Mathematics of Data: From Theory to Computation

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Lecture 6: From stochastic gradient descent to non-smooth optimization

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Outline

- Stochastic optimization
- Deficiency of smooth models
- Sparsity and compressive sensing
- Non-smooth minimization via Subgradient descent
- *Atomic norms

Recall: Gradient descent

Problem (Unconstrained optimization problem)

Consider the following minimization problem:

$$f^{\star} = \min_{\mathbf{x} \in \mathbb{R}^p} f(\mathbf{x})$$

 $f(\mathbf{x})$ is proper and closed.

Gradient descent

Choose a starting point \mathbf{x}^0 and iterate

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

where α_k is a step-size to be chosen so that \mathbf{x}^k converges to \mathbf{x}^\star .

	f is L-smooth & convex	f is L-gradient Lipschitz & non-convex
GD	O(1/k) (fast)	O(1/k) (optimal)
AGD	$O(1/k^2)$ (optimal)	O(1/k) (optimal) [16]



Recall: Gradient descent

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Why should we study anything else?



Statistical learning with streaming data

 \circ Recall that statistical learning seeks to find a $h^{\star} \in \mathcal{H}$ that minimizes the expected risk,

$$h^* \in \operatorname*{arg\,min}_{h \in \mathcal{H}} \left\{ R(h) := \mathbb{E}_{(\mathbf{a},b)} \left[\mathcal{L}(h(\mathbf{a}),b) \right] \right\}.$$

Abstract gradient method

$$h^{k+1} = h^k - \alpha_k \nabla R(h^k) = h^k - \alpha_k \mathbb{E}_{(\mathbf{a},b)}[\nabla \mathcal{L}(h^k(\mathbf{a}),b)].$$

Remark: • This algorithm can not be implemented as the distribution of (\mathbf{a}, b) is unknown.



Statistical learning with streaming data

 \circ Recall that statistical learning seeks to find a $h^{\star} \in \mathcal{H}$ that minimizes the *expected* risk,

$$h^{\star} \in \underset{h \in \mathcal{H}}{\operatorname{arg\,min}} \left\{ R(h) := \mathbb{E}_{(\mathbf{a},b)} \left[\mathcal{L}(h(\mathbf{a}),b) \right] \right\}.$$

Abstract gradient method

$$h^{k+1} = h^k - \alpha_k \nabla R(h^k) = h^k - \alpha_k \mathbb{E}_{(\mathbf{a},b)}[\nabla \mathcal{L}(h^k(\mathbf{a}),b)].$$

Remark: • This algorithm can not be implemented as the distribution of (\mathbf{a}, b) is unknown.

• In practice, data can arrive in a *streaming* way.

A parametric example: Markowitz portfolio optimization

$$\mathbf{x}^{\star} := \min_{\mathbf{x} \in \mathcal{X}} \left\{ \mathbb{E} \left[|b - \langle \mathbf{x}, \mathbf{a} \rangle|^2 \right] \right\}$$

 $\blacktriangleright h_{\mathbf{x}}(\cdot) = \langle \mathbf{x}, \cdot \rangle$

- ▶ $b \in \mathbb{R}$ is the desired return & $\mathbf{a} \in \mathbb{R}^p$ are the stock returns
- ▶ \mathcal{X} is intersection of the standard simplex and the constraint: $\langle \mathbf{x}, \mathbb{E}[\mathbf{a}] \rangle \ge \rho$.

Problem (Mathematical formulation)

Consider the following convex minimization problem:

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

- θ is a random vector whose probability distribution is supported on set Θ .
- $f(\mathbf{x}) := \mathbb{E}[f(\mathbf{x}, \theta)]$ is proper, closed, and convex.
- The solution set $S^* := {\mathbf{x}^* \in \text{dom}(f) : f(\mathbf{x}^*) = f^*}$ is nonempty.

Stochastic gradient descent (SGD)

 Stochastic gradient descent (SGD)

 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:

 $\mathbf{x}^{k+1} = \mathbf{x}^k - \alpha_k G(\mathbf{x}^k, \theta_k).$

• $G(\mathbf{x}^k, \theta_k)$ is an unbiased estimate of the full gradient:

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



Stochastic gradient descent (SGD)

Stochastic gradient descent (SGD) 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: $\mathbf{x}^{k+1} = \mathbf{x}^k - \alpha_k G(\mathbf{x}^k, \theta_k).$

• $G(\mathbf{x}^k, \theta_k)$ is an unbiased estimate of the full gradient:

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

Remarks:

 \circ The cost of computing $G(\mathbf{x}^k, heta_k)$ is n times cheaper than that of $abla f(\mathbf{x}^k)$.

 \circ As $G(\mathbf{x}^k, \theta_k)$ is an unbiased estimate of the full gradient, SGD would perform well.

• We assume $\{\theta_k\}$ are jointly independent.

 \circ SGD is not a monotonic descent method.

Example: Convex optimization with finite sums

Convex optimization with finite sums

The problem

$$\underset{\mathbf{x}\in\mathbb{R}^p}{\operatorname{arg\,min}}\left\{f(\mathbf{x}):=\frac{1}{n}\sum_{j=1}^n f_j(\mathbf{x})\right\},\$$

can be rewritten as

 $\underset{\mathbf{x} \in \mathbb{R}^p}{\arg\min} \left\{ f(\mathbf{x}) := \mathbb{E}_i[f_i(\mathbf{x})] \right\}, \qquad i \text{ is uniformly distributed over } \{1, 2, \cdots, n\}.$

A stochastic gradient descent (SGD) variant for finite sums

 $\mathbf{x}^{k+1} = \mathbf{x}^k - \alpha_k \nabla f_i(\mathbf{x}^k) \qquad i \text{ is uniformly distributed over}\{1,...,n\}$

Remarks:

0

Note:
$$\mathbb{E}_i[\nabla f_i(\mathbf{x}^k)] = \sum_{j=1}^n \nabla f_j(\mathbf{x}^k)/n = \nabla f(\mathbf{x}^k).$$

 \circ The computational cost of SGD per iteration is p.



Synthetic least-squares problem

$$\min_{\mathbf{x}} \left\{ f(\mathbf{x}) := \frac{1}{2n} \|\mathbf{A}\mathbf{x} - \mathbf{b}\|_2^2 : \mathbf{x} \in \mathbb{R}^p \right\}$$

Setup

- $\mathbf{A} := \operatorname{randn}(n, p)$ standard Gaussian $\mathcal{N}(0, \mathbb{I})$, with $n = 10^4$, $p = 10^2$.
- \mathbf{x}^{\natural} is 50 sparse with zero mean Gaussian i.i.d. entries, normalized to $\|\mathbf{x}^{\natural}\|_{2} = 1$.
- $\mathbf{b} := \mathbf{A} \mathbf{x}^{\natural} + \mathbf{w}$, where \mathbf{w} is Gaussian white noise with variance 1.



 $\circ 1 \text{ epoch} = 1 \text{ pass over the full gradient}$



Convergence of SGD when the objective is not strongly convex

Theorem (decaying step-size [28])

Assume

•
$$\mathbb{E}[\|\mathbf{x}^k - \mathbf{x}^\star\|^2] \le D^2$$
 for all k ,

•
$$\mathbb{E}[\|G(\mathbf{x}^k, \theta_k)\|^2] \le M^2$$
 (bounded gradient),

$$\blacktriangleright \ \alpha_k = \alpha_0 / \sqrt{k}.$$

Then

$$\mathbb{E}[f(\mathbf{x}^k) - f(\mathbf{x}^\star)] \le \left(\frac{D^2}{\alpha_0} + \alpha_0 M^2\right) \frac{2 + \log k}{\sqrt{k}}.$$

Observation: $\circ O(1/\sqrt{k})$ rate is optimal for SGD if we do not consider the strong convexity.



