

Computational Principles for High-dim Data Analysis

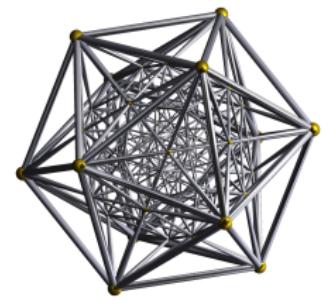
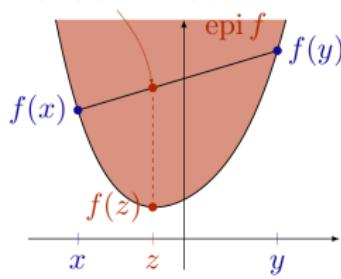
(Lecture Thirteen)

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October 12, 2021

$$(1 - \lambda)f(x) + \lambda f(y)$$



Unconstrained Convex Optimization for Structured Data Recovery

- 1 Challenges and Opportunities
- 2 Proximal Gradient Methods
- 3 Accelerated Proximal Gradient Methods

“Since the fabric of the universe is most perfect and the work of a most wise Creator, nothing at all takes place in the universe in which some rule of maximum or minimum does not appear.”

– Leonhard Euler

Optimization Problems for Structured Data Recovery

Sparse Vector Recovery: recover a sparse x_o from $\mathbf{y} = \mathbf{A}x_o \in \mathbb{R}^m$ or $\mathbf{y} = \mathbf{A}x_o + \mathbf{z} \in \mathbb{R}^m$ via convex programs:

- **Basis Pursuit (BP):**

$$\min_{\mathbf{x}} \|\mathbf{x}\|_1 \quad \text{subject to} \quad \mathbf{A}\mathbf{x} = \mathbf{y}. \quad (1)$$

- **LASSO:**

$$\min_{\mathbf{x}} \frac{1}{2} \|\mathbf{y} - \mathbf{A}\mathbf{x}\|_2^2 + \lambda \|\mathbf{x}\|_1. \quad (2)$$

Optimization Problems for Structured Data Recovery

Matrix Completion or Recovery: recover a low-rank \mathbf{L}_o from incomplete $\mathbf{Y} = \mathcal{P}_\Omega[\mathbf{X}_o]$ or corrupted $\mathbf{Y} = \mathbf{L}_o + \mathbf{S}_o \in \mathbb{R}^{m \times n}$ via convex programs:

- **Matrix Completion:**

$$\min \|\mathbf{X}\|_* \quad \text{subject to} \quad \mathcal{P}_\Omega[\mathbf{X}] = \mathbf{Y}. \quad (3)$$

- **Principal Component Pursuit (PCP):**

$$\min_{\mathbf{L}, \mathbf{S}} \|\mathbf{L}\|_* + \lambda \|\mathbf{S}\|_1 \quad \text{subject to} \quad \mathbf{L} + \mathbf{S} = \mathbf{Y}. \quad (4)$$

- **Stable PCP:**

$$\min_{\mathbf{L}, \mathbf{S}} \|\mathbf{L}\|_* + \lambda \|\mathbf{S}\|_1 + \frac{\mu}{2} \|\mathbf{Y} - \mathbf{L} - \mathbf{S}\|_F^2. \quad (5)$$

Optimization Challenges for Structured Data Recovery

$$\min_{\mathbf{x} \in \mathbb{R}^n} F(\mathbf{x}) \doteq \underbrace{f(\mathbf{x})}_{\text{smooth convex}} + \underbrace{g(\mathbf{x})}_{\text{nonsmooth convex}}. \quad (6)$$

- **Challenge of Scale:** scale algorithms to when n is very large.

$$\text{Second order methods} \implies \text{First order methods...} \quad (7)$$

- **Nonsmoothness:** first order methods are slow for nonsmooth.

$$O(1/\sqrt{k}) \implies O(1/k) \implies O(1/k^2) \implies O(e^{-\alpha k}) \quad (8)$$

- **Equality Constraints:** augmented Lagrange multiplier (ALM).
- **Separable Structures:** alternating direction of multipliers method (ADMM).

