Computational Principles for High-dim Data Analysis

(Lecture Thirteen)

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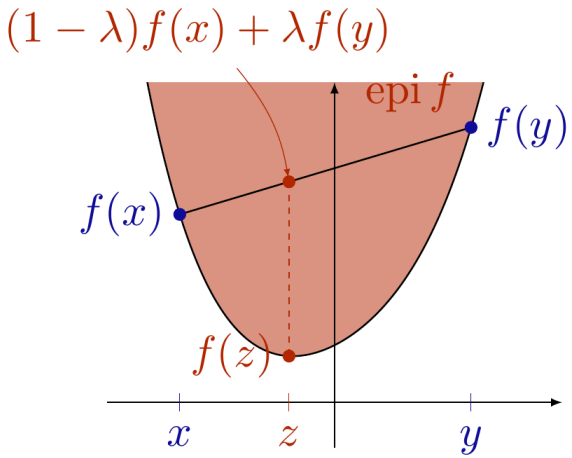
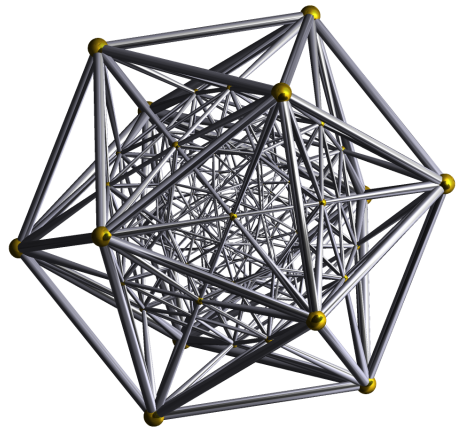




Unconstrained Convex Optimization
for Structured Data Recovery

"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 $\boldsymbol{x}_o$ from $\boldsymbol{y} = \boldsymbol{A}\boldsymbol{x}_o \in \mathbb{R}^m$ or $\boldsymbol{y} = \boldsymbol{A}\boldsymbol{x}_o + \boldsymbol{z} \in \mathbb{R}^m$ via convex programs:

- **Basis Pursuit** (BP):

$$\min_{\boldsymbol{x}} \|\boldsymbol{x}\|_1 \quad \text{subject to} \quad \boldsymbol{A}\boldsymbol{x} = \boldsymbol{y}. \tag{1}$$

- **LASSO**:

$$\min_{\boldsymbol{x}} \frac{1}{2}\|\boldsymbol{y} - \boldsymbol{A}\boldsymbol{x}\|_2^2 + \lambda\|\boldsymbol{x}\|_1. \tag{2}$$

Optimization Problems for Structured Data Recovery

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

- **Matrix Completion**:

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

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

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

- **Stable PCP**:

$$\min_{\boldsymbol{L},\boldsymbol{S}} \|\boldsymbol{L}\|_* + \lambda \|\boldsymbol{S}\|_1 + \frac{\mu}{2} \|\boldsymbol{Y} - \boldsymbol{L} - \boldsymbol{S}\|_F^2 . \tag{5}$$

Optimization Challenges for Structured Data Recovery

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

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

$$\text{Second order methods} \quad \Longrightarrow \quad \text{First order methods...} \tag{7}$$

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

$$O(1/\sqrt{k}) \quad \Longrightarrow \quad O(1/k) \quad \Longrightarrow \quad O(1/k^2)... \tag{8}$$

- **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):

$$\min f(\boldsymbol{x}), \quad \boldsymbol{x} \in \mathsf{C} \text{ (a convex set)}, \tag{9}$$

