## Mathematics of Data: From Theory to Computation

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## Lecture 9: Composite convex minimization I <br> Laboratory for Information and Inference Systems (LIONS) <br> École Polytechnique Fédérale de Lausanne (EPFL)

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## Outline

- Today

1. Motivation for non-smooth optimization
2. Composite convex minimization
3. Proximal operator and computational complexity
4. Proximal gradient methods

- Next week

1. Proximal Newton-type methods
2. Stochastic proximal methods

## Recommended reading material

- A. Beck and M. Tebulle, A Fast Iterative Shrinkage-Thresholding Algorithm for Linear Inverse Problems, SIAM J. Imaging Sciences, 2(1), 183-202, 2009.
- Y. Nesterov, Smooth minimization of non-smooth functions, Math. Program, 103(1), 127-152, 2005.
- Q. Tran-Dinh, A. Kyrillidis and V. Cevher, Composite Self-Concordant Minimization, LIONS-EPFL Tech. Report. http://arxiv.org/abs/1308.2867, 2013.
- N. Parikh and S. Boyd, Proximal Algorithms, Foundations and Trends in Optimization, 1(3):123-231, 2014.


## Convex minimization: non-smooth and composite

## Motivation

Data analytics problems in various disciplines can often be simplified to nonsmooth composite convex minimization problems. To this end, this lecture provides efficient numerical solution methods for such problems.

Intriguingly, composite minimization problems are far from generic nonsmooth problems and we can exploit individual function structures to obtain numerical solutions nearly as efficiently as if they are smooth problems.

## Nonsmooth: When smooth models are deficient

## Example: Linear Regression

Consider the classical linear regression problem:

$$
\mathbf{b}=\mathbf{A} \mathbf{x}^{\natural}+\mathbf{w}
$$

with $\mathbf{b} \in \mathbb{R}^{n}, \mathbf{A} \in \mathbb{R}^{n \times p}$ are known, $\mathbf{x}^{\natural}$ is unknown, and $\mathbf{w}$ is noise. Assume for now that $n \geq p$ (more later).

Standard approach: Least squares: $\hat{\mathbf{x}}_{\mathrm{LS}} \in \arg \min _{\mathbf{x}}\|\mathbf{b}-\mathbf{A x}\|_{2}^{2}$

- Convex, smooth, and an explicit solution: $\hat{\mathbf{x}}_{\mathrm{LS}}=\left(\mathbf{A}^{T} \mathbf{A}\right)^{-1} \mathbf{A}^{T} \mathbf{b}=\mathbf{A}^{\dagger} \mathbf{b}$


## Practical performance of an estimator $\hat{\mathbf{x}}$

Denote the numerical approximation by $\mathbf{x}_{\epsilon}^{\star}$. The practical performance is determined by

$$
\left\|\mathbf{x}_{\epsilon}^{\star}-\mathbf{x}^{\natural}\right\|_{2} \leq \underbrace{\left\|\mathbf{x}_{\epsilon}^{\star}-\hat{\mathbf{x}}\right\|_{2}}_{\text {approximation error }}+\underbrace{\left\|\hat{\mathbf{x}}-\mathbf{x}^{\natural}\right\|_{2}}_{\text {statistical error }}
$$

Motivation: non-smooth estimators of $\mathbf{x}^{\natural}$ can help reduce the statistical error.

## Non-smooth unconstrained convex minimization

Alternative approach for Linear Regression: Least absolute value deviation:

$$
\hat{\mathbf{x}} \in \arg \min _{\mathbf{x}}\|\mathbf{b}-\mathbf{A x}\|_{1} .
$$

- The advantage: Improved robustness against outliers (high noise values)
- The bad (!) news: A non-differentiable objective function


## Problem (Mathematical formulation)

How can we find an optimal solution to the following optimization problem?

$$
\begin{equation*}
F^{\star}:=\min _{\mathbf{x} \in \mathbb{R}^{p}} f(\mathbf{x}) \tag{1}
\end{equation*}
$$

where $f$ is proper, closed, convex, but not everywhere differentiable, $f \in \mathcal{F}$.

## Subdifferentials: A generalization of the gradient

## Definition

Let $f: \mathcal{Q} \rightarrow \mathbb{R} \cup\{+\infty\}$ be a convex function. The subdifferential of $f$ at a point $\mathbf{x} \in \mathcal{Q}$ is defined by the set:

$$
\partial f(\mathbf{x})=\left\{\mathbf{v} \in \mathbb{R}^{p}: f(\mathbf{y}) \geq f(\mathbf{x})+\langle\mathbf{v}, \mathbf{y}-\mathbf{x}\rangle \text { for all } \mathbf{y} \in \mathcal{Q}\right\} .
$$

Each element $\mathbf{v}$ of $\partial f(\mathbf{x})$ is called subgradient of $f$ at $\mathbf{x}$.

## Lemma

Let $f: \mathcal{Q} \rightarrow \mathbb{R} \cup\{+\infty\}$ be a differentiable convex function. Then, the subdifferential of $f$ at a point $\mathbf{x} \in \mathcal{Q}$ contains only the gradient, i.e., $\partial f(\mathbf{x})=\{\nabla f(\mathbf{x})\}$.



Figure: (Left) Non-differentiability at point y. (Right) Gradient as a subdifferential with a singleton entry.
(Sub)gradients in convex functions

## Example

$$
f(x)=|x| \quad \longrightarrow \partial|x|=\{\operatorname{sgn}(x)\}, \text { if } x \neq 0, \text { but }[-1,1], \text { if } x=0 \text {. }
$$



Figure: Subdifferentials of $f(x)=|x|$ in $\mathbb{R}$.