Gradient Descent [Cauchy, 1847]

For minimizing a smooth convex function (App. B):

$$\min f(\mathbf{x}), \quad \mathbf{x} \in \mathcal{C} \text{ (a convex set)}, \quad (9)$$

conduct **local gradient descent search** (App. D):

$$\mathbf{x}_{k+1} = \mathbf{x}_k - \gamma_k \nabla f(\mathbf{x}_k), \quad (10)$$



where a rule of thumb: $\gamma \approx 1/L$, where L the Lipschitz constant (why?).

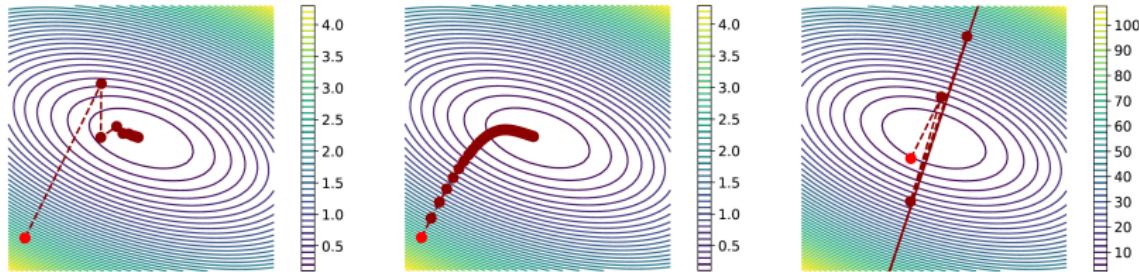


figure courtesy of prof. Carlos Fernandez of NYU.

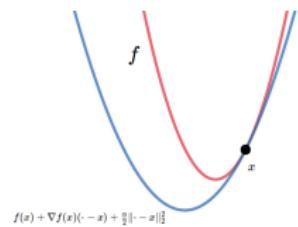
Gradient Descent

For $f(\mathbf{x})$ has L -Lipschitz continuous gradients if

$$\|\nabla f(\mathbf{x}') - \nabla f(\mathbf{x})\|_2 \leq L\|\mathbf{x}' - \mathbf{x}\|_2, \quad \forall \mathbf{x}', \mathbf{x} \in \mathbb{R}^n. \quad (11)$$

This gives a matching **quadratic upper bound**:

$$\begin{aligned} f(\mathbf{x}') &\leq \hat{f}(\mathbf{x}', \mathbf{x}) \\ &\doteq f(\mathbf{x}) + \langle \nabla f(\mathbf{x}), \mathbf{x}' - \mathbf{x} \rangle + \frac{L}{2} \|\mathbf{x}' - \mathbf{x}\|_2^2 \\ &= \frac{L}{2} \|\mathbf{x}' - (\mathbf{x} - \frac{1}{L} \nabla f(\mathbf{x}))\|_2^2 + h(\mathbf{x}). \end{aligned}$$



Take a step to the **minimizer of this bound**:

$$\mathbf{x}_{k+1} = \arg \min_{\mathbf{x}'} \hat{f}(\mathbf{x}', \mathbf{x}_k) = \mathbf{x}_k - \frac{1}{L} \nabla f(\mathbf{x}_k). \quad (12)$$

Fact: this gives a convergence rate of $O(1/k)$.

Proximal Gradient Descent

The same (local) strategy for a convex function with a nonsmooth term:

$$\min_{\mathbf{x} \in \mathbb{R}^n} F(\mathbf{x}) \doteq \underbrace{f(\mathbf{x})}_{\text{smooth convex}} + \underbrace{g(\mathbf{x})}_{\text{nonsmooth convex}}. \quad (13)$$

Upper bound:

$$\hat{F}(\mathbf{x}, \mathbf{x}_k) = f(\mathbf{x}_k) + \langle \nabla f(\mathbf{x}_k), \mathbf{x} - \mathbf{x}_k \rangle + \frac{L}{2} \|\mathbf{x} - \mathbf{x}_k\|_2^2 + g(\mathbf{x}) \quad (14)$$

$$= \frac{L}{2} \|\mathbf{x} - (\mathbf{x}_k - \frac{1}{L} \nabla f(\mathbf{x}_k))\|_2^2 + g(\mathbf{x}) + h(\mathbf{x}_k). \quad (15)$$