Convergence of SGD for strongly convex problems I

Theorem (strongly convex objective, fixed step-size [4])

Assume

- ▶ f is µ-strongly convex and L-smooth,
- $\blacktriangleright \mathbb{E}[\|G(\mathbf{x}^k, \theta_k)\|^2]_2 \le \sigma^2 + M \|\nabla f(\mathbf{x}^k)\|_2^2 \text{ (bounded variance),}$

$$\qquad \bullet \ \alpha_k = \alpha \le \frac{1}{LM}$$

Then

$$\mathbb{E}[f(\mathbf{x}^k) - f(\mathbf{x}^\star)] \le \frac{\alpha L \sigma^2}{2\mu} + (1 - \mu \alpha)^{k-1} \left(f(\mathbf{x}^1) - f^\star \right).$$

Observations: \circ Converge fast (linearly) to a neighborhood around \mathbf{x}^* .

 \circ Smaller step-sizes $\alpha \Longrightarrow$ converge to a better point, but with a slower rate.

 \circ Zero variance ($\sigma = 0$) \Longrightarrow linear convergence.

- \circ This is also known as the relative noise model [25] or the strong growth condition [8].
- The growth condition is in fact a necessary and sufficient condition for linear convergence [8].
- \circ The theory applies to the Kaczmarz algorithm (see advanced material).



Convergence of SGD for strongly convex problems II

Theorem (strongly convex objective, decaying step-size [4])

Assume

- f is μ-strongly convex and L-smooth,
- $\blacktriangleright \mathbb{E}[\|G(\mathbf{x}^k, \theta_k)\|^2]_2 \leq \sigma^2 + M \|\nabla f(\mathbf{x}^k)\|_2^2 \text{ (bounded variance),}$
- $\alpha_k = \frac{c}{k_0 + k}$ with some appropriate constants c and k_0 .

Then

$$\mathbb{E}[\|\mathbf{x}^k - \mathbf{x}^\star\|^2] \le \frac{C}{k+1},$$

where C is a constant independent of k.

Observations: • Using the *L*-smooth property,

$$\mathbb{E}[f(\mathbf{x}^k) - f(\mathbf{x}^\star)] \le L\mathbb{E}[\|\mathbf{x}^k - \mathbf{x}^\star\|^2] \le \frac{C}{k+1}.$$

 \circ The rate is optimal if $\sigma^2>0$ with the assumption of strongly-convexity.



Example: SGD with different step sizes



Setup

- Synthetic least-squares problem as before.
- \circ We use $\alpha_k = \alpha_0/(k+k_0)$.

Example: SGD with different step sizes



Setup

 \circ Synthetic least-squares problem as before.

• We use $\alpha_k = \alpha_0/(k+k_0)$.

Observation: $\circ \alpha_0 = 1/\mu$ is the best choice.



Comparison with GD

$$f^{\star} := \min_{\mathbf{x} \in \mathbb{R}^p} \bigg\{ f(\mathbf{x}) := \frac{1}{n} \sum_{j=1}^n f_j(\mathbf{x}) \bigg\}.$$

 \circ *f*: μ -strongly convex with *L*-Lipschitz smooth.

	rate	iteration complexity	cost per iteration	total cost
GD	ρ^k	$\log(1/\epsilon)$	n	$n\log(1/\epsilon)$
SGD	1/k	$1/\epsilon$	1	$1/\epsilon$

Remark: \circ SGD is more favorable when n is large — large-scale optimization problems

Motivation for SGD with Averaging

 \circ SGD iterates tend to oscillate around global minimizers

o Averaging iterates can reduce the oscillation effect

• Two types of averaging:

$$\begin{split} \bar{\mathbf{x}}^k &= \frac{1}{k} \sum_{j=1}^k \alpha_j \mathbf{x}^j \quad \text{(vanilla averaging)} \\ \bar{\mathbf{x}}^k &= \frac{\sum_{j=1}^k \alpha_j \mathbf{x}^j}{\sum_{j=1}^k \alpha_j} \quad \text{(weighted averaging)} \end{split}$$

Remark:

• Do not confuse the averaging above with the ones used in Federated Learning.

Convergence for SGD-A I: non-strongly convex case

Stochastic gradient method with averaging (SGD-A) **1.** Choose $\mathbf{x}^0 \in \mathbb{R}^p$ and $(\alpha_k)_{k \in \mathbb{N}} \in [0, +\infty]^{\mathbb{N}}$. **2a.** For k = 0, 1, ... perform: $\mathbf{x}^{k+1} = \mathbf{x}^k - \alpha_k G(\mathbf{x}^k, \theta_k).$ **2b.** $\bar{\mathbf{x}}^k = (\sum_{j=0}^k \alpha_j)^{-1} \sum_{j=0}^k \alpha_j \mathbf{x}^j.$

Theorem (Convergence of SGD-A [24]) Let $D = \|\mathbf{x}^0 - \mathbf{x}^{\star}\|$ and $\mathbb{E}[\|G(\mathbf{x}^k, \theta_k)\|^2] < M^2$. Then.

$$\mathbb{E}[f(\bar{\mathbf{x}}^{k+1}) - f(\mathbf{x}^{\star})] \le \frac{D^2 + M^2 \sum_{j=0}^{k} \alpha_j^2}{2 \sum_{j=0}^{k} \alpha_j}$$

In addition, choosing $\alpha_k = D/(M\sqrt{k+1})$, we get.

$$\mathbb{E}[f(\bar{\mathbf{x}}^k) - f(\mathbf{x}^\star)] \le \frac{MD(2 + \log k)}{\sqrt{k}}.$$

Observation: • Same convergence rate with vanilla SGD.

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Convergence for SGD-A II: strongly convex case

Stochastic gradient method with averaging (SGD-A) 1. Choose $\mathbf{x}^0 \in \mathbb{R}^p$ and $(\alpha_k)_{k \in \mathbb{N}} \in]0, +\infty[^{\mathbb{N}}.$ 2a. For $k = 0, 1, \dots$ perform: $\mathbf{x}^{k+1} = \mathbf{x}^k - \alpha_k G(\mathbf{x}^k, \theta_k).$ 2b. $\bar{\mathbf{x}}^k = \frac{1}{k} \sum_{j=1}^k \mathbf{x}^j.$

Theorem (Convergence of SGD-A [27]) Assume

• f is μ -strongly convex,

$$\blacktriangleright \mathbb{E}[\|G(\mathbf{x}^k, \theta_k)\|^2] \le M^2$$

•
$$\alpha_k = \alpha_0/k$$
 for some $\alpha_0 \ge 1/\mu$.

Then

$$\mathbb{E}[f(\bar{\mathbf{x}}^k) - f(\mathbf{x}^\star)] \le \frac{\alpha_0 M^2 (1 + \log k)}{2k}$$

Observation: • Same convergence rate with vanilla SGD.

Example: SGD-A method with different step sizes



Setup

o Synthetic least-squares problem as before

$$\circ \ \alpha_k = \alpha_0 / (k + k_0).$$

Example: SGD-A method with different step sizes



Setup

 \circ Synthetic least-squares problem as before

$$\circ \ \alpha_k = \alpha_0 / (k + k_0).$$

Observations:

 \circ SGD-A is more stable than SGD.

 $\circ \alpha_0 = 2/\mu$ is the best choice.