## Subdifferentials: Two basic results

## Lemma (Necessary and sufficient condition)

$$
\mathbf{x}^{\star} \in \operatorname{dom}(F) \text { is a globally optimal solution to }(1) \quad \text { iff } \quad 0 \in \partial F\left(\mathbf{x}^{\star}\right)
$$

## Sketch of the proof.

- $\Rightarrow$ : For any $\mathbf{x} \in \mathbb{R}^{p}$, by definition of $\partial F\left(\mathbf{x}^{\star}\right)$ :

$$
F(\mathbf{x})-F\left(\mathbf{x}^{\star}\right) \geq 0^{T}\left(\mathbf{x}-\mathbf{x}^{\star}\right)=0
$$

that is, $\mathrm{x}^{\star}$ is a global solution to (1).

- $\Leftarrow$ : If $\mathbf{x}^{\star}$ is a global of (1) then for every $\mathbf{x} \in \operatorname{dom}(F), F(\mathbf{x}) \geq F\left(\mathbf{x}^{\star}\right)$ and hence

$$
F(\mathbf{x})-F\left(\mathbf{x}^{\star}\right) \geq 0^{T}\left(\mathbf{x}-\mathbf{x}^{\star}\right), \forall \mathbf{x} \in \mathbb{R}^{p}
$$

which leads to $0 \in \partial F\left(\mathbf{x}^{\star}\right)$.

## Theorem (Moreau-Rockafellar's theorem [8])

Let $\partial f$ and $\partial g$ be the subdiffierential of $f$ and $g$, respectively. If $f, g \in \mathcal{F}\left(\mathbb{R}^{p}\right)$ and $\operatorname{dom}(f) \cap \operatorname{dom}(g) \neq \emptyset$, then:

$$
\partial(f+g)=\partial f+\partial g
$$

## Non-smooth unconstrained convex minimization

## Problem (Non-smooth convex minimization)

$$
\begin{equation*}
F^{\star}:=\min _{\mathbf{x} \in \mathbb{R}^{p}} f(\mathbf{x}) \tag{2}
\end{equation*}
$$

## Subgradient method

The subgradient method relies on the fact that even though $f$ is non-smooth, we can still compute its subgradients, informing of the local descent directions.

## Subgradient method

1. Choose $\mathbf{x}^{0} \in \mathbb{R}^{p}$ as a starting point.
2. For $k=0,1, \cdots$, perform:

$$
\begin{equation*}
\left\{\mathbf{x}^{k+1}=\mathbf{x}^{k}-\alpha_{k} \mathbf{d}^{k}\right. \tag{3}
\end{equation*}
$$

where $\mathbf{d}^{k} \in \partial f\left(\mathbf{x}^{k}\right)$ and $\alpha_{k} \in(0,1]$ is a given step size.

## Convergence of the subgradient method

## Theorem

Assume that the following conditions are satisfied:

1. $\|\mathbf{g}\|_{2} \leq G$ for all $\mathbf{g} \in \partial f(\mathbf{x})$ for any $\mathbf{x} \in \mathbb{R}^{p}$.
2. $\left\|\mathbf{x}^{0}-\mathbf{x}^{\star}\right\|_{2} \leq R$

Let the stepsize be chosen as

$$
\alpha_{k}=\frac{R}{G \sqrt{k}}
$$

then the iterates generated by the subgradient method satisfy

$$
\min _{0 \leq i \leq k} f\left(\mathbf{x}^{i}\right)-f^{\star} \leq \frac{R G}{\sqrt{k}} .
$$

## Remarks

- Condition (1) holds, for example, when $f$ is $G$-Lipschitz.
- The convergence rate of $\mathcal{O}(1 / \sqrt{k})$ is the slowest we have seen so far!

Next lecture: Achieving guarantees for (many) non-smooth optimization problems that are just as good as those for smooth ones

## Stochastic subgradient methods

- An unbiased stochastic subgradient

$$
\mathbb{E}[G(\mathbf{x}) \mid \mathbf{x}] \in \partial f(\mathbf{x})
$$

- Algorithms in Lecture 7 can be extended using unbiased subgradients instead of unbiased gradients.

The classic stochastic subgradient methods (SG)

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

$$
\mathbf{x}_{k+1}=\mathbf{x}_{k}-\gamma_{k} G\left(\mathbf{x}_{k}\right)
$$

## Theorem (Convergence in expectation [10])

Suppose that:

1. $\mathbb{E}\left[\left\|G\left(\mathbf{x}^{k}\right)\right\|^{2}\right] \leq M^{2}$,
2. $\gamma_{k}=\gamma_{0} / \sqrt{k}$.

Then,

$$
\mathbb{E}\left[f\left(\mathbf{x}^{k}\right)-f\left(\mathbf{x}^{\star}\right)\right] \leq\left(\frac{D^{2}}{\gamma_{0}}+\gamma_{0} M^{2}\right) \frac{2+\log k}{\sqrt{k}} .
$$

- Note: Rate is $\mathcal{O}(\log k / \sqrt{k})$ instead of $\mathcal{O}(1 / \sqrt{k})$ for the deterministic algorithm.