A step to the minimizer of the bound $\hat{F}(\mathbf{x}, \mathbf{x}_k)$:

$$\mathbf{x}_{k+1} = \arg \min_{\mathbf{x}} \frac{L}{2} \|\mathbf{x} - \underbrace{(\mathbf{x}_k - \frac{1}{L} \nabla f(\mathbf{x}_k))}_{\mathbf{w}_k}\|_2^2 + g(\mathbf{x}) \quad (16)$$

$$= \arg \min_{\mathbf{x}} g(\mathbf{x}) + \frac{L}{2} \|\mathbf{x} - \mathbf{w}_k\|_2^2. \quad (17)$$

Proximal Operators

Definition (Proximal Operator)

The proximal operator of a convex function g is

$$\text{prox}_g[\mathbf{w}] \doteq \arg \min_{\mathbf{x}} \left\{ g(\mathbf{x}) + \frac{1}{2} \|\mathbf{x} - \mathbf{w}\|_2^2 \right\}. \quad (18)$$

Iteration (17) can be written as:

$$\mathbf{x}_{k+1} = \text{prox}_{g/L}[\mathbf{w}_k]. \quad (19)$$

For many convex functions g :

$\text{prox}_g[\mathbf{w}]$ has a closed form or can be computed efficiently.

Proximal Operators

Proposition

Proximal operators for the ℓ^1 norm and nuclear norm are given by:

- Let $g(\mathbf{x}) = \lambda \|\mathbf{x}\|_1$ be the ℓ^1 norm. Then $\text{prox}_g[\mathbf{w}]$ is the soft-thresholding function applied element-wise:

$$(\text{prox}_g[\mathbf{w}])_i = \text{soft}\{w_i, \lambda\} \doteq \text{sign}(w_i) \max(|w_i| - \lambda, 0).$$

- Let $g(\mathbf{X}) = \lambda \|\mathbf{X}\|_*$ be the matrix nuclear norm. Then $\text{prox}_g[\mathbf{W}]$ is the singular-value soft thresholding function:

$$\text{prox}_g[\mathbf{W}] = \mathbf{U} \text{soft}\{\mathbf{\Sigma}, \lambda\} \mathbf{V}^*,$$

where $(\mathbf{U}, \mathbf{\Sigma}, \mathbf{V})$ are the SVD of \mathbf{W} . In other words, $\text{prox}_g[\mathbf{W}]$ applies component-wise soft thresholding on the singular values of \mathbf{W} .

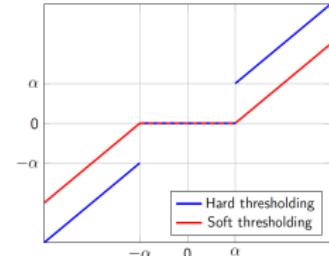
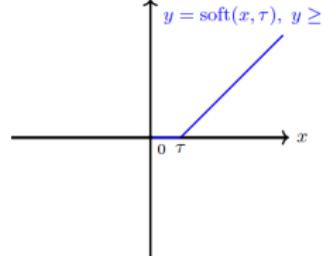
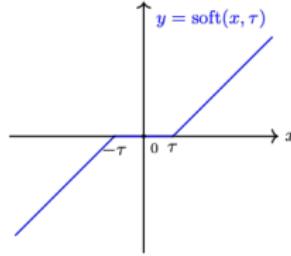
Proximal Operators

Proof ideas: The objective function reaches minimum when the subdifferential of $\lambda\|\mathbf{x}\|_1 + \frac{1}{2}\|\mathbf{x} - \mathbf{w}\|_2^2$ contains zero,

$$0 \in (\mathbf{x} - \mathbf{w}) + \lambda \partial \|\mathbf{x}\|_1 = \begin{cases} x_i - w_i + \lambda, & x_i > 0 \\ -w_i + \lambda[-1, 1], & x_i = 0, \quad i = 1, \dots, n. \\ x_i - w_i - \lambda, & x_i < 0 \end{cases}$$

□

Thresholding:



Proximal Gradient Algorithm

Proximal Gradient (PG)

Problem Class: $\min_{\mathbf{x}} F(\mathbf{x}) = f(\mathbf{x}) + g(\mathbf{x})$

$f, g : \mathbb{R}^n \rightarrow \mathbb{R}$ convex, ∇f L -Lipschitz and g nonsmooth.