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

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

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

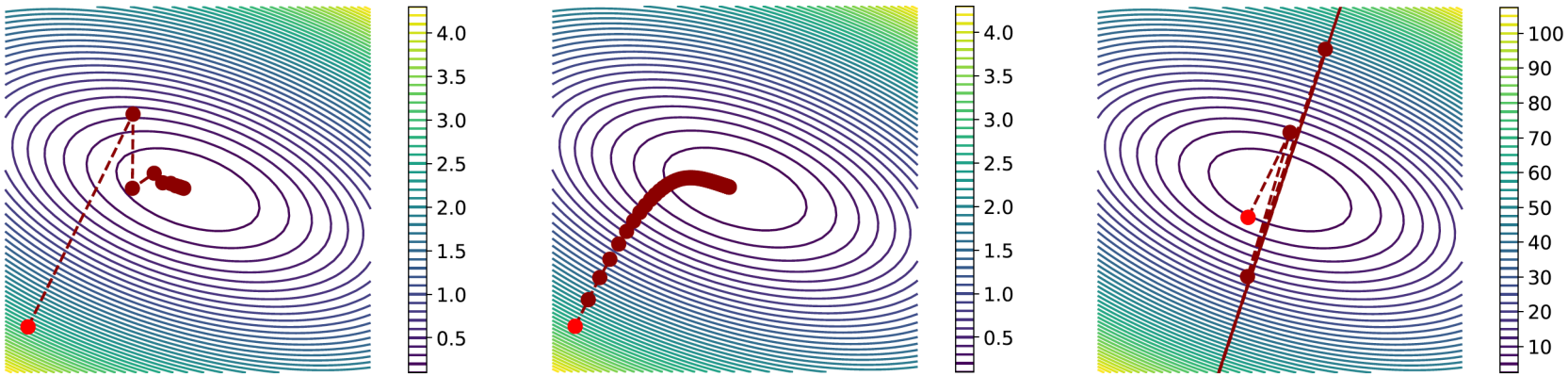


figure courtesy of prof. Carlos Fernandez of NYU.

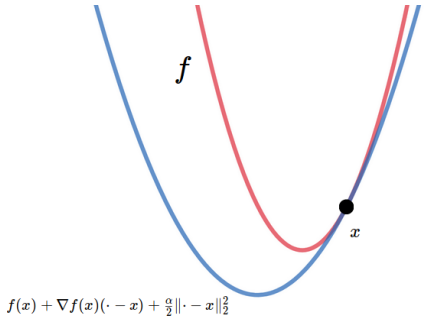
Gradient Descent

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

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

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

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



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

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

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:

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

Upper bound:

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

$$= \frac{L}{2}\left\|\boldsymbol{x} - (\boldsymbol{x}_k - \tfrac{1}{L}\nabla f(\boldsymbol{x}_k))\right\|_2^2 + g(\boldsymbol{x}) + h(\boldsymbol{x}_k). \tag{15}$$

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

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

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

Proximal Operators

Definition (Proximal Operator)

The proximal operator of a convex function g is

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

Iteration (17) can be written as:

$$\boldsymbol{x}_{k+1} = \text{prox}_{g/L}[\boldsymbol{w}_k]. \tag{19}$$

For many convex functions g:

$\text{prox}_g[w]$ 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:

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

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

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

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

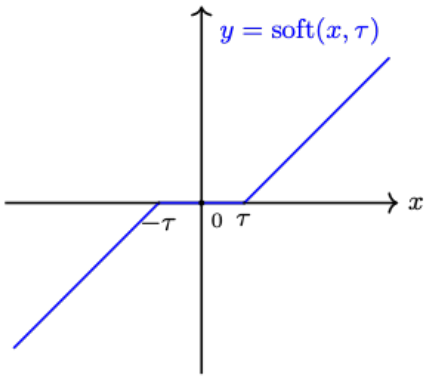
where $(\boldsymbol{U}, \boldsymbol{\Sigma}, \boldsymbol{V})$ are the SVD of $\boldsymbol{W}$. In other words, $\mathrm{prox}_g[\boldsymbol{W}]$ applies component-wise soft thresholding on the singular values of $\boldsymbol{W}$.

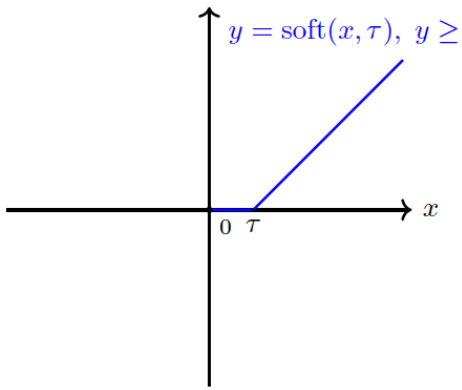
Proximal Operators

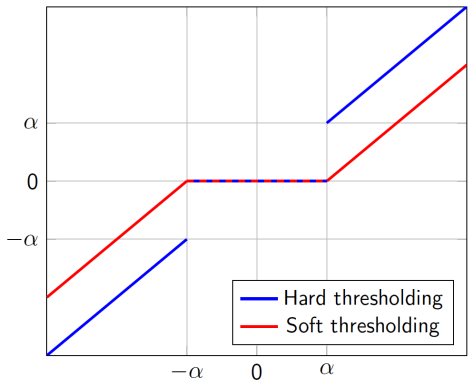
Proof ideas: The objective function reaches minimum when the subdifferential of $\lambda\|\boldsymbol{x}\|_1 + \frac{1}{2}\|\boldsymbol{x} - \boldsymbol{w}\|_2^2$ contains zero,