## Composite convex minimization

## Problem (Unconstrained composite convex minimization)

$$
\begin{equation*}
F^{\star}:=\min _{\mathbf{x} \in \mathbb{R}^{p}}\{F(\mathbf{x}):=f(\mathbf{x})+g(\mathbf{x})\} \tag{4}
\end{equation*}
$$

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


## Two remarks

- Nonsmoothness: At least one of the two functions $f$ and $g$ is nonsmooth
- General nonsmooth convex optimization methods (e.g., classical subgradient methods, level, or bundle methods) lack efficiency and numerical robustness.
- Require $\mathcal{O}\left(\epsilon^{-2}\right)$ iterations to reach a point $\mathbf{x}_{\epsilon}^{\star}$ such that $F\left(\mathbf{x}_{\epsilon}^{\star}\right)-F^{\star} \leq \epsilon$. Hence, to reach $\mathbf{x}_{0.01}^{\star}$ such that $F\left(\mathbf{x}_{0.01}^{\star}\right)-F^{\star} \leq 0.01$, we need $\mathcal{O}\left(10^{4}\right)$ iterations.
- Generality: it covers a wider range of problems than smooth unconstrained problems, e.g., when handling regularized $M$-estimation,
- $f$ is a loss function, a data fidelity, or negative log-likelihood function.
- $g$ is a regularizer, encouraging structure and/or constraints in the solution.


## Example 1: 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 $\left\{b_{i}\right\}_{i=1}^{n}$ and $\left\{\mathbf{a}_{i}\right\}_{i=1}^{n}$, knowing that the likelihood function at $y_{i}$ given $\mathbf{a}_{i}$ and $\mathbf{x}^{\natural}$ is given by $\mathcal{L}\left(b_{i} ;\left\langle\mathbf{a}_{i}, \mathbf{x}^{\natural}\right\rangle\right)$, and that $\mathbf{x}^{\natural}$ is sparse.


## Optimization formulation

$$
\min _{\mathbf{x} \in \mathbb{R}^{p}}\{\underbrace{-\sum_{i=1}^{n} \log \mathcal{L}\left(b_{i} ;\left\langle\mathbf{a}_{i}, \mathbf{x}\right\rangle\right)}_{f(\mathbf{x})}+\underbrace{\rho_{n}\|\mathbf{x}\|_{1}}_{g(\mathbf{x})}\}
$$

where $\rho_{n}>0$ is a parameter which controls the strength of sparsity regularization.

## Theorem (cf. [5] for details)

Under some technical conditions, there exists $\left\{\rho_{i}\right\}_{i=1}^{\infty}$ such that with high probability,

$$
\begin{aligned}
\left\|\mathbf{x}^{\star}-\mathbf{x}^{\natural}\right\|_{2}^{2}=\mathcal{O}\left(\frac{s \log p}{n}\right), \quad \operatorname{supp} \mathbf{x}^{\star}=\operatorname{supp} \mathbf{x}^{\natural} \\
\text { Recall } M L:\left\|\mathbf{x}_{M L}-\mathbf{x}^{\natural}\right\|_{2}^{2}=\mathcal{O}(p / n) .
\end{aligned}
$$

## Example 2: Image processing

## Problem (Imaging denoising/deblurring)

Our goal is to obtain a clean image $\mathbf{x}$ given "dirty" observations $\mathbf{b} \in \mathbb{R}^{n \times 1}$ via $\mathbf{b}=\mathcal{A}(\mathbf{x})+\mathbf{w}$, where $\mathcal{A}$ is a linear operator, which, e.g., captures camera blur as well as image subsampling, and $\mathbf{w}$ models perturbations, such as Gaussian or Poisson noise.

Optimization formulation

$$
\begin{aligned}
& \text { Gaussian : } \min _{\mathbf{x} \in \mathbb{R}^{n \times p}}\{\underbrace{(1 / 2)\|\mathcal{A}(\mathbf{x})-\mathbf{b}\|_{2}^{2}}_{f(\mathbf{x})}+\underbrace{\rho\|\mathbf{x}\|_{\mathrm{TV}}}_{g(\mathbf{x})}\} \\
& \text { Poisson : } \min _{\mathbf{x} \in \mathbb{R}^{n \times p}}\{\underbrace{\frac{1}{n} \sum_{i=1}^{n}\left[\left\langle\mathbf{a}_{i}, \mathbf{x}\right\rangle-b_{i} \ln \left(\left\langle\mathbf{a}_{i}, \mathbf{x}\right\rangle\right)\right]}_{f(\mathbf{x})}+\underbrace{\rho\|\mathbf{x}\|_{\mathrm{TV}}}_{g(\mathbf{x})}\}
\end{aligned}
$$

where $\rho>0$ is a regularization parameter and $\|\cdot\|_{\mathrm{TV}}$ is the total variation (TV) norm:

$$
\|\mathbf{x}\|_{\mathrm{TV}}:= \begin{cases}\sum_{i, j}\left|\mathbf{x}_{i, j+1}-\mathbf{x}_{i, j}\right|+\left|\mathbf{x}_{i+1, j}-\mathbf{x}_{i, j}\right| & \text { anisotropic case } \\ \sum_{i, j} \sqrt{\left|\mathbf{x}_{i, j+1}-\mathbf{x}_{i, j}\right|^{2}+\left|\mathbf{x}_{i+1, j}-\mathbf{x}_{i, j}\right|^{2}} & \text { isotropic case }\end{cases}
$$

## Example 3: Confocal microscopy with camera blur and Poisson observations



Observed image b


Estimate $\hat{\mathbf{x}}$


## Example 4: Sparse inverse covariance estimation

## Problem (Graphical model selection)

Given a data set $\mathcal{D}:=\left\{\mathbf{x}_{1}, \cdots, \mathbf{x}_{N}\right\}$, where $\mathbf{x}_{i}$ is a Gaussian random variable. Let $\Sigma$ be the covariance matrix corresponding to the graphical model of the Gaussian Markov random field. Our goal is to learn a sparse precision matrix $\Theta$ (i.e., the inverse covariance matrix $\Sigma^{-1}$ ) that captures the Markov random field structure..