Basic Iteration: set $\mathbf{x}_0 \in \mathbb{R}^n$.

Repeat:

$$\begin{aligned}\mathbf{w}_k &\leftarrow \mathbf{x}_k - \frac{1}{L} \nabla f(\mathbf{x}_k), \\ \mathbf{x}_{k+1} &\leftarrow \text{prox}_{g/L}[\mathbf{w}_k].\end{aligned}$$

Convergence Guarantee:

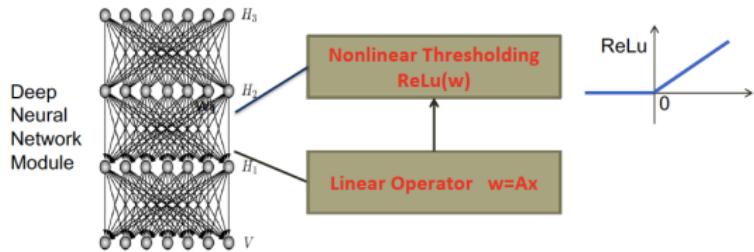
$F(\mathbf{x}_k) - F(\mathbf{x}_*)$ converges at a rate of $O(1/k)$.

Proximal Gradient for LASSO

Iterative soft-thresholding algorithm (ISTA):

- 1: **Problem:** $\min_{\mathbf{x}} \frac{1}{2} \|\mathbf{y} - \mathbf{A}\mathbf{x}\|_2^2 + \lambda \|\mathbf{x}\|_1$, given $\mathbf{y} \in \mathbb{R}^m$, $\mathbf{A} \in \mathbb{R}^{m \times n}$.
- 2: **Input:** $\mathbf{x}_0 \in \mathbb{R}^n$ and $L \geq \lambda_{\max}(\mathbf{A}^* \mathbf{A})$.
- 3: **for** $(k = 0, 1, 2, \dots, K - 1)$ **do**
- 4: $\mathbf{w}_k \leftarrow \mathbf{x}_k - \frac{1}{L} \mathbf{A}^* (\mathbf{A}\mathbf{x}_k - \mathbf{y})$.
- 5: $\mathbf{x}_{k+1} \leftarrow \text{soft}(\mathbf{w}_k, \lambda/L)$.
- 6: **end for**
- 7: **Output:** $\mathbf{x}_* \leftarrow \mathbf{x}_K$.

The unrolled iterations resemble a deep neural network!¹



¹Learning Fast Approximations of Sparse Coding, Karol Gregor and Yann LeCun, ICML 2010. Also known as the Learned ISTA (LISTA).

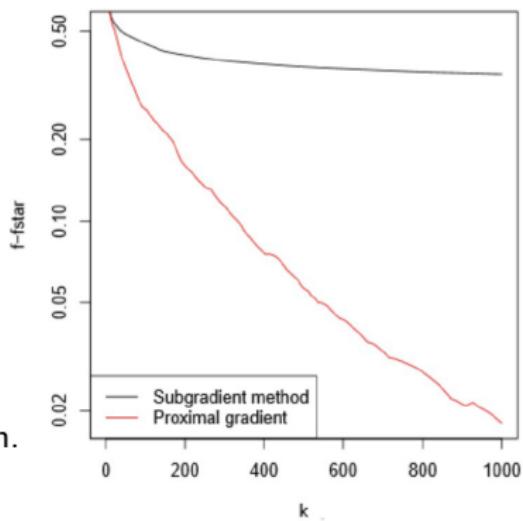
Proximal Gradient for LASSO

Iterative soft-thresholding algorithm (ISTA):

- 1: **Problem:** $\min_{\mathbf{x}} \frac{1}{2} \|\mathbf{y} - \mathbf{A}\mathbf{x}\|_2^2 + \lambda \|\mathbf{x}\|_1$, given $\mathbf{y} \in \mathbb{R}^m$, $\mathbf{A} \in \mathbb{R}^{m \times n}$.
- 2: **Input:** $\mathbf{x}_0 \in \mathbb{R}^n$ and $L \geq \lambda_{\max}(\mathbf{A}^* \mathbf{A})$.
- 3: **for** $(k = 0, 1, 2, \dots, K - 1)$ **do**
- 4: $\mathbf{w}_k \leftarrow \mathbf{x}_k - \frac{1}{L} \mathbf{A}^* (\mathbf{A}\mathbf{x}_k - \mathbf{y})$.
- 5: $\mathbf{x}_{k+1} \leftarrow \text{soft}(\mathbf{w}_k, \lambda/L)$.
- 6: **end for**
- 7: **Output:** $\mathbf{x}_* \leftarrow \mathbf{x}_K$.