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

Thresholding:







Proximal Gradient Algorithm

Proximal Gradient (PG)

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

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

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

Repeat:

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

Convergence Guarantee:

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

Proximal Gradient for LASSO

Iterative soft-thresholding algorithm (ISTA):

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

The unrolled iterations resemble a deep neural network![1]

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

The Heavy Ball Method [Polyak, 1964]

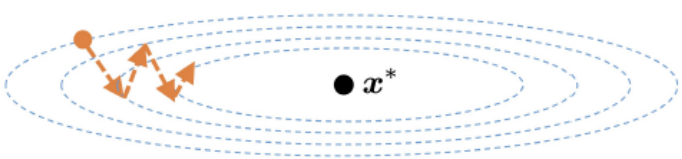
Gradient descent:

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

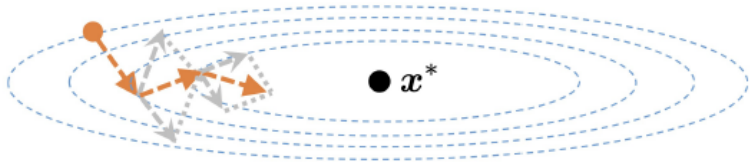
The **heavy ball method** (a.k.a the *momentum method*):

$$\boldsymbol{x}_{k+1} = \boldsymbol{x}_k - \alpha \nabla f(\boldsymbol{x}_k) + \underbrace{\beta\left(\boldsymbol{x}_k - \boldsymbol{x}_{k-1}\right)}_{\text{momentum}}. \tag{21}$$

- Basis for popular ADAM for train deep neural networks.
- Worst convergence rate is still $O(1/k)$.



gradient descent



heavy-ball method

Accelerated Gradient Descent [Nesterov, 1983]

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

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

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

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

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

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

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

Accelerated Gradient Descent [Nesterov, 1983]

Accelerated Proximal Gradient (APG)

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

f, g convex, with ∇f L-Lipschitz and g nonsmooth.

Basic Iteration: set $\boldsymbol{x}_0 \in \mathbb{R}^n$, $\boldsymbol{p}_1 = \boldsymbol{x}_1 \leftarrow \boldsymbol{x}_0$, and $t_1 \leftarrow 1$.

Repeat for $k = 1, 2, \ldots, K$:

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

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

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

Convergence Guarantee:

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

GD versus Accelerated GD

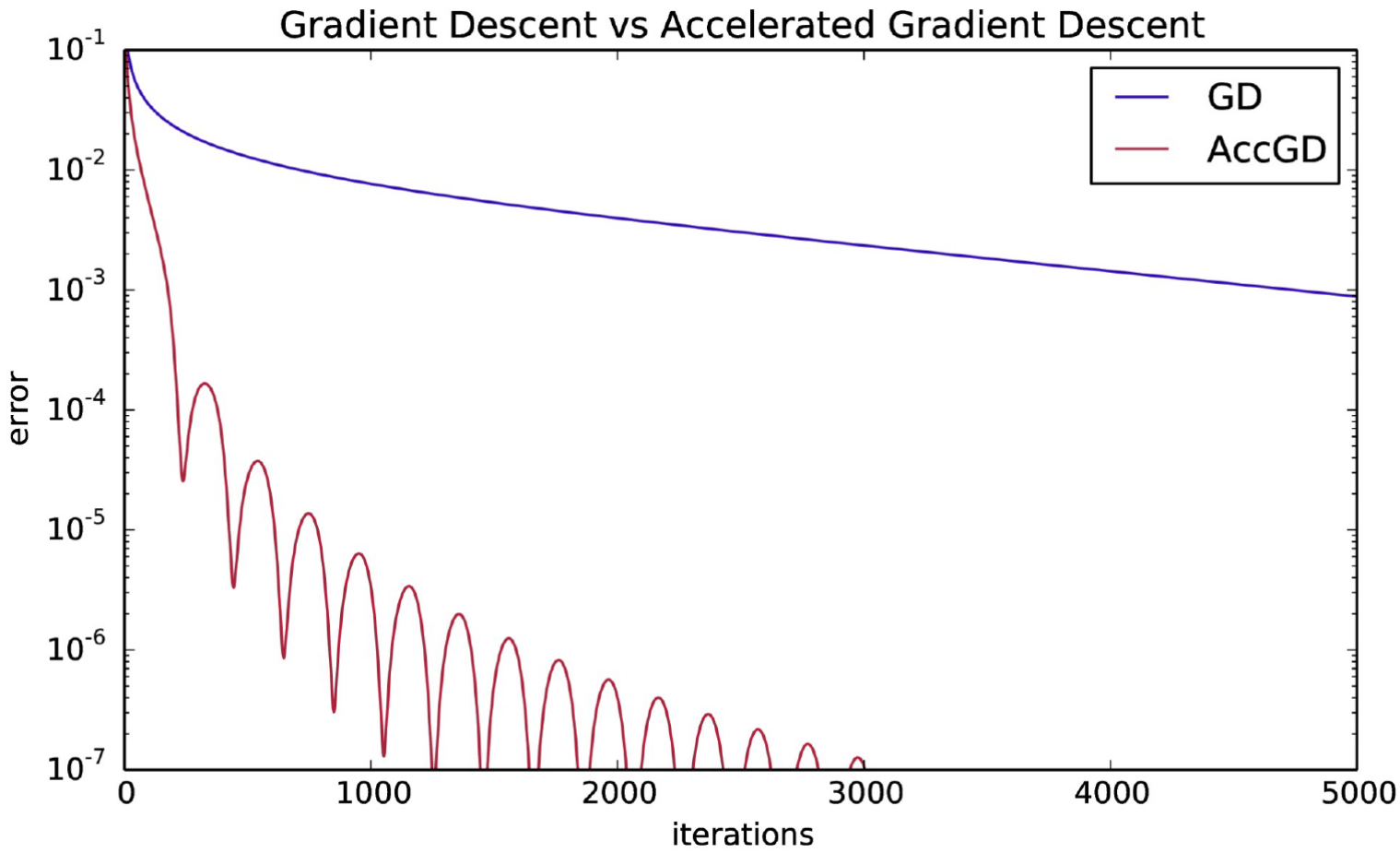


Image courtesy of Prof. Qing Qu of Univ. Michigan.

APG for LASSO

FISTA: Accelerated Proximal Gradient (APG) for LASSO

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

APG for Stable PCP

Accelerated Proximal Gradient (APG) for Stable PCP

Problem: $\min_{\boldsymbol{L},\boldsymbol{S}} \|\boldsymbol{L}\|_* + \lambda\|\boldsymbol{S}\|_1 + \frac{\mu}{2}\|\boldsymbol{Y} - \boldsymbol{L} - \boldsymbol{S}\|_F^2$, given $\boldsymbol{Y}$.

Input: $\boldsymbol{L}_0, \boldsymbol{S}_0 \in \mathbb{R}^{m\times n}$, $\boldsymbol{P}_1^S = \boldsymbol{S}_1 \leftarrow \boldsymbol{S}_0$, $\boldsymbol{P}_1^L = \boldsymbol{L}_1 \leftarrow \boldsymbol{L}_0$, $t_1 \leftarrow 1$.

for $(k = 1, 2, \ldots, K-1)$ **do**

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

  $\boldsymbol{P}_{k+1}^L \leftarrow \boldsymbol{L}_k + \beta_{k+1}\big(\boldsymbol{L}_k - \boldsymbol{L}_{k-1}\big)$; $\boldsymbol{P}_{k+1}^S \leftarrow \boldsymbol{S}_k + \beta_{k+1}\big(\boldsymbol{S}_k - \boldsymbol{S}_{k-1}\big)$.

  $\boldsymbol{W}_{k+1} \leftarrow \boldsymbol{Y} - \boldsymbol{P}_{k+1}^S$ and compute SVD: $\boldsymbol{W}_{k+1} = \boldsymbol{U}_{k+1}\boldsymbol{\Sigma}_{k+1}\boldsymbol{V}_{k+1}^*$.