## Optimization formulation

$$
\begin{equation*}
\min _{\Theta \succ 0}\{\underbrace{\operatorname{tr}(\Sigma \Theta)-\log \operatorname{det}(\Theta)}_{f(\mathbf{x})}+\underbrace{\lambda\|\operatorname{vec}(\Theta)\|_{1}}_{g(\mathbf{x})}\} \tag{5}
\end{equation*}
$$

where $\Theta \succ 0$ means that $\Theta$ is symmetric and positive definite and $\lambda>0$ is a regularization parameter and vec is the vectorization operator.

## Question: How do we design algorithms for finding a solution $\mathrm{x}^{\star}$ ?

## Philosophy

- We cannot immediately design algorithms just based on the original formulation

$$
\begin{equation*}
F^{\star}:=\min _{\mathbf{x} \in \mathbb{R}^{p}}\{F(\mathbf{x}):=f(\mathbf{x})+g(\mathbf{x})\} \tag{6}
\end{equation*}
$$

- We need intermediate tools to characterize the solutions $\mathbf{x}^{\star}$ of this problem
- One key tool is called the optimality condition


## A short detour: Proximal-point operators

## Definition (Proximal operator [9])

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

$$
\begin{equation*}
\operatorname{prox}_{g}(\mathbf{x}) \equiv \arg \min _{\mathbf{y} \in \mathbb{R}^{p}}\left\{g(\mathbf{y})+\frac{1}{2}\|\mathbf{y}-\mathbf{x}\|_{2}^{2}\right\} . \tag{7}
\end{equation*}
$$

## A short detour: Proximal-point operators

## Definition (Proximal operator [9])

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

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\end{equation*}
$$

Numerical efficiency: Why do we need proximal operator?
For problem (4):

- For many well-known convex functions $g$, we can compute $\operatorname{prox}_{g}(\mathbf{x})$ analytically or very efficiently.
- If $f \in \mathcal{F}_{L}^{1,1}\left(\mathbb{R}^{p}\right)$, and $\operatorname{prox}_{g}(\mathbf{x})$ is cheap to compute, then solving (4) is as efficient as solving $\min _{\mathbf{x} \in \mathbb{R}^{p}} f(\mathbf{x})$ in terms of complexity.
- If $\operatorname{prox}_{f}(\mathbf{x})$ and $\operatorname{prox}_{g}(\mathbf{x})$ are both cheap to compute, then convex splitting (4) is also efficient.


## Tractable prox-operators

## Processing non-smooth terms in (4)

- We handle the nonsmooth term $g$ in (4) using the proximal mapping principle.
- Computing proximal operator prox $_{g}$ of a general convex function $g$

$$
\operatorname{prox}_{g}(\mathbf{x}) \equiv \arg \min _{\mathbf{y} \in \mathbb{R}^{p}}\left\{g(\mathbf{y})+(1 / 2)\|\mathbf{y}-\mathbf{x}\|_{2}^{2}\right\} .
$$

can be computationally demanding.

- If we can efficiently compute $\operatorname{prox}_{F}$, we can use the proximal-point algorithm (PPA) $[4,9]$ to solve (4). Unfortunately, PPA is hardly used in practice to solve (4) since computing $\operatorname{prox}_{\lambda F}(\cdot)$ can be as almost hard as solving (4).


## Definition (Tractable proximity)

Given $g \in \mathcal{F}\left(\mathbb{R}^{p}\right)$. We say that $g$ is proximally tractable if prox $_{g}$ defined by (7) can be computed efficiently.

- "efficiently" $=$ \{closed form solution, low-cost computation, polynomial time $\}$.
- We denote $\mathcal{F}_{\text {prox }}\left(\mathbb{R}^{p}\right)$ the class of proximally tractable convex functions.


## Tractable prox-operators

## Example

- For separable functions, the prox-operator can be efficient. For instance, $g(\mathbf{x}):=\|\mathbf{x}\|_{1}=\sum_{i=1}^{n}\left|\mathbf{x}_{i}\right|$, we have

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

- For smooth functions, we can computer the prox-operator via basic algebra. For instance, $g(\mathbf{x}):=(1 / 2)\|\mathbf{A x}-\mathbf{b}\|_{2}^{2}$, one has

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

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

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

the projection of $\mathbf{x}$ onto $\mathcal{X}$. For instance, when $\mathcal{X}=\left\{\mathbf{x}:\|\mathbf{x}\|_{1} \leq \lambda\right\}$, the projection can be obtained efficiently.

## Computational efficiency - Example

## Proximal operator of quadratic function

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

$$
\begin{equation*}
\operatorname{prox}_{\lambda g}(\mathbf{x}):=\arg \min _{\mathbf{y} \in \mathbb{R}^{p}}\left\{\frac{1}{2}\|\mathbf{A} \mathbf{y}-\mathbf{b}\|_{2}^{2}+\frac{1}{2 \lambda}\|\mathbf{y}-\mathbf{x}\|_{2}^{2}\right\} \tag{8}
\end{equation*}
$$

## Computational efficiency - Example

## Proximal operator of quadratic function

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

$$
\begin{equation*}
\operatorname{prox}_{\lambda g}(\mathbf{x}):=\arg \min _{\mathbf{y} \in \mathbb{R}^{p}}\left\{\frac{1}{2}\|\mathbf{A y}-\mathbf{b}\|_{2}^{2}+\frac{1}{2 \lambda}\|\mathbf{y}-\mathbf{x}\|_{2}^{2}\right\} \tag{8}
\end{equation*}
$$

## How to compute $\operatorname{prox}_{\lambda g}(\mathbf{x})$ ?

The optimality condition implies that the solution of (8) should satisfy the following linear system: $\mathbf{A}^{T}(\mathbf{A y}-\mathbf{b})+\lambda^{-1}(\mathbf{y}-\mathbf{x})=0$. As a result, we obtain