Slide 18/ 46

Least mean squares algorithm

Least-square regression problem

Solve

$$\mathbf{x}^{\star} \in \operatorname*{arg\,min}_{\mathbf{x} \in \mathbb{R}^p} \left\{ f(\mathbf{x}) := rac{1}{2} \mathbb{E}_{(\mathbf{a},b)} (\langle \mathbf{a}, \mathbf{x} \rangle - b)^2
ight\},$$

given i.i.d. samples $\{(\mathbf{a}_j, b_j)\}_{j=1}^n$ (particularly in a streaming way).

Stochastic gradient method with averaging 1. Choose $\mathbf{x}^0 \in \mathbb{R}^p$ and $\alpha > 0$. 2a. For k = 1, ..., n perform: $\mathbf{x}^k = \mathbf{x}^{k-1} - \alpha \left(\langle \mathbf{a}_k, \mathbf{x}^{k-1} \rangle - b_k \right) \mathbf{a}_k.$ 2b. $\bar{\mathbf{x}}^k = \frac{1}{k+1} \sum_{j=0}^k \mathbf{x}^j.$

O(1/k) convergence rate, without strongly convexity [2]

Let $\|\mathbf{a}_j\|_2 \leq R$ and $|\langle \mathbf{a}_j, \mathbf{x}^* \rangle - b_j| \leq \sigma$ a.s.. Pick $\alpha = 1/(4R^2)$. Then, the average sequence $\bar{\mathbf{x}}^{k-1}$ satisfies the following

$$\mathbb{E}f(\bar{\mathbf{x}}^{k-1}) - f^* \leq \frac{2}{k} \left(\sigma \sqrt{p} + R \| \mathbf{x}^0 - \mathbf{x}^* \|_2 \right)^2.$$

Popular SGD Variants

• Mini-batch SGD: For each iteration,

$$\mathbf{x}^{k+1} = \mathbf{x}^k - \alpha_k \frac{1}{b} \sum_{\theta \in \Gamma} G(\mathbf{x}^k, \theta).$$

- ▶ *b* : mini-batch size
- Γ : a set of random variables θ of size b
- Accelerated SGD (Nesterov accelerated technique)
- \circ SGD with Momentum
- \circ Adaptive stochastic methods: AdaGrad...

SGD - Non-convex stochastic optimization

• SGD and several variants are also well-studied for non-convex problems [21].

Sometimes, there are gaps between SGD's practical performance and theoretical understanding (more later!).
Recall SGD update rule:

$$\mathbf{x}^{k+1} = \mathbf{x}^k - \alpha_k G(\mathbf{x}^k, \theta)$$

Theorem (A well-known result for SGD & Non-convex problems [15]) Let f be a non-convex and L-smooth function. Set $\alpha_k = \min\left\{\frac{1}{L}, \frac{C}{\sigma\sqrt{T}}\right\}$, $\forall k = 1, ..., T$, where σ^2 is the variance of the gradients and C > 0 is constant. Then, it holds that

$$\mathbb{E}[\|\nabla f(\mathbf{x}^R)\|^2] = O\left(\frac{\sigma}{\sqrt{T}}\right),\$$

where
$$\mathbb{P}(R=k) = \frac{2\alpha_k - L\alpha_k^2}{\sum_{k=1}^T (2\alpha_k - L\alpha_k^2)}$$
.

Lower bounds in non-convex optimization

Assumptions on f	Additional assumptions	Sample complexity	
L-smooth	Deterministic Oracle $f(\mathbf{x}^0) - \inf_{\mathbf{x}} f(\mathbf{x}) \leq \Delta$	$\Omega(\Delta L \epsilon^{-2})[6]$	
L_1 -smooth	Deterministic Oracle	$\Omega(\Delta L^{3/7} L^{2/7} e^{-12/7})$ [6]	
L_2 -Lipschitz Hessian	$f(\mathbf{x}^0) - \inf_{\mathbf{x}} f(\mathbf{x}) \le \Delta$	$\mathbb{I}(\Delta L_1 \ L_2 \ \epsilon \)[0]$	
L-smooth	$ \begin{split} \mathbb{E}[G(\mathbf{x}, \theta)] &= \nabla f(x) \\ \mathbb{E}[\ G(\mathbf{x}, \theta) - \nabla f(\mathbf{x})\ ^2] \leq \sigma^2 \\ f(\mathbf{x}^0) &- \inf_{\mathbf{x}} f(\mathbf{x}) \leq \Delta \end{split} $	$\Omega(\Delta L \sigma^2 \epsilon^{-4})[1]$	
$G(\mathbf{x}, \theta)$ has averaged <i>L</i> -Lipschitz gradient \implies <i>L</i> -smooth	$ \begin{split} \mathbb{E}[G(\mathbf{x}, \theta)] &= \nabla f(x) \\ \mathbb{E}[\ G(\mathbf{x}, \theta) - \nabla f(\mathbf{x})\ ^2] \leq \sigma^2 \\ f(\mathbf{x}^0) - \inf_{\mathbf{x}} f(\mathbf{x}) \leq \Delta \end{split} $	$\Omega(\Delta L\sigma\epsilon^{-3} + \sigma^2\epsilon^{-2})[1]$	
$\begin{aligned} f(\mathbf{x}) &:= \frac{1}{n} \sum_{i=1}^{n} f_i(\mathbf{x}) \\ f_i(\mathbf{x}) \text{ has averaged } L\text{-Lipschitz gradient} \\ &\implies L\text{-smooth} \end{aligned}$	$\begin{array}{c} \operatorname{Access to} \nabla f_i(\mathbf{x}) \\ f(\mathbf{x}^0) - \inf_{\mathbf{x}} f(\mathbf{x}) \leq \Delta \\ n \leq O(\epsilon^{-4})^1 \end{array}$	$\Omega(\Delta L \sqrt{n} \epsilon^{-2})[12]$	

 $\circ \text{ Measure of stationarity: } \|\nabla f(\mathbf{x})\| \leq \epsilon \text{ or } \mathbb{E}[\|\nabla f(\mathbf{x})\| \leq \epsilon$

• Sample complexity: # of total oracle calls (deterministic or stochastic gradients)

 $\circ \text{ Averaged } L\text{-Lipschitz gradient: } \mathbb{E}\left[\|\nabla f_i(\mathbf{x}) - \nabla f_i(\mathbf{y})\|^2\right] \leq L^2 \|\mathbf{x} - \mathbf{y}\|^2$

 $\circ G(\mathbf{x}, \theta)$ denotes a stochastic gradient estimate for f at \mathbf{x} with randomness governed by θ .

¹We have $n \leq O(\epsilon^{-4})$ in order to match the respective *upper bound* of $O(n + \sqrt{n}\epsilon^{-2})$ achieved by [12]



Non-smooth minimization: A simple example

What if we simultaneously want $f_1(x), f_2(x), \ldots, f_k(x)$ to be small?

A natural approach in some cases: Minimize $f(x) = \max\{f_1(x), \dots, f_k(x)\}$

- The good news: If each $f_i(x)$ is convex, then f(x) is convex
- The bad (!) news: Even if each $f_i(x)$ is smooth, f(x) may be non-smooth

• e.g., $f(x) = \max\{x, x^2\}$

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Figure: Maximum of two smooth convex functions.

A statistical learning motivation for non-smooth optimization

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 $n \ge p$ (more later).



A statistical learning motivation for non-smooth optimization

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 $n \ge p$ (more later).