Proximal Gradient versus Projected Gradient Descent.

Image courtesy of Prof. Qing Qu of Univ. Michigan.



The Heavy Ball Method [Polyak, 1964]

Gradient descent:

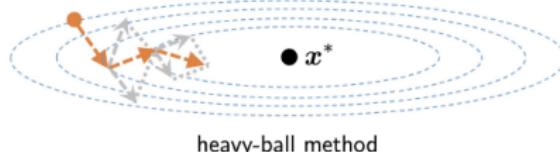
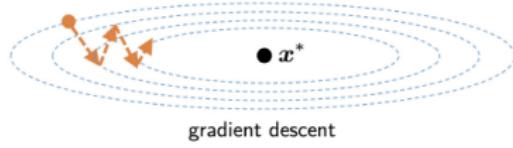
$$\mathbf{x}_{k+1} = \mathbf{x}_k - \alpha \nabla f(\mathbf{x}_k). \quad (20)$$

The **heavy ball method** (a.k.a the *momentum method*):

$$\mathbf{x}_{k+1} = \mathbf{x}_k - \alpha \nabla f(\mathbf{x}_k) + \underbrace{\beta(\mathbf{x}_k - \mathbf{x}_{k-1})}_{\text{momentum}}. \quad (21)$$



- Basis for popular ADAM for train deep neural networks.
- Worst convergence rate is still $O(1/k)$, yet best possible is $O(1/k^2)$.



Accelerated Gradient Descent [Nesterov, 1983]

Generate an auxiliary point \mathbf{p}_{k+1} of the form:

$$\mathbf{p}_{k+1} \doteq \mathbf{x}_k + \beta_{k+1}(\mathbf{x}_k - \mathbf{x}_{k-1}).$$

Move from \mathbf{x}_k to \mathbf{p}_{k+1} , and gradient descend from it:

$$\mathbf{x}_{k+1} = \mathbf{p}_{k+1} - \alpha \underbrace{\nabla f(\mathbf{p}_{k+1})}_{\text{a stroke of genius}}. \quad (22)$$



The weights α and $\{\beta_{k+1}\}$ are carefully chosen:

$$t_1 = 1, \quad t_{k+1} = \frac{1 + \sqrt{1 + 4t_k^2}}{2}, \quad \beta_{k+1} = \frac{t_k - 1}{t_{k+1}}, \quad \alpha = 1/L. \quad (23)$$

- We may not always have $f(\mathbf{x}_{k+1}) \leq f(\mathbf{x}_k)$.
- Achieve optimal convergence rate $O(1/k^2)$ among 1st order methods.

Accelerated Gradient Descent [Nesterov, 1983]

Accelerated Proximal Gradient (APG)

Problem Class: $\min_{\mathbf{x}} F(\mathbf{x}) = f(\mathbf{x}) + g(\mathbf{x})$,
 f, g convex, with ∇f L -Lipschitz and g **nonsmooth**.

Basic Iteration: set $\mathbf{x}_0 \in \mathbb{R}^n$, $\mathbf{p}_1 = \mathbf{x}_1 \leftarrow \mathbf{x}_0$, and $t_1 \leftarrow 1$.
 Repeat for $k = 1, 2, \dots, K$:

$$t_{k+1} \leftarrow \frac{1 + \sqrt{1 + 4t_k^2}}{2}, \quad \beta_{k+1} \leftarrow \frac{t_k - 1}{t_{k+1}}.$$

$$\mathbf{p}_{k+1} \leftarrow \mathbf{x}_k + \beta_{k+1}(\mathbf{x}_k - \mathbf{x}_{k-1}).$$

$$\mathbf{x}_{k+1} \leftarrow \text{prox}_{g/L} \left[\underbrace{\mathbf{p}_{k+1} - \frac{1}{L} \nabla f(\mathbf{p}_{k+1})}_{\text{proximal gradient}} \right].$$

Convergence Guarantee:

$F(\mathbf{x}_k) - F(\mathbf{x}_*)$ converges at a rate of $O(1/k^2)$.