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

- When $\mathbf{A}^{T} \mathbf{A}$ is efficiently diagonalizable (e.g., $\mathbf{U}^{T} \mathbf{A}^{T} \mathbf{A U}:=\Lambda$, where $\mathbf{U}$ is a unitary matrix and $\Lambda$ is a diagonal matrix) then $\operatorname{prox}_{\lambda g}(\mathbf{x})$ can be cheap $\operatorname{prox}_{\lambda g}(\mathbf{x})=\mathbf{U}(\mathbb{I}+\lambda \Lambda)^{-1} \mathbf{U}^{T}(\mathbf{x}+\lambda \mathbf{A b})$.
- Matrices A such as TV operator with periodic boundary conditions, index subsampling operators (e.g., as in matrix completion), and circulant matrices (e.g., typical image blur operators) are efficiently diagonalizable with the Fast Fourier transform U.
- If $\mathbf{A} \mathbf{A}^{T}$ is diagonalizable (e.g., a tight frame $\mathbf{A}$ ), then we can use the identity

$$
\left(\mathbb{I}+\lambda \mathbf{A}^{T} \mathbf{A}\right)^{-1}=\mathbb{I}-\mathbf{A}^{T}\left(\lambda^{-1} \mathbb{I}+\mathbf{A} \mathbf{A}^{T}\right)^{-1} \mathbf{A} .
$$

## A non-exhaustive list of proximal tractability functions

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

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 $[1,7]$.

## A short detour: Basic properties of prox-operator

## Property (Basic properties of prox-operator)

1. $\operatorname{prox}_{g}(\mathbf{x})$ is well-defined and single-valued (i.e., the prox-operator (7) has a unique solution since $g(\cdot)+(1 / 2)\|\cdot-\mathbf{x}\|_{2}^{2}$ is strongly convex).
2. Optimality condition:

$$
\mathbf{x} \in \operatorname{prox}_{g}(\mathbf{x})+\partial g\left(\operatorname{prox}_{g}(\mathbf{x})\right), \mathbf{x} \in \mathbb{R}^{p}
$$

3. $\mathbf{x}^{\star}$ is a fixed point of $\operatorname{prox}_{g}(\cdot)$ :

$$
0 \in \partial g\left(\mathbf{x}^{\star}\right) \quad \Leftrightarrow \quad \mathbf{x}^{\star}=\operatorname{prox}_{g}\left(\mathbf{x}^{\star}\right)
$$

4. Nonexpansiveness:

$$
\left\|\operatorname{prox}_{g}(\mathbf{x})-\operatorname{prox}_{g}(\tilde{\mathbf{x}})\right\|_{2} \leq\|\mathbf{x}-\tilde{\mathbf{x}}\|_{2}, \quad \forall \mathbf{x}, \tilde{\mathbf{x}} \in \mathbb{R}^{p}
$$

Choices of solution methods


- $\mathcal{F}_{L}^{1,1}$ and $\mathcal{F}_{2}$ are the class of convex functions with Lipschitz gradient and self-concordant, respectively.
- $\mathcal{F}_{\text {prox }}$ is the class of convex functions with proximity operator (defined in the next slides).
- "smoothable" is defined in the next lectures.


## Solution methods

## Composite convex minimization

$$
\begin{equation*}
F^{\star}:=\min _{\mathbf{x} \in \mathbb{R}^{p}}\{F(\mathbf{x}):=f(\mathbf{x})+g(\mathbf{x})\} \tag{1}
\end{equation*}
$$

## Choice of numerical solution methods

- Solve (4) $=$ Find $\mathbf{x}^{k} \in \mathbb{R}^{p}$ such that

$$
F\left(\mathrm{x}^{k}\right)-F^{\star} \leq \varepsilon
$$

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

Using different oracle leads to different types of algorithms

## Proximal-gradient method: A quadratic majorization perspective

Definition (Proximal operator [9])
Let $g \in \mathcal{F}\left(\mathbb{R}^{p}\right)$. The proximal operator (or prox-operator) of $g$ is defined as:

$$
\operatorname{prox}_{g}(\mathbf{x}) \equiv \arg \min _{\mathbf{y} \in \mathbb{R}^{p}}\left\{g(\mathbf{y})+\frac{1}{2}\|\mathbf{y}-\mathbf{x}\|_{2}^{2}\right\}
$$

## Quadratic upper bound for $f$

For $f \in \mathcal{F}_{L}^{1,1}\left(\mathbb{R}^{p}\right)$, we have, $\forall \mathbf{x}, \mathbf{y} \in \mathbb{R}^{p}$

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

Quadratic majorizer for $f+g$
Of course, $\forall \mathbf{x}, \mathbf{y} \in \mathbb{R}^{p}$,

$$
f(\mathbf{x}) \leq Q_{L}(\mathbf{x}, \mathbf{y}) \Rightarrow f(\mathbf{x})+g(\mathbf{x}) \leq Q_{L}(\mathbf{x}, \mathbf{y})+g(\mathbf{x}):=P_{L}(\mathbf{x}, \mathbf{y})
$$

Proximal-gradient from the majorize-minimize perspective

$$
\mathbf{x}^{k+1}=\arg \min _{\mathbf{x}} P_{L}\left(\mathbf{x}, \mathbf{x}^{k}\right)=\operatorname{prox}_{g / L}\left(\mathbf{x}-\nabla f\left(\mathbf{x}^{k}\right) / L\right)
$$

## Geometric illustration



## Proximal-gradient algorithm

Basic proximal-gradient scheme (ISTA)

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

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

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

## Proximal-gradient algorithm

## Basic proximal-gradient scheme (ISTA)

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

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

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

## Theorem (Convergence of ISTA [2])

Let $\left\{\mathrm{x}^{k}\right\}$ be generated by ISTA. Then:

$$
F\left(\mathbf{x}^{k}\right)-F^{\star} \leq \frac{L_{f}\left\|\mathbf{x}^{0}-\mathbf{x}^{\star}\right\|_{2}^{2}}{2(k+1)}
$$

The worst-case complexity to reach $F\left(\mathbf{x}^{k}\right)-F^{\star} \leq \varepsilon$ of (ISTA) is $\mathcal{O}\left(\frac{L_{f} R_{0}^{2}}{\varepsilon}\right)$, where $R_{0}:=\max _{\mathbf{x}^{\star} \in \mathcal{S}^{\star}}\left\|\mathbf{x}^{0}-\mathbf{x}^{\star}\right\|_{2}$.