- Standard approach: Least squares: $\mathbf{x}_{LS}^{\star} \in \arg \min_{\mathbf{x}} \|\mathbf{b} \mathbf{Ax}\|_2^2$
 - Convex, smooth, and an explicit solution: $\mathbf{x}_{LS}^{\star} = (\mathbf{A}^T \mathbf{A})^{-1} \mathbf{A}^T \mathbf{b} = \mathbf{A}^{\dagger} \mathbf{b}$

 \circ Alternative approach: Least absolute value deviation: $\mathbf{x}^{\star} \in \arg\min_{\mathbf{x}} \|\mathbf{b} - \mathbf{A}\mathbf{x}\|_1$

- The advantage: Improved robustness against outliers (i.e., less sensitive to high noise values)
- ▶ The bad (!) news: A non-differentiable objective function

Our main motivating example this lecture: The case $n \ll p$

Deficiency of smooth models

Recall the practical performance of an estimator \mathbf{x}^{\star} .

Practical performance

Denote the numerical approximation at time t by \mathbf{x}^t . The practical performance is determined by

$$\|\mathbf{x}^{t} - \mathbf{x}^{\natural}\|_{2} \leq \underbrace{\|\mathbf{x}^{t} - \mathbf{x}^{\star}\|_{2}}_{\text{numerical error}} + \underbrace{\|\mathbf{x}^{\star} - \mathbf{x}^{\natural}\|_{2}}_{\text{statistical error}} .$$

Remarks:

- $\,\circ\,$ Non-smooth estimators of \mathbf{x}^{\natural} can help reduce the statistical error.
- This improvement *may* require higher computational costs.

Example: Least-squares estimation in the linear model

 \circ Recall the linear model and the LS estimator.

LS estimation in the linear model

Let $\mathbf{x}^{\natural} \in \mathbb{R}^{p}$ and $\mathbf{A} \in \mathbb{R}^{n \times p}$. The samples are given by $\mathbf{b} = \mathbf{A}\mathbf{x}^{\natural} + \mathbf{w}$, where \mathbf{w} denotes the unknown noise. The LS estimator for \mathbf{x}^{\natural} given \mathbf{A} and \mathbf{b} is defined as

$$\mathbf{x}_{\mathsf{LS}}^{\star} \in rg\min_{\mathbf{x}\in\mathbb{R}^p}\left\{\|\,\mathbf{b}-\mathbf{Ax}\,\|_2^2
ight\}.$$

 $\begin{array}{ll} \textbf{Remarks:} & \circ \mbox{ If } \textbf{A} \mbox{ has full column rank, } \textbf{x}^{\star}_{\text{LS}} = \textbf{A}^{\dagger}\textbf{b} \mbox{ is uniquely defined.} \\ & \circ \mbox{ When } n < p, \mbox{ A cannot have full column rank, and hence } \textbf{x}^{\star}_{\text{LS}} \in \Big\{ \textbf{A}^{\dagger}\textbf{b} + \textbf{h} : \textbf{h} \in \mbox{null} (\textbf{A}) \Big\}. \end{array}$

Observation: • The estimation error $\|\mathbf{x}_{LS}^{\star} - \mathbf{x}^{\natural}\|_{2}$ can be *arbitrarily large*!

A candidate solution

Continuing the LS example:

- There exist infinitely many x's such that $\mathbf{b} = \mathbf{A}\mathbf{x}$
- Suppose that $\mathbf{w} = 0$ (i.e. no noise). Let us just choose the one $\hat{\mathbf{x}}_{candidate}$ with the smallest norm $\|\mathbf{x}\|_2$.



Observation: \circ Unfortunately, *this still fails when* n < p

A candidate solution contd.

Proposition ([17])

Suppose that $\mathbf{A} \in \mathbb{R}^{n \times p}$ is a matrix of i.i.d. standard Gaussian random variables, and $\mathbf{w} = \mathbf{0}$. We have

$$(1-\epsilon)\left(1-\frac{n}{p}\right) \|\mathbf{x}^{\natural}\|_{2}^{2} \leq \|\hat{\mathbf{x}}_{\text{candidate}} - \mathbf{x}^{\natural}\|_{2}^{2} \leq (1-\epsilon)^{-1}\left(1-\frac{n}{p}\right) \|\mathbf{x}^{\natural}\|_{2}^{2}$$

with probability at least $1 - 2 \exp\left[-(1/4)(p-n)\epsilon^2\right] - 2 \exp\left[-(1/4)p\epsilon^2\right]$, for all $\epsilon > 0$ and $\mathbf{x}^{\natural} \in \mathbb{R}^p$.

Summarizing the findings so far

The message so far:

- Even in the absence of noise, we cannot recover x^{\natural} from the observations $b = Ax^{\natural}$ unless $n \ge p$
- But in applications, p might be thousands, millions, billions...
- Can we get away with $n \ll p$ under some further assumptions on x?

A natural signal model

Definition (s-sparse vector)

A vector $\mathbf{x} \in \mathbb{R}^p$ is *s*-sparse if it has at most *s* non-zero entries.



Sparse representations

 \mathbf{x}^{\natural} : *sparse* transform coefficients

- Basis representations $\Psi \in \mathbb{R}^{p \times p}$
 - Wavelets, DCT, ...
- Frame representations $\Psi \in \mathbb{R}^{m \times p}$, m > p
 - Gabor, curvelets, shearlets, …
- Other *dictionary* representations...










 $\blacktriangleright \ \mathbf{b} \in \mathbb{R}^n \text{, } \tilde{\mathbf{A}} \in \mathbb{R}^{n \times p} \text{, and } n < p$



- $\blacktriangleright \ \mathbf{b} \in \mathbb{R}^n \text{, } \tilde{\mathbf{A}} \in \mathbb{R}^{n \times p} \text{, and } n < p$
- $\blacktriangleright \ \Psi \in \mathbb{R}^{p \times p} \text{, } \mathbf{x}^{\natural} \in \mathbb{R}^{p} \text{, and } \|\mathbf{x}^{\natural}\|_{0} \leq s < n$



 $\blacktriangleright \ \mathbf{b} \in \mathbb{R}^n, \ \mathbf{A} \in \mathbb{R}^{n \times p}, \ \text{and} \ \mathbf{x}^{\natural} \in \mathbb{R}^p, \ \text{and} \ \|\mathbf{x}^{\natural}\|_0 \le s < n < p$





Observations: The matrix A effectively becomes overcomplete. We could solve for x^β if we knew the location of the non-zero entries of x^β.



Compressible signals

• Real signals may not be exactly sparse, but approximately sparse, or *compressible*.

Definition (Compressible signals [7])

Roughly speaking, a vector $\mathbf{x} := (x_1, \ldots, x_p)^T \in \mathbb{R}^p$ is compressible if the number of its significant components (i.e., entries larger than some $\epsilon > 0$: $|\{k : |x_k| \ge \epsilon, 1 \le k \le p\}|$) is small.



Cameraman@MIT.



- **Solid curve**: Sorted wavelet coefficients of the cameraman image.
- Dashed curve: Expected order statistics of generalized Pareto distribution with shape parameter 1.67.



A different tale of the linear model $\mathbf{b} = \mathbf{A}\mathbf{x} + \mathbf{w}$

A *realistic* linear model

Let $\mathbf{b} := \tilde{\mathbf{A}} \mathbf{y}^{\natural} + \tilde{\mathbf{w}} \in \mathbb{R}^n$.