GD versus Accelerated GD

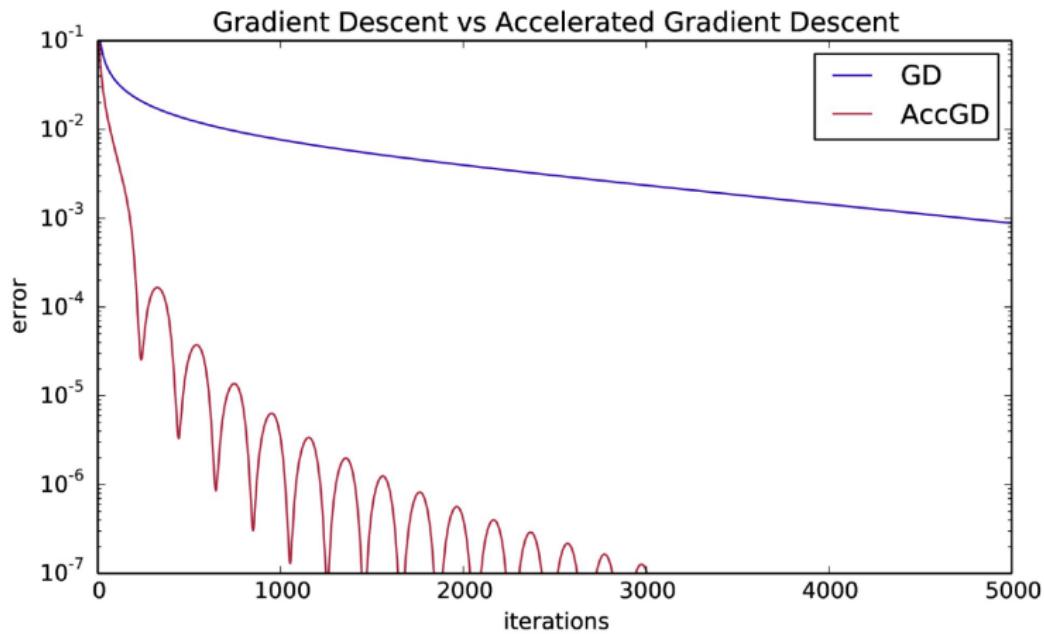


Image courtesy of Prof. Qing Qu of Univ. Michigan.

APG for LASSO

FISTA: Accelerated Proximal Gradient (APG) for LASSO

- 1: **Problem:** $\min_{\mathbf{x}} \frac{1}{2} \|\mathbf{y} - \mathbf{A}\mathbf{x}\|_2^2 + \lambda \|\mathbf{x}\|_1$, given $\mathbf{y} \in \mathbb{R}^m$, $\mathbf{A} \in \mathbb{R}^{m \times n}$.
- 2: **Input:** $\mathbf{x}_0 \in \mathbb{R}^n$, $\mathbf{p}_1 = \mathbf{x}_1 \leftarrow \mathbf{x}_0$, and $t_1 \leftarrow 1$, and $L \geq \lambda_{\max}(\mathbf{A}^* \mathbf{A})$.
- 3: **for** $(k = 1, 2, \dots, K - 1)$ **do**
- 4: $t_{k+1} \leftarrow \frac{1 + \sqrt{1 + 4t_k^2}}{2}$; $\beta_{k+1} \leftarrow \frac{t_k - 1}{t_{k+1}}$.
- 5: $\mathbf{p}_{k+1} \leftarrow \mathbf{x}_k + \beta_{k+1}(\mathbf{x}_k - \mathbf{x}_{k-1})$.
- 6: $\mathbf{w}_{k+1} \leftarrow \mathbf{p}_{k+1} - \frac{1}{L} \mathbf{A}^*(\mathbf{A}\mathbf{p}_{k+1} - \mathbf{y})$.
- 7: $\mathbf{x}_{k+1} \leftarrow \text{soft}[\mathbf{w}_{k+1}, \lambda/L]$.
- 8: **end for**
- 9: **Output:** $\mathbf{x}_* \leftarrow \mathbf{x}_K$.