- A line-search procedure can be used to estimate $L_{k}$ for $L$ based on $(0<c \leq 1)$ :

$$
f\left(\mathbf{x}^{k+1}\right) \leq f\left(\mathbf{x}^{k}\right)-\frac{c}{2 L_{k}}\left\|\nabla f\left(\mathbf{x}^{k}\right)\right\|^{2}
$$

## Fast proximal-gradient algorithm

## Fast proximal-gradient scheme (FISTA)

1. Choose $\mathbf{x}^{0} \in \operatorname{dom}(F)$ arbitrarily as a starting point.
2. Set $\mathbf{y}^{0}:=\mathbf{x}^{0}$ and $t_{0}:=1$.
3. For $k=0,1, \ldots$, generate two sequences $\left\{\mathbf{x}^{k}\right\}_{k \geq 0}$ and $\left\{\mathbf{y}^{k}\right\}_{k \geq 0}$ as:

$$
\begin{cases}\mathbf{x}^{k+1} & :=\operatorname{prox}_{\alpha g}\left(\mathbf{y}^{k}-\alpha \nabla f\left(\mathbf{y}^{k}\right)\right) \\ t_{k+1} & :=\left(1+\sqrt{4 t_{k}^{2}+1}\right) / 2 \\ \mathbf{y}^{k+1} & :=\mathbf{x}^{k+1}+\frac{t_{k}-1}{t_{k+1}}\left(\mathbf{x}^{k+1}-\mathbf{x}^{k}\right)\end{cases}
$$

where $\alpha:=L^{-1}$.
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 $\nabla f\left(\mathbf{y}^{k}\right)$ and one prox-operator of $g$;
- 8 arithmetic operations for $t_{k+1}$ and $\gamma_{k+1}$;
- 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: $\ell_{1}$-regularized least squares

## Problem ( $\ell_{1}$-regularized least squares)

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

$$
\begin{equation*}
F^{\star}:=\min _{\mathbf{x} \in \mathbb{R}^{p}}\left\{F(\mathbf{x}):=\frac{1}{2}\|\mathbf{A} \mathbf{x}-\mathbf{b}\|_{2}^{2}+\lambda\|\mathbf{x}\|_{1}\right\} \tag{9}
\end{equation*}
$$

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

## Complexity per iterations

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


## Synthetic data generation

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


## Example 1: Theoretical bounds vs practical performance

(Theoretical bounds) FISTA $:=\frac{2 L_{f} R_{0}^{2}}{(k+2)^{2}}$ and ISTA $:=\frac{L_{f} R_{0}^{2}}{2(k+2)}$.


descent directions

restricted descent directions

- $\ell_{1}$-regularized least squares formulation has restricted strong convexity. The proximal-gradient method can automatically exploit this structure.


## Adaptive Restart

It is possible the preserve $\mathcal{O}\left(1 / k^{2}\right)$ convergence guarantee!
One needs to slightly modify the algorithm as below.

## Generalized fast proximal-gradient scheme

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

$$
\left\{\begin{array}{l}
\mathbf{y}^{k}:=\mathbf{x}^{k}+\theta_{k}\left(\theta_{k-1}^{-1}-1\right)\left(\mathbf{x}^{k}-\mathbf{x}^{k-1}\right)  \tag{10}\\
\mathbf{x}^{k+1}:=\operatorname{prox}_{\lambda g}\left(\mathbf{y}^{k}-\lambda \nabla f\left(\mathbf{y}^{k}\right)\right) \\
\text { if restart test holds } \\
\quad \theta_{k-1}=\theta_{k}=1 \\
\quad \mathbf{y}^{k}=\mathbf{x}^{k} \\
\quad \mathbf{x}^{k+1}:=\operatorname{prox}_{\lambda g}\left(\mathbf{y}^{k}-\lambda \nabla f\left(\mathbf{y}^{k}\right)\right)
\end{array}\right.
$$

where $\lambda:=L_{f}^{-1}$.

## $\theta_{k}$ 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 [3])

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

$$
\begin{equation*}
F\left(\mathbf{x}^{k}\right)-F^{\star} \leq \frac{2 L_{f}}{(k+2)^{2}}\left(R_{0}^{2}+\sum_{k_{i} \leq k}\left(\left\|\mathbf{x}^{\star}-\mathbf{x}^{k_{i}}\right\|_{2}^{2}-\left\|\mathbf{x}^{\star}-\mathbf{z}^{k_{i}}\right\|_{2}^{2}\right)\right) \forall k \geq 0 \tag{11}
\end{equation*}
$$

where $R_{0}:=\min _{\mathbf{x}^{\star} \in \mathcal{S}^{\star}}\left\|\mathbf{x}^{0}-\mathbf{x}^{\star}\right\|, \mathbf{z}^{k}=\mathbf{x}^{k-1}+\theta_{k-1}^{-1}\left(\mathbf{x}^{k}-\mathbf{x}^{k-1}\right)$ and $k_{i}, i=1 \ldots$ are the iterations for which the restart test holds.