- Let $\mathbf{y}^{\natural} := \Psi \mathbf{x}_{\mathsf{real}} \in \mathbb{R}^m$ that admits a *compressible* representation $\mathbf{x}_{\mathsf{real}}$.
- Let $\mathbf{x}_{real} \in \mathbb{R}^p$ that is *compressible* and let \mathbf{x}^{\natural} be its *best s-term approximation*.
- Let $\tilde{\mathbf{w}} \in \mathbb{R}^n$ denote the possibly nonzero *noise* term.
- Assume that $\Psi \in \mathbb{R}^{m \times p}$ and $\tilde{\mathbf{A}} \in \mathbb{R}^{n \times m}$ are known.

Then we have

$$\begin{split} \mathbf{b} &= \tilde{\mathbf{A}} \Psi \left(\mathbf{x}^{\natural} + \mathbf{x}_{\mathsf{real}} - \mathbf{x}^{\natural} \right) + \tilde{\mathbf{w}}. \\ &:= \underbrace{\left(\tilde{\mathbf{A}} \Psi \right)}_{\mathbf{A}} \mathbf{x}^{\natural} + \underbrace{\left[\underbrace{\tilde{\mathbf{w}} + \tilde{\mathbf{A}} \Psi \left(\mathbf{x}_{\mathsf{real}} - \mathbf{x}^{\natural} \right) \right]}_{\mathbf{w}}, \end{split}$$

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

Peeling the onion

• The *realistic* linear model uncovers yet another level of difficulty

Practical performance

The practical performance at time t is determined by

$$\|\mathbf{x}^{t} - \mathbf{x}_{\mathsf{real}}\|_{2} \leq \underbrace{\|\mathbf{x}^{t} - \mathbf{x}^{\star}\|_{2}}_{\mathsf{numerical error}} + \underbrace{\|\mathbf{x}^{\star} - \mathbf{x}^{\flat}\|_{2}}_{\mathsf{statistical error}} + \underbrace{\|\mathbf{x}_{\mathsf{real}} - \mathbf{x}^{\flat}\|_{2}}_{\mathsf{model error}}.$$

numerical error statistical error

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Approach 1: Sparse recovery via exhaustive search

Approach 1 for estimating \mathbf{x}^{\natural} from $\mathbf{b}=\mathbf{A}\mathbf{x}^{\natural}+\mathbf{w}$

We may search over all $\binom{p}{s}$ subsets $S \subset \{1, \ldots, p\}$ of cardinality s, solve the restricted least-squares problem $\min_{\mathbf{x}S} \|\mathbf{b} - \mathbf{A}_S \mathbf{x}_S\|_2^2$, and return the resulting \mathbf{x} corresponding to the smallest error, putting zeros in the entries of \mathbf{x} outside S.

 \circ Stable and robust recovery of any s-sparse signal is possible using just n = 2s measurements.



Approach 1: Sparse recovery via exhaustive search

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 \circ Stable and robust recovery of any s-sparse signal is possible using just n=2s measurements.

Issues

- (p) is a huge number too many to search!
- s is not known in practice

The ℓ_1 -norm heuristic

Heuristic: The ℓ_1 -ball with radius c_{∞} is an "approximation" of the set of sparse vectors $\hat{\mathbf{x}} \in {\mathbf{x} : \|\mathbf{x}\|_0 \le s, \|\mathbf{x}\|_{\infty} \le c_{\infty}}$ parameterized by their sparsity s and maximum amplitude c_{∞} .

 $\hat{\mathbf{x}} \in {\{\mathbf{x} : \| \mathbf{x} \|_1 \le c_\infty\}}$ with some $c_\infty > 0$.



Remark: • This heuristic leads to the so-called *Lasso* optimization problem.



Sparse recovery via the Lasso

Definition (Least absolute shrinkage and selection operator (Lasso))

$$\mathbf{x}_{Lasso}^{\star} := \arg\min_{\mathbf{x}\in\mathbb{R}^{p}} \|\mathbf{b} - \mathbf{A}\mathbf{x}\|_{2}^{2} + \rho \|\mathbf{x}\|_{1}$$

with some $\rho \geq 0$.

• The second term in the objective function is called the *regularizer*.

• The parameter ρ is called the *regularization parameter*. It is used to trade off the objectives:

- Minimize $\|\mathbf{b} \mathbf{A}\mathbf{x}\|_2^2$, so that the solution is consistent with the observations
- Minimize $\|\mathbf{x}\|_1$, so that the solution has the desired sparsity structure

Remark: • The Lasso has a *convex* but *non-smooth* objective function

Performance of the Lasso

Theorem (Existence of a stable solution in polynomial time [23])

This Lasso convex formulation is a second order cone program, which can be solved in polynomial time in terms of the inputs n and p. Surprisingly, if the signal \mathbf{x}^{\natural} is s-sparse and the noise \mathbf{w} is sub-Gaussian (e.g., Gaussian

or bounded) with parameter σ , then choosing $ho = \sqrt{rac{16\sigma^2\log p}{n}}$ yields an error of

$$\|\mathbf{x}_{Lasso}^{\star} - \mathbf{x}^{\natural}\|_{2} \leq \frac{8\sigma}{\kappa(\mathbf{A})} \sqrt{\frac{s\ln p}{n}},$$

with probability at least $1 - c_1 \exp(-c_2 n \rho^2)$, where c_1 and c_2 are absolute constants, and $\kappa(\mathbf{A}) > 0$ encodes the difficulty of the problem.

Remark: • The number of measurements is $O(s \ln p)$ – this may be *much* smaller than p!

Non-smooth unconstrained convex minimization

Problem (Mathematical formulation)

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

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

where f is proper, closed, convex, but not everywhere differentiable.



(1)

Subdifferentials: A generalization of the gradient

Definition

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

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

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

Lemma

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Let $f : \mathcal{Q} \to \mathbb{R} \cup \{+\infty\}$ 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

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



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

Subdifferentials: Two basic results

Lemma (Necessary and sufficient condition)

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

Sketch of the proof.

• \Leftarrow : For any $\mathbf{x} \in \mathbb{R}^p$, by definition of $\partial F(\mathbf{x}^{\star})$:

$$F(\mathbf{x}) - F(\mathbf{x}^{\star}) \ge 0^T (\mathbf{x} - \mathbf{x}^{\star}) = 0,$$

that is, \mathbf{x}^* is a global solution to (1).

• \Rightarrow : If \mathbf{x}^* is a global of (1) then for every $\mathbf{x} \in \text{dom}(F)$, $F(\mathbf{x}) \ge F(\mathbf{x}^*)$ and hence

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

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

Theorem (Moreau-Rockafellar's theorem [26])

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

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

Slide 42/46

Non-smooth unconstrained convex minimization

Problem (Non-smooth convex minimization)

$$\mathcal{T}^{\star} := \min_{\mathbf{x} \in \mathbb{R}^p} f(\mathbf{x})$$
 (2)

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:	
$\left\{ \begin{array}{c} \mathbf{x}^{k+1} & = \mathbf{x}^k - \mathbf{c} \end{array} \right.$	$\alpha_k \mathbf{d}^k,$ (3)
where $\mathbf{d}^k \in \partial f(\mathbf{x}^k)$ 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.
$$\|\mathbf{x}^0 - \mathbf{x}^{\star}\|_2 \le R$$

Let the stepsize be chosen as

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

then the iterates generated by the subgradient method satisfy

$$\min_{0 \le i \le k} f(\mathbf{x}^i) - f^* \le \frac{RG}{\sqrt{k}}$$

Remarks

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

Stochastic subgradient methods

• An unbiased stochastic subgradient

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

o Stochastic gradient methods using unbiased subgradients instead of unbiased gradients work

The classic stochastic subgradient methods (SG) 1. Choose $\mathbf{x}_1 \in \mathbb{R}^p$ and $(\gamma_k)_{k \in \mathbb{N}} \in (0, +\infty)^{\mathbb{N}}$. 2. For k = 1, ... perform: $\mathbf{x}_{k+1} = \mathbf{x}_k - \gamma_k G(\mathbf{x}_k)$.