  $\boldsymbol{L}_{k+1} \leftarrow \boldsymbol{U}_{k+1}\mathsf{soft}[\boldsymbol{\Sigma}_{k+1}, 1/\mu]\boldsymbol{V}_{k+1}^*$; $\boldsymbol{S}_{k+1} \leftarrow \mathsf{soft}[(\boldsymbol{Y} - \boldsymbol{P}_{k+1}^L), \lambda/\mu]$.

end for

Output: $\boldsymbol{L}_\star \leftarrow \boldsymbol{L}_K$; $\boldsymbol{S}_\star \leftarrow \boldsymbol{S}_K$.

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 1000x1000 matrix of rank 50, with 10% (100,000) entries randomly corrupted: $\min \|A\|_* + \lambda\|E\|_1 \quad \text{subj} \quad A + E = D.$

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

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

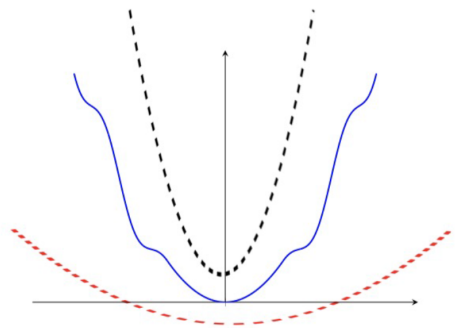
$$\min_{\boldsymbol{x}} f(\boldsymbol{x}), \quad \boldsymbol{x} \in \mathbb{R}^n. \tag{24}$$

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

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

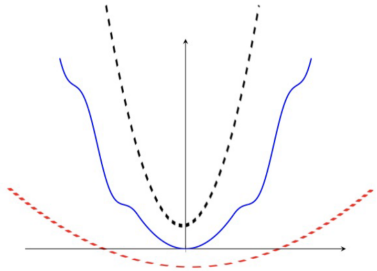
This implies (assuming f is twice differentiable):

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



Convergence of GD for Strongly Convex Problems

Theorem (see Appendix D).
$f(\boldsymbol{x})$: μ-strongly convex and L-Lipschitz continuous.
For gradient descent with a step size $t = \frac{2}{L+\mu}$, we have:



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

where $\kappa = L/\mu$ and $\boldsymbol{x}_\star$ 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]

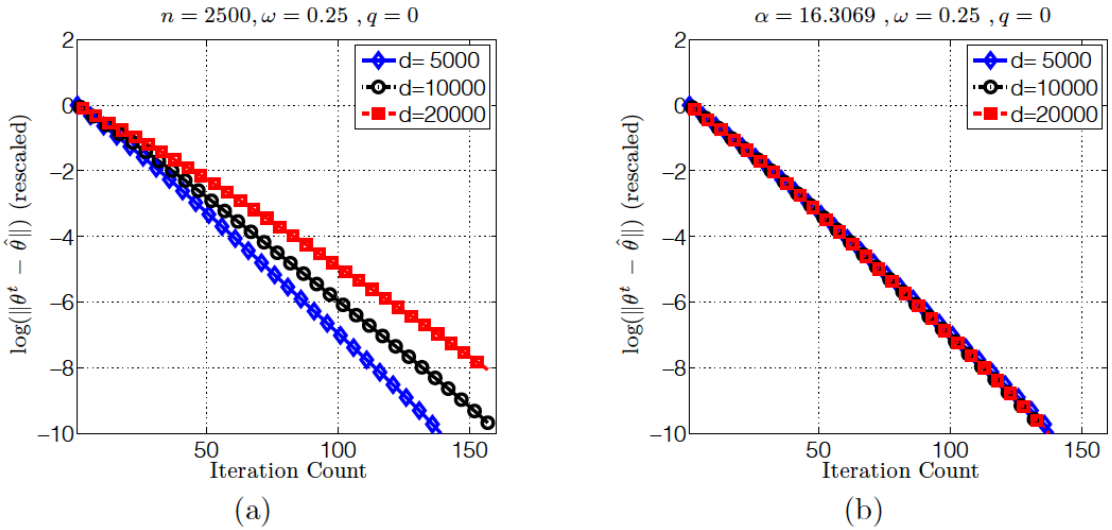


Figure 1. Convergence rates of projected gradient descent in application to Lasso programs (ℓ_1-constrained least-squares). Each panel shows the log optimization error $\log \|\theta^t - \widehat{\theta}\|$ versus the iteration number t. Panel (a) shows three curves, corresponding to dimensions $d \in \{5000, 10000, 20000\}$, 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.

[2] Fast 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.