## Various restarts tests that might coincide with $\left\|\mathrm{x}^{*}-\mathrm{x}^{k_{i}}\right\|_{2}^{2} \leq\left\|\mathrm{x}^{*}-\mathrm{z}^{k_{i}}\right\|_{2}^{2}$

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


## 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:

$$
F^{\star}:=\min _{\mathbf{x}, \beta}\left\{F(\mathbf{x}):=\frac{1}{n} \sum_{j=1}^{n} \log \left(1+\exp \left(-\mathbf{b}_{j}\left(\mathbf{a}_{j}^{T} \mathbf{x}+\beta\right)\right)\right)+\rho\|\mathbf{x}\|_{1}\right\}
$$

## Real data

- Real data: w8a with $n=49^{\prime} 749$ 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 $\mathbf{x}^{\star}$ and $F^{\star}$.


## 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 $\left(\times 10^{-7}\right)$ | 29370 | 2.774 | 1.000 | 0.998 | 0.961 | 0.985 |

## Strong convexity case: Algorithms

| Proximal-gradient scheme $\left(\right.$ ISTA $\left._{\mu}\right)$ |
| :--- |
| 1. Given $\mathbf{x}^{0} \in \mathbb{R}^{p}$ as a starting point. |
| 2. For $k=0,1, \cdots$, generate a sequence $\left\{\mathbf{x}^{k}\right\}_{k \geq 0}$ as: |
| $\qquad \mathbf{x}^{k+1}:=\operatorname{prox}_{\alpha_{k} g}\left(\mathbf{x}^{k}-\alpha_{k} \nabla f\left(\mathbf{x}^{k}\right)\right)$, |
| where $\alpha_{k}:=2 /\left(L_{f}+\mu\right)$ 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 $k=0,1, \cdots$, generate two sequences $\left\{\mathbf{x}^{k}\right\}_{k \geq 0}$ and $\left\{\mathbf{y}^{k}\right\}_{k \geq 0}$ as:

$$
\left\{\begin{array}{l}
\mathbf{x}^{k+1}:=\operatorname{prox}_{\alpha_{k} g}\left(\mathbf{y}^{k}-\alpha_{k} \nabla f\left(\mathbf{y}^{k}\right)\right) \\
\mathbf{y}^{k+1}:=\mathbf{x}^{k+1}+\left(\frac{\sqrt{c_{f}}-1}{\sqrt{c_{f}}+1}\right)\left(\mathbf{x}^{k+1}-\mathbf{x}^{k}\right)
\end{array}\right.
$$

where $\alpha_{k}:=L_{f}^{-1}$ is the optimal step-size.

## Strong convexity case: Convergence

## Assumption

$f$ is strongly convex with parameter $\mu>0$, i.e., $f \in \mathcal{F}_{L, \mu}^{1,1}\left(\mathbb{R}^{p}\right)$.
Condition number: $c_{f}:=\frac{L_{f}}{\mu} \geq 0$.

## Theorem (ISTA ${ }_{\mu}[6]$ )

$$
F\left(\mathbf{x}^{k}\right)-F^{\star} \leq \frac{L_{f}}{2}\left(\frac{c_{f}-1}{c_{f}+1}\right)^{2 k}\left\|\mathbf{x}^{0}-\mathbf{x}^{\star}\right\|_{2}^{2} .
$$

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 ${ }_{\mu}$ [6])

$$
F\left(\mathbf{x}^{k}\right)-F^{\star} \leq \frac{L_{f}+\mu}{2}\left(1-\sqrt{\frac{\mu}{L_{f}}}\right)^{k}\left\|\mathbf{x}^{0}-\mathbf{x}^{\star}\right\|_{2}^{2}
$$

Convergence rate: Linear with contraction factor: $\omega_{f}=\frac{\sqrt{L_{f}}-\sqrt{\mu}}{\sqrt{L_{f}}}<\omega$.

## A practical issue

## Stopping criterion

Fact: If $\mathcal{P} \mathcal{G}_{\mathcal{L}}\left(\mathrm{x}^{\star}\right)=0$, then $\mathrm{x}^{\star}$ is optimal to (4), where

$$
\mathcal{P} \mathcal{G}_{\mathcal{L}}(\mathbf{x})=L\left(\mathbf{x}-\operatorname{prox}_{(1 / L) g}(\mathbf{x}-(1 / L) \nabla f(\mathbf{x}))\right) .
$$

Stopping criterion: (relative solution change)

$$
L_{k}\left\|\mathbf{x}^{k+1}-\mathbf{x}^{k}\right\|_{2} \leq \varepsilon \max \left\{L_{0}\left\|\mathbf{x}^{1}-\mathbf{x}^{0}\right\|_{2}, 1\right\},
$$

where $\varepsilon$ is a given tolerance.

## Summary of the worst-case complexities

## Software

TFOCS is a good software package to learn about first order methods.
http://cvxr.com/tfocs/

Comparison with gradient scheme ( $F\left(\mathrm{x}^{k}\right)-F^{\star} \leq \varepsilon$ )

| Complexity | Proximal-gradient scheme | Fast <br> scheme |
| :--- | :--- | :--- |
| Complexity $[\mu=0]$ | $\mathcal{O}\left(R_{0}^{2}\left(L_{f} / \varepsilon\right)\right)$ | $\mathcal{O}\left(R_{0} \sqrt{\left.L_{f} / \varepsilon\right)}\right.$ |
| Per iteration | 1-gradient, 1-prox, 1-sv, 1- <br> $v+$ | 1-gradient, 1-prox, 2-sv, 3- <br> $v+$ |
| Complexity $[\mu>0]$ | $\mathcal{O}\left(\kappa \log \left(\varepsilon^{-1}\right)\right)$ | $\mathcal{O}\left(\sqrt{\kappa} \log \left(\varepsilon^{-1}\right)\right)$ |
| Per iteration | 1-gradient, 1-prox, 1-sv, 1- <br> $v+$ | 1-gradient, 1-prox, 1-sv, 2- <br> $v+$ |

Here: $s v=$ scalar-vector multiplication, $v+=$ vector addition. $R_{0}:=\max _{\mathbf{x}^{\star} \in \mathcal{S}^{\star}}\left\|\mathbf{x}^{0}-\mathbf{x}^{\star}\right\|$ and $\kappa=L_{f} / \mu_{f}$ is the condition number.