APG for Stable PCP

Accelerated Proximal Gradient (APG) for Stable PCP

- 1: **Problem:** $\min_{\mathbf{L}, \mathbf{S}} \|\mathbf{L}\|_* + \lambda \|\mathbf{S}\|_1 + \frac{\mu}{2} \|\mathbf{Y} - \mathbf{L} - \mathbf{S}\|_F^2$, given \mathbf{Y} .
- 2: **Input:** $\mathbf{L}_0, \mathbf{S}_0 \in \mathbb{R}^{m \times n}$, $\mathbf{P}_1^S = \mathbf{S}_1 \leftarrow \mathbf{S}_0$, $\mathbf{P}_1^L = \mathbf{L}_1 \leftarrow \mathbf{L}_0$, $t_1 \leftarrow 1$.
- 3: **for** $(k = 1, 2, \dots, K - 1)$ **do**
- 4: $t_{k+1} \leftarrow \frac{1 + \sqrt{1 + 4t_k^2}}{2}$, $\beta_{k+1} \leftarrow \frac{t_k - 1}{t_{k+1}}$.
- 5: $\mathbf{P}_{k+1}^L \leftarrow \mathbf{L}_k + \beta_{k+1}(\mathbf{L}_k - \mathbf{L}_{k-1})$; $\mathbf{P}_{k+1}^S \leftarrow \mathbf{S}_k + \beta_{k+1}(\mathbf{S}_k - \mathbf{S}_{k-1})$.
- 6: $\mathbf{W}_{k+1} \leftarrow \mathbf{Y} - \mathbf{P}_{k+1}^S$ and compute SVD: $\mathbf{W}_{k+1} = \mathbf{U}_{k+1} \boldsymbol{\Sigma}_{k+1} \mathbf{V}_{k+1}^*$.
- 7: $\mathbf{L}_{k+1} \leftarrow \mathbf{U}_{k+1} \text{soft}[\boldsymbol{\Sigma}_{k+1}, 1/\mu] \mathbf{V}_{k+1}^*$; $\mathbf{S}_{k+1} \leftarrow \text{soft}[(\mathbf{Y} - \mathbf{P}_{k+1}^L), \lambda/\mu]$.
- 8: **end for**
- 9: **Output:** $\mathbf{L}_* \leftarrow \mathbf{L}_K$; $\mathbf{S}_* \leftarrow \mathbf{S}_K$.

Algorithm: A Little Lesson from History

Comparison from chronological development of algorithms for solving the PCP problem: **the older the algorithm, the more efficient!**

GOOD NEWS: Scalable first-order gradient-descent algorithms:

- Proximal Gradient [Osher, Mao, Dong, Yin '09, Wright et. al.'09, Cai et. al.'09].
- Accelerated Proximal Gradient [Nesterov '83, Beck and Teboulle '09]:
- Augmented Lagrange Multiplier [Hestenes '69, Powell '69]:
- Alternating Direction Method of Multipliers [Gabay and Mercier '76].

For a 1000×1000 matrix of rank 50, with 10% (100,000) entries randomly corrupted: $\min \|A\|_* + \lambda \|E\|_1$ subj $A + E = D$.

| Algorithms | Accuracy | Rank | $\ E\ _0$ | # iterations | time (sec) | |
|-------------------|-----------|------|-----------|--------------|------------|--|
| IT | 5.99e-006 | 50 | 101,268 | 8,550 | 119,370.3 | |
| DUAL | 8.65e-006 | 50 | 100,024 | 822 | 1,855.4 | |
| APG | 5.85e-006 | 50 | 100,347 | 134 | 1,468.9 | |
| APG _P | 5.91e-006 | 50 | 100,347 | 134 | 82.7 | |
| EALM _P | 2.07e-007 | 50 | 100,014 | 34 | 37.5 | |
| IALM _P | 3.83e-007 | 50 | 99,996 | 23 | 11.8 | |

10,000 times speedup!

GD for Strongly Convex Problems

A troubling fact though: Not supposed to be this fast!