Theorem (Convergence in expectation [28])

Suppose that:

1.
$$\mathbb{E}[\|G(\mathbf{x}^k)\|^2] \le M^2$$
,

2.
$$\gamma_k = \gamma_0 / \sqrt{k}$$
.

Then,

$$\mathbb{E}[f(\mathbf{x}^k) - f(\mathbf{x}^\star)] \le \left(\frac{D^2}{\gamma_0} + \gamma_0 M^2\right) \frac{2 + \log k}{\sqrt{k}}.$$

Remark: • The rate is $O(\log k/\sqrt{k})$ instead of $O(1/\sqrt{k})$ for the deterministic algorithm.

Wrap up!

- \circ Three supplementary lectures to take a look once the course is over!
 - One on compressive sensing (Math of Data Lecture 4 from 2014): https://archive-wp.epfl.ch/lions/wp-content/uploads/2019/01/lecture-4-2014.pdf
 - One on source separation (Math of Data Lecture 6 from 2014) https://archive-wp.epfl.ch/lions/wp-content/uploads/2019/01/lecture-6-2014.pdf
 - One on convexification of structured sparsity models (research presentation) https://www.epfl.ch/labs/lions/wp-content/uploads/2019/01/volkan-TU-view-web.pdf

*Adaptive methods for stochastic optimization

Remark

- Adaptive methods have extensive applications in stochastic optimization.
- We will see another nature of adaptive methods in this lecture.
- Mild additional assumption: bounded variance of gradient estimates.

*AdaGrad for stochastic optimization

• Only modification: $\nabla f(\mathbf{x}) \Rightarrow G(\mathbf{x}, \theta)$

AdaGrad with $\mathbf{H}_{k} = \lambda_{k} \mathbf{I}$ [18] 1. Set $Q^{0} = 0$. 2. For $k = 0, 1, \dots$, iterate $\begin{cases} Q^{k} = Q^{k-1} + \|G(\mathbf{x}^{k}, \theta)\|^{2} \\ \mathbf{H}_{k} = \sqrt{Q^{k}} \mathbf{I} \\ \mathbf{x}^{k+1} = \mathbf{x}_{t} - \alpha_{k} \mathbf{H}_{k}^{-1} G(\mathbf{x}^{k}, \theta) \end{cases}$

Theorem (Convergence rate: stochastic, convex optimization [18])

Assume f is convex and L-smooth, such that minimizer of f lies in a convex, compact set \mathcal{K} with diameter D. Also consider bounded variance for unbiased gradient estimates, i.e., $\mathbb{E}\left[\|G(\mathbf{x}, \theta) - \nabla f(\mathbf{x})\|^2 |\mathbf{x}|\right] \leq \sigma^2$. Then,

$$\mathbb{E}[f(\mathbf{x}^k)] - \min_{\mathbf{x} \in \mathbb{R}^d} f(\mathbf{x}) = O\left(\frac{\sigma D}{\sqrt{k}}\right)$$

o AdaGrad is adaptive also in the sense that it adapts to nature of the oracle.



*AcceleGrad for stochastic optimization

 \circ Similar to AdaGrad, replace $\nabla f(\mathbf{x}) \Rightarrow G(\mathbf{x}, \theta)$

 $\label{eq:constraint} \begin{array}{|c|c|c|} \hline \textbf{AcceleGrad (Accelerated Adaptive Gradient Method)} \\ \hline \textbf{Input: } \mathbf{x}^0 \in \mathcal{K}, \text{ diameter } D, \text{ weights } \{\alpha_k\}_{k \in \mathbb{N}}, \text{ learning} \\ \hline \textbf{rate } \{\eta_k\}_{k \in \mathbb{N}} \\ \hline \textbf{1. Set } \mathbf{y}^0 = \mathbf{z}^0 = \mathbf{x}^0 \\ \hline \textbf{2. For } k = 0, 1, \dots, \text{ iterate} \\ \hline & \mathbf{x}^{k+1} = \tau_t \mathbf{z}^k + (1 - \tau_k) \mathbf{y}^k, \text{ define } \mathbf{g}_k := \nabla f(\mathbf{x}^{k+1}) \\ & \mathbf{z}^{k+1} = \Pi_{\mathcal{K}}(\mathbf{z}^k - \alpha_k \eta_k \mathbf{g}_k) \\ & \mathbf{y}^{k+1} = \mathbf{x}^{k+1} - \eta_k \mathbf{g}_k \\ \hline \\ \hline \textbf{Output : } \overline{\mathbf{y}}^k \propto \sum_{i=0}^{k-1} \alpha_i \mathbf{y}^{i+1} \end{array}$

Theorem (Convergence rate [19])

Assume f is convex and G-Lipschitz and that minimizer of f lies in a convex, compact set \mathcal{K} with diameter D. Also consider bounded variance for unbiased gradient estimates, i.e., $\mathbb{E}\left[\|G(\mathbf{x}, \theta) - \nabla f(\mathbf{x})\|^2 |\mathbf{x}|\right] \leq \sigma^2$. Then,

$$\mathbb{E}[f(\overline{\mathbf{y}}^k)] - \min_{\mathbf{x}} f(\mathbf{x}) = O\left(\frac{GD\sqrt{\log k}}{\sqrt{k}}\right)$$

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Slide 3/ 24

*Example: Synthetic least squares

 $\circ \mathbf{A} \in \mathbb{R}^{n \times d}$, where n = 200 and d = 50.

 \circ Number of epochs: 20.

• Algorithms: SGD, AdaGrad & AcceleGrad.



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***UniXGrad** for stochastic optimization



Theorem (Convergence rate of UniXGrad)

Let the sequence $\{\mathbf{x}^{k+1/2}\}$ be generated by UniXGrad. Under the assumptions

- ▶ f is convex and L-smooth,
- Constraint set \mathcal{X} has bounded diameter, i.e., $D = \max_{\mathbf{x}, \mathbf{y} \in \mathcal{X}} \|\mathbf{x} \mathbf{y}\|$,

$$\blacktriangleright \mathbb{E}[\tilde{\nabla}f(\mathbf{x})|\mathbf{x}] = \nabla f(\mathbf{x}) \text{ and } \mathbb{E}[\|\tilde{\nabla}f(\mathbf{x}) - \nabla f(\mathbf{x})\|^2|\mathbf{x}] \le \sigma^2$$

UniXGrad guarantees the following:

$$f(\bar{\mathbf{x}}^{k+1/2}) - \min_{\mathbf{x}\in\mathcal{X}} f(\mathbf{x}) \le O\left(\frac{LD^2}{k^2} + \frac{\sigma D}{\sqrt{k}}\right).$$

*Randomized Kaczmarz algorithm

Problem

Given a full-column-rank matrix $\mathbf{A} \in \mathbb{R}^{n \times p}$ and $b \in \mathbb{R}^n$, solve the linear system

Ax = b.

Notations: $\mathbf{b} := (b_1, \dots, b_n)^T$ and \mathbf{a}_j^T is the *j*-th row of \mathbf{A} .

Randomized Kaczmarz algorithm (RKA)	
1. Choose $\mathbf{x}^0 \in \mathbb{R}^p$. 2. For $k = 0, 1,$ perform: 2a. Pick $j_k \in \{1, \dots, n\}$ randomly with $\Pr(j_k = i) = \ \mathbf{a}_i\ _2^2 / \ \mathbf{A}\ _F^2$ 2b. $\mathbf{x}^{k+1} = \mathbf{x}^k - (\langle \mathbf{a}_i, \mathbf{x}^k \rangle - b_i, \rangle \mathbf{a}_i, /\ \mathbf{a}_i, \ _2^2$.	