## Summary of the worst-case complexities

## Software

TFOCS is a good software package to learn about first order methods.
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Comparison with gradient scheme $\left(F\left(\mathbf{x}^{k}\right)-F^{\star} \leq \varepsilon\right)$

| Complexity | Proximal-gradient scheme | Fast <br> scheme |
| :--- | :--- | :--- |
| Complexity $[\mu=0]$ | $\mathcal{O}\left(R_{0}^{2}\left(L_{f} / \varepsilon\right)\right)$ | $\mathcal{O}\left(R_{0} \sqrt{\left.L_{f} / \varepsilon\right)}\right.$ |
| Per iteration | 1-gradient, 1-prox, 1-sv, 1- <br> $v+$ | 1-gradient, 1-prox, 2-sv, 3- <br> $v+$ |
| Complexity $[\mu>0]$ | $\mathcal{O}\left(\kappa \log \left(\varepsilon^{-1}\right)\right)$ | $\mathcal{O}\left(\sqrt{\kappa} \log \left(\varepsilon^{-1}\right)\right)$ |
| Per iteration | 1-gradient, 1-prox, 1-sv, 1- <br> $v+$ | 1-gradient, 1-prox, 1- $s v, ~ 2-$ <br> $v+$ |

Here: $s v=$ scalar-vector multiplication, $v+=$ vector addition. $R_{0}:=\max _{\mathbf{x}^{\star} \in \mathcal{S}^{\star}}\left\|\mathbf{x}^{0}-\mathbf{x}^{\star}\right\|$ and $\kappa=L_{f} / \mu_{f}$ is the condition number.

## Need alternatives when

- $f$ is only self-concordant
- computing $\nabla f(\mathbf{x})$ is much costlier than computing prox ${ }_{g}$


## *Examples

## Example (Sparse graphical model selection)

$$
\min _{\Theta \succ 0}\{\underbrace{\operatorname{tr}(\Sigma \Theta)-\log \operatorname{det}(\Theta)}_{f(\mathbf{x})}+\underbrace{\rho\|\operatorname{vec}(\Theta)\|_{1}}_{g(\mathbf{x})}\}
$$

where $\Theta \succ 0$ means that $\Theta$ is symmetric and positive definite, and $\rho>0$ is a regularization parameter and vec is the vectorization operator.

- Computing the gradient is expensive: $\nabla f(\Theta)=\Theta^{-1}$.
- $f \in \mathcal{F}_{2}$ is self-concordant. However, if $\alpha \mathbf{I} \preceq \Theta \preceq \beta \mathbf{I}$, then $f \in \mathcal{F}_{L, \mu}^{2,1}$ with $L=\sqrt{p} / \alpha^{2}$ and $\mu=\left(\beta^{2} \sqrt{p}\right)^{-1}$.


## Example ( $\ell_{1}$-regularized Lasso)

$$
\min _{\mathbf{x}} \underbrace{\frac{1}{2}\|\mathbf{b}-\mathbf{A} \mathbf{x}\|_{2}^{2}}_{f(\mathbf{x})}+\underbrace{\rho\|\mathbf{x}\|_{1}}_{g(\mathbf{x})}
$$

where $n \gg p, \mathbf{A} \in \mathbb{R}^{n \times p}$ is a full column-rank matrix, and $\rho>0$ is a regularization parameter.

- $f \in \mathcal{F}_{L, \mu}^{2,1}$ and computing the gradient is $\mathcal{O}(n)$.



## $\star$ Examples (Learned ISTA)



Figure: a) Traditional machine learning approaches b) End-to-end deep learning methods [?]

## Example

In sparse coding, given a an overcomplete family basis vectors, we would like to find the optimal sparse code vector $Z^{*} \in \mathbb{R}^{m}$ to reconstruct the input vector $X \in \mathbb{R}^{n}$

$$
\begin{equation*}
Z^{*}=\underset{Z}{\arg \min } \frac{1}{2}\left\|X-W_{d} Z\right\|_{2}^{2}+\alpha\|Z\|_{1}, \tag{12}
\end{equation*}
$$

where $W_{d}$ is $n \times m$ dictionary matrix, whose columns are normalized basis vectors.

- Too slow for real-time applications


## * Examples (Learned ISTA)



ISTA method for sparse coding


Learned ISTA - time unfolded version of the ISTA block diagram

## Example

$$
\begin{equation*}
\mathcal{L}(W)=\frac{1}{P} \sum_{p=0}^{(P-1)} \underbrace{\frac{1}{2}\left\|Z^{* p}-f_{e}\left(W, X_{p}\right)\right\|^{2}}_{L\left(W, X_{p}\right)} \tag{13}
\end{equation*}
$$

where $\left(X_{1}, \ldots, X_{P}\right)$ are some samples, and $Z^{* p}$ is the optimal code for sample $X^{p}$. Parameters of the encoder are chosen as minimizers of $\mathcal{L}(W)$.

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