathbf{A}^T(\mathbf{Ax}^k - \mathbf{b})$ requires one \mathbf{Ax} and one $\mathbf{A}^T\mathbf{y}$.
- ▶ One soft-thresholding operator $\text{prox}_{\lambda g}(\mathbf{x}) = \text{sign}(\mathbf{x}) \otimes \max\{|\mathbf{x}| - \rho, 0\}$.
- ▶ **Optional:** Evaluating $L = \|\mathbf{A}^T\mathbf{A}\|$ (spectral norm) - via **power iterations** (e.g., 20 iterations, each iteration requires one \mathbf{Ax} and one $\mathbf{A}^T\mathbf{y}$).

Synthetic data generation

- ▶ $\mathbf{A} := \text{randn}(n, p)$ - standard Gaussian $\mathcal{N}(0, \mathbb{I})$.
- ▶ \mathbf{x}^* is a s -sparse vector generated randomly.
- ▶ $\mathbf{b} := \mathbf{Ax}^* + \mathcal{N}(0, 10^{-3})$.

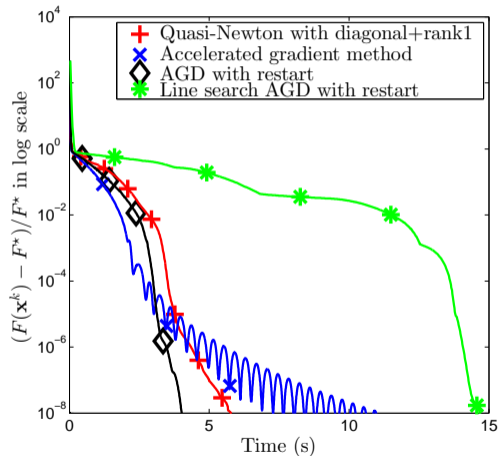
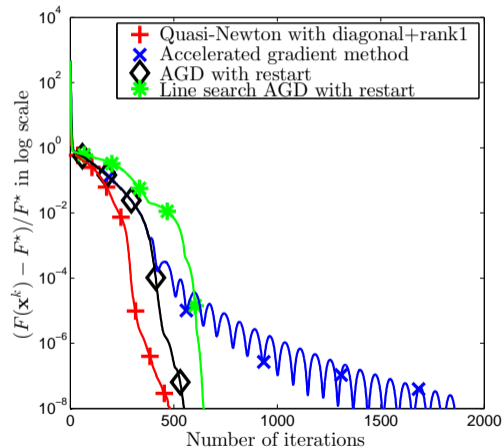
* Example 2: ℓ_1 -regularized least squares - Numerical results - Trial 1

Parameters: $n = 750, p = 2000, s = 200, \rho = 1$



* Example 2: ℓ_1 -regularized least squares - Numerical results - Trial 2

Parameters: $n = 750, p = 2000, s = 200, \rho = 1$



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