Linear convergence [29]

Let \mathbf{x}^{\star} be the solution of $\mathbf{A}\mathbf{x} = \mathbf{b}$ and $\kappa = \|\mathbf{A}\|_F \|\mathbf{A}^{-1}\|$. Then

$$\mathbb{E} \| \mathbf{x}^k - \mathbf{x}^\star \|_2^2 \leq (1 - \kappa^{-2})^k \| \mathbf{x}^0 - \mathbf{x}^\star \|_2^2$$

 \circ RKA can be seen as a particular case of SGD [22].



*Other models with simplicity



There are many models extending far beyond sparsity, coming with other non-smooth regularizers.



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*Generalization via simple representations

Definition (Atomic sets & atoms [9])

An *atomic set* A is a set of vectors in \mathbb{R}^p . An *atom* is an element in an atomic set.

Terminology (Simple representation [9])

A parameter $\mathbf{x}^{\natural} \in \mathbb{R}^{p}$ admits a simple representation with respect to an atomic set $\mathcal{A} \subseteq \mathbb{R}^{p}$, if it can be represented as a non-negative combination of few atoms, i.e., $\mathbf{x}^{\natural} = \sum_{i=1}^{k} c_{i} \mathbf{a}_{i}$, $\mathbf{a}_{i} \in \mathcal{A}$, $c_{i} \ge 0$.

Example (Sparse parameter)

Let \mathbf{x}^{\natural} be *s*-sparse. Then \mathbf{x}^{\natural} can be represented as the non-negative combination of *s* elements in \mathcal{A} , with $\mathcal{A} := \{\pm \mathbf{e}_1, \dots, \pm \mathbf{e}_p\}$, where $\mathbf{e}_i := (\delta_{1,i}, \delta_{2,i}, \dots, \delta_{p,i})$ for all *i*.

Example (Sparse parameter with a dictionary)

Let $\Psi \in \mathbb{R}^{m \times p}$, and let $\mathbf{y}^{\natural} := \Psi \mathbf{x}^{\natural}$ for some *s*-sparse \mathbf{x}^{\natural} . Then \mathbf{y}^{\natural} can be represented as the non-negative combination of *s* elements in \mathcal{A} , with $\mathcal{A} := \{\pm \psi_1, \ldots, \pm \psi_p\}$, where ψ_k denotes the *k*th column of Ψ .

*Atomic norms

• Recall the Lasso problem

$$\mathbf{x}_{\mathsf{Lasso}}^{\star} := \arg\min_{\mathbf{x} \in \mathbb{R}^{p}} \|\mathbf{b} - \mathbf{A}\mathbf{x}\|_{2}^{2} + \rho \|\mathbf{x}\|_{1}$$

Observations: $\circ \ell_1$ -norm is the *atomic norm* associated with the atomic set $\mathcal{A} := \{\pm \mathbf{e}_1, \dots, \pm \mathbf{e}_p\}$.

 \circ The norm is closely tied with the convex hull of the set.

 \circ We can extend the same principle for a wide range of regularizers

$$\mathcal{A} := \left\{ \begin{bmatrix} 1\\0 \end{bmatrix}, \begin{bmatrix} 0\\1 \end{bmatrix}, \begin{bmatrix} -1\\0 \end{bmatrix}, \begin{bmatrix} 0\\-1 \end{bmatrix} \right\}.$$
$$\mathcal{C} := \operatorname{conv}\left(\mathcal{A}\right).$$



*Gauge functions and atomic norms

Definition (Gauge function)

Let \mathcal{C} be a convex set in \mathbb{R}^p , the gauge function associated with \mathcal{C} is given by

$$g_{\mathcal{C}}(\mathbf{x}) := \inf \left\{ t > 0 : \mathbf{x} = t\mathbf{c} \text{ for some } \mathbf{c} \in \mathcal{C} \right\}.$$

Definition (Atomic norm)

Let \mathcal{A} be a symmetric *atomic set* in \mathbb{R}^p such that if $\mathbf{a} \in \mathcal{A}$ then $-\mathbf{a} \in \mathcal{A}$ for all $\mathbf{a} \in \mathcal{A}$. Then, the **atomic norm** associated with a symmetric atomic set \mathcal{A} is given by

$$\|\mathbf{x}\|_{\mathcal{A}} := g_{\operatorname{conv}(\mathcal{A})}(\mathbf{x}), \quad \forall \mathbf{x} \in \mathbb{R}^p,$$

where $\operatorname{conv}(\mathcal{A})$ denotes the *convex hull* of \mathcal{A} .

A generalization of the Lasso

Given an atomic set \mathcal{A} , solve the following regularized least-squares problem:

$$\mathbf{x}^{\star} = \arg\min_{\mathbf{x}\in\mathbb{R}^{p}} \|\mathbf{b} - \mathbf{A}\mathbf{x}\|_{2}^{2} + \rho \|\mathbf{x}\|_{\mathcal{A}}$$
(4)



Let
$$\mathcal{A} := \left\{ (1,0)^T, (0,1)^T, (-1,0)^T, (0,-1)^T \right\}$$
, and let $\mathbf{x} := (-\frac{1}{5}, 1)^T$. What is $\|\mathbf{x}\|_{\mathcal{A}}$?





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Let
$$\mathcal{A} := \left\{ (1,0)^T, (0,1)^T, (-1,0)^T, (0,-1)^T \right\}$$
, and let $\mathbf{x} := (-\frac{1}{5}, 1)^T$. What is $\|\mathbf{x}\|_{\mathcal{A}}$?
ANS: $\|\mathbf{x}\|_{\mathcal{A}} = \frac{6}{5}$.





What is the expression of $\|\mathbf{x}\|_{\mathcal{A}}$ for any $\mathbf{x} := (x_1, x_2, x_3)^T \in \mathbb{R}^3$?



What is the expression of $\| \mathbf{x} \|_{\mathcal{A}}$ for any $\mathbf{x} := (x_1, x_2, x_3)^T \in \mathbb{R}^3$? **ANS:** $\| \mathbf{x} \|_{\mathcal{A}} = |x_1| + \| (x_2, x_3)^T \|_2$.



*Application: Multi-knapsack feasibility problem

Problem formulation [20]

Let $\mathbf{x}^{\natural} \in \mathbb{R}^p$ which is a convex combination of k vectors in $\mathcal{A} := \{-1, +1\}^p$, and let $\mathbf{A} \in \mathbb{R}^{n \times p}$. How can we recover \mathbf{x}^{\natural} given \mathbf{A} and $\mathbf{b} = \mathbf{A}\mathbf{x}^{\natural}$?

The answer: • We can use the ℓ_{∞} -norm, $\|\cdot\|_{\mathcal{A}}$ as $\|\cdot\|_{\mathcal{A}}$. The regularized estimator is given by

 $\mathbf{x}^{\star} \in \arg\min_{\mathbf{x} \in \mathbb{R}^{\rho}} \| \mathbf{b} - \mathbf{A}\mathbf{x} \|_{2}^{2} + \rho \| \mathbf{x} \|_{\infty}, \rho > 0.$

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Let $\mathbf{x}^{\natural} \in \mathbb{R}^p$ which is a convex combination of k vectors in $\mathcal{A} := \{-1, +1\}^p$, and let $\mathbf{A} \in \mathbb{R}^{n \times p}$. How can we recover \mathbf{x}^{\natural} given \mathbf{A} and $\mathbf{b} = \mathbf{A}\mathbf{x}^{\natural}$?