Reason? Consider minimizing a **L -Lipschitz continuous** function

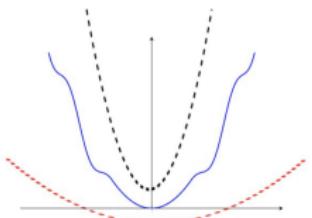
$$\min_{\mathbf{x}} f(\mathbf{x}), \quad \mathbf{x} \in \mathbb{R}^n. \quad (24)$$

Assume $f(\mathbf{x})$ is **μ -strongly convex**:

$$f((\mathbf{x}') \geq f(\mathbf{x}) + \langle \nabla f(\mathbf{x}), \mathbf{x}' - \mathbf{x} \rangle + \frac{\mu}{2} \|\mathbf{x}' - \mathbf{x}\|_2^2. \quad (25)$$

This implies (assuming f is twice differentiable):

$$\mathbf{0} \prec \mu \mathbf{I} \preceq \nabla^2 f(\mathbf{x}) \preceq L \mathbf{I}.$$

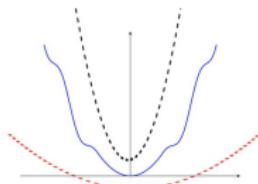


Convergence of GD for Strongly Convex Problems

Theorem (see Appendix D).

$f(\mathbf{x})$: μ -strongly convex and L -Lipschitz continuous.

For gradient descent with a step size $t = \frac{2}{L+\mu}$, we have:



$$\|\mathbf{x}_k - \mathbf{x}_\star\|_2 \leq \left(\frac{\kappa - 1}{\kappa + 1} \right)^k \|\mathbf{x}_0 - \mathbf{x}_\star\|_2, \quad (26)$$

where $\kappa = L/\mu$ and \mathbf{x}_\star is the minimizer.

Convergence Rates for Gradient Descent:

- ① f non-smooth: $O(1/\sqrt{k})$.
- ② f differentiable: $O(1/k)$.
- ③ f smooth, ∇f Lipschitz: $O(1/k^2)$.
- ④ f strongly convex: $O(e^{-\alpha k})$.

Convergence of Restricted Strong Convex Problems

Fact: Structured signal recovery problems such as LASSO and PCP satisfy **restricted strong convexity**. Hence, gradient descent enjoys **globally linear convergence** up to the statistical precision of the model.²

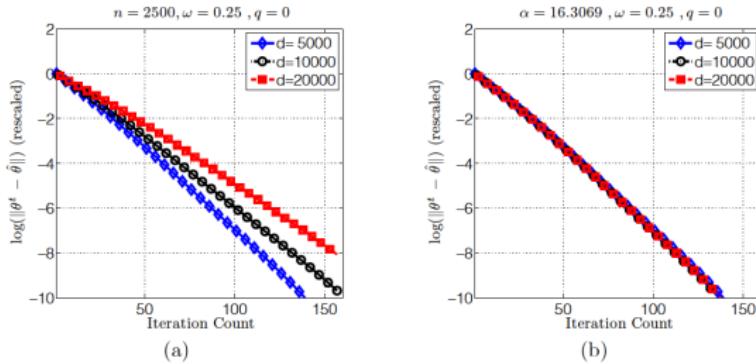


Figure 1. Convergence rates of projected gradient descent in application to Lasso programs (ℓ_1 -constrained least-squares). Each panel shows the log optimization error $\log\|\theta^t - \hat{\theta}\|$ versus the iteration number t . Panel (a) shows three curves, corresponding to dimensions $d \in \{5000, 10000, 20000\}$, sparsity $s = \lceil \sqrt{d} \rceil$, and all with the same sample size $n = 2500$. All cases show geometric convergence, but the rate for larger problems becomes progressively slower. (b) For an appropriately rescaled sample size ($\alpha = \frac{n}{s \log d}$), all three convergence rates should be roughly the same, as predicted by the theory.

²Fast global convergence of gradient methods for high-dimensional statistical recovery, Agarwal, Negahban, Wainwright, NIPS 2010.

Assignments

- Reading: Section 8.1 - 8.3 of Chapter 8. Appendix B, C, and D.
- Programming Homework #3.