The answer: \circ We can use the ℓ_{∞} -norm, $\|\cdot\|_{\infty}$ as $\|\cdot\|_{\mathcal{A}}$. The regularized estimator is given by $\mathbf{x}^{\star} \in \arg\min_{\mathbf{x}\in\mathbb{R}^p} \|\mathbf{b} - \mathbf{A}\mathbf{x}\|_2^2 + \rho \|\mathbf{x}\|_{\infty}, \rho > 0.$

The derivation: \circ In this case, we have $\mathsf{conv}(\mathcal{A}) = [-1,1]^p$ and

 $g_{\operatorname{conv}(\mathcal{A})}(\mathbf{x}) = \inf \left\{ t > 0 : \mathbf{x} = t\mathbf{c} \text{ for some } \mathbf{c} \text{ such that } |c_i| \le 1 \ \forall i \right\}.$

 \circ We also have, $\forall \mathbf{x} \in \mathbb{R}^p, \mathbf{c} \in \mathsf{conv}(\mathcal{A}), t > 0$,

$$\begin{split} \mathbf{x} &= t\mathbf{C} \Rightarrow \forall i, |x_i| = |tc_i| \leq t \\ &\Rightarrow g_{\mathsf{conv}(\mathcal{A})}(\mathbf{x}) \geq \max_i |x_i| \end{split}$$

◦ Let $\mathbf{x} \neq 0$, let $j \in \arg \max_i |x_i|$ and choose $t = \max_i |x_i|$, $c_i = x_i/t \in [-1, 1]^p$. ◦ Then, $\mathbf{x} = t\mathbf{c}$, and so $g_{\mathsf{conv}(\mathcal{A})}(\mathbf{x}) \leq \max_i |x_i|$.


*Application: Matrix completion

Problem formulation [5, 13]

Let $\mathbf{X}^{\natural} \in \mathbb{R}^{p \times p}$ with $\operatorname{rank}(\mathbf{X}^{\natural}) = r$, and let $\mathbf{A}_1, \dots, \mathbf{A}_n$ be matrices in $\mathbb{R}^{p \times p}$. How do we estimate \mathbf{X}^{\natural} given $\mathbf{A}_1, \dots, \mathbf{A}_n$ and $b_i = \operatorname{Tr} \left(\mathbf{A}_i \mathbf{X}^{\natural} \right) + w_i$, $i = 1, \dots, n$, where $\mathbf{w} := (w_1, \dots, w_n)^T$ denotes unknown noise?

The answer: • We can use the *nuclear norm*, $\|\cdot\|_*$ as $\|\cdot\|_{\mathcal{A}}$. The regularized estimator is given by

$$\mathbf{x}^{\star} \in \arg\min_{\mathbf{X} \in \mathbb{R}^{p \times p}} \sum_{i=1}^{n} (b_i - \operatorname{Tr}(\mathbf{A}_i \mathbf{X}))^2 + \rho \| \mathbf{X} \|_*, \rho > 0.$$



*Application: Matrix completion

Problem formulation [5, 13]

Let $\mathbf{X}^{\natural} \in \mathbb{R}^{p \times p}$ with $\operatorname{rank}(\mathbf{X}^{\natural}) = r$, and let $\mathbf{A}_1, \dots, \mathbf{A}_n$ be matrices in $\mathbb{R}^{p \times p}$. How do we estimate \mathbf{X}^{\natural} given $\mathbf{A}_1, \dots, \mathbf{A}_n$ and $b_i = \operatorname{Tr} \left(\mathbf{A}_i \mathbf{X}^{\natural} \right) + w_i$, $i = 1, \dots, n$, where $\mathbf{w} := (w_1, \dots, w_n)^T$ denotes unknown noise?

The answer: • We can use the *nuclear norm*, $\|\cdot\|_*$ as $\|\cdot\|_{\mathcal{A}}$. The regularized estimator is given by

$$\mathbf{x}^{\star} \in \arg\min_{\mathbf{X}\in\mathbb{R}^{p\times p}} \sum_{i=1}^{n} (b_{i} - \operatorname{Tr}(\mathbf{A}_{i}\mathbf{X}))^{2} + \rho \|\mathbf{X}\|_{*}, \rho > 0.$$

The derivation: \circ Let us use the following atomic set $\mathcal{A} = \left\{ \mathbf{X} : \operatorname{rank} (\mathbf{X}) = 1, \|\mathbf{X}\|_F = 1, \mathbf{X} \in \mathbb{R}^{p \times p} \right\}.$

$$\circ \text{ Let } \forall \mathbf{X} \in \mathbb{R}^{p \times p}, \mathbf{C} = \sum_{i} \lambda_i \mathbf{C}_i \in \text{conv}(\mathcal{A}), \\ \sum_{i} \lambda_i = 1, \mathbf{C}_i \in \mathcal{A}, t > 0. \text{ Then, we have} \\ \mathbf{X} = t \sum_{i} \lambda_i \mathbf{C}_i \Rightarrow \left\| \mathbf{X} \right\|_* = t \left\| \sum_{i} \lambda_i \mathbf{C}_i \right\|_* \le t \sum_{i} \lambda_i \left\| \mathbf{C}_i \right\|_* \le t \Rightarrow g_{\text{conv}(\mathcal{A})}(\mathbf{X}) \ge \left\| \mathbf{X} \right\|_*.$$

• Let $\mathbf{X} \neq 0$, let $\mathbf{X} = \sum_{i} \sigma_{i} \mathbf{u}_{i} \mathbf{v}_{i}^{t}$ be its SVD decomposition, where σ_{i} 's are its singular values. • Let $t = \|\mathbf{X}\|_{*} = \sum_{i} |\sigma_{i}|$, $\mathbf{C}_{i} = \mathbf{u}_{i} \mathbf{v}_{i}^{T} \in \mathcal{A}$, $\forall i$. Then, $\mathbf{X} = t \sum_{i} \lambda_{i} \mathbf{C}_{i}$, $\lambda_{i} = \frac{|\sigma_{i}|}{t}$. • Since t is feasible and $\sum_{i} \lambda_{i} = 1$, it follows that $g_{\text{conv}(\mathcal{A})}(\mathbf{X}) \leq \|\mathbf{X}\|_{*}$.

*Structured Sparsity

There exist many more structures that we have not covered here, each of which is handled using different non-smooth regularizers. Some examples [3, 11]:

- Group Sparsity: Many signals are not only sparse, but the non-zero entries tend to cluster according to known patterns.
- Tree Sparsity: When natural images are transformed to the Wavelet domain, their significant entries form a rooted connected tree.





Figure: (Left panel) Natural image in the Wavelet domain. (Right panel) Rooted connected tree containing the significant coefficients.



*Selection of the Parameters

In all of these problems, there remain the issues of how to design A and how to choose ρ .

Design of A:

- Sometimes A is given "by nature", whereas sometimes it can be designed
- ▶ For the latter case, i.i.d. Gaussian designs provide good theoretical guarantees, whereas in practice we must resort to structured matrices permitting more efficient storage and computation
- See [14] for an extensive study in the context of compressive sensing

Selection of ρ :

- ▶ Theoretical bounds provide some insight, but usually the direct use of the theoretical choice does not suffice
- In practice, a common approach is cross-validation [10], which involves searching for a parameter that performs well on a set of known training signals
- ▶ Other approaches include *covariance penalty* [10] and *upper bound heuristic* [30]

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