

Mathematics of Data: From Theory to Computation

Prof. Volkan Cevher
volkan.cevher@epfl.ch

Lecture 6: Time-data tradeoffs and variance reduction

Laboratory for Information and Inference Systems (LIONS)
École Polytechnique Fédérale de Lausanne (EPFL)

EE-556 (Fall 2020)



License Information for Mathematics of Data Slides

- ▶ This work is released under a [Creative Commons License](#) with the following terms:
- ▶ **Attribution**
 - ▶ The licensor permits others to copy, distribute, display, and perform the work. In return, licensees must give the original authors credit.
- ▶ **Non-Commercial**
 - ▶ The licensor permits others to copy, distribute, display, and perform the work. In return, licensees may not use the work for commercial purposes – unless they get the licensor's permission.
- ▶ **Share Alike**
 - ▶ The licensor permits others to distribute derivative works only under a license identical to the one that governs the licensor's work.
- ▶ [Full Text of the License](#)

Outline

- ▶ This class
 1. Time-data trade-offs
 2. Rate iteration-cost trade-offs
 3. Variance reduction
- ▶ Next class
 1. Deep learning introduction

A simple *regression* model

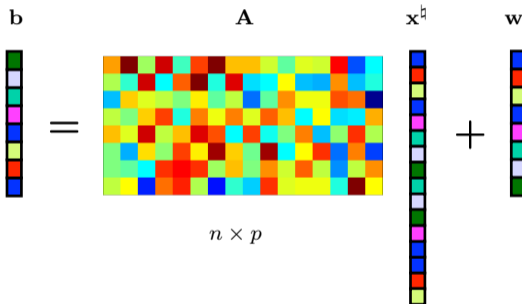
$$b_i = h_{\mathbf{x}^{\natural}}(\mathbf{a}_i)$$

\mathbf{x}^{\natural} : unknown function parameters

\mathbf{a}_i : input

b_i : response / output

Linear model:



$$\mathbf{b}_i = \langle \mathbf{a}_i, \mathbf{x}^{\natural} \rangle + \mathbf{w}_i$$

Applications: **Compressive sensing, machine learning, theoretical computer science...**

A simple *regression* model and many *practical* questions

$$\mathbf{b}_i = \langle \mathbf{a}_i, \mathbf{x}^{\natural} \rangle + \mathbf{w}_i$$

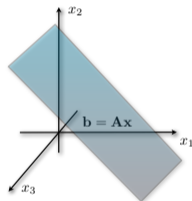
\mathbf{x}^{\natural} : unknown function parameters

\mathbf{a}_i : input

\mathbf{b}_i : response / output

\mathbf{w}_i : perturbations / noise

- Estimation: find \mathbf{x}^* to minimize $\|\mathbf{x}^* - \mathbf{x}^{\natural}\|$
- Prediction: find \mathbf{x}^* to minimize $L(\langle \mathbf{a}_i, \mathbf{x}^* \rangle, \langle \mathbf{a}_i, \mathbf{x}^{\natural} \rangle)$
- Decision: choose \mathbf{a}_i for estimation or prediction



A difficult estimation challenge when $n < p$:

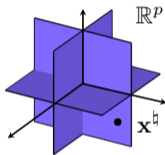
Nullspace (null) of \mathbf{A} : $\mathbf{x}^{\natural} + \mathbf{v} \rightarrow \mathbf{b}, \quad \forall \mathbf{v} \in \text{null}(\mathbf{A})$

- Needle in a haystack: **We need additional information on \mathbf{x}^{\natural} !**

A natural signal model

Definition (s -sparse vector)

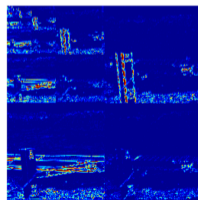
A vector $\mathbf{x} \in \mathbb{R}^p$ is s -sparse if it has at most s non-zero entries.



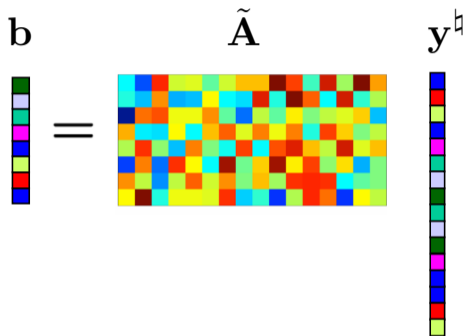
Sparse representations

- \mathbf{x}^h : *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...

$$\mathbf{y}^h = \Psi \mathbf{x}^h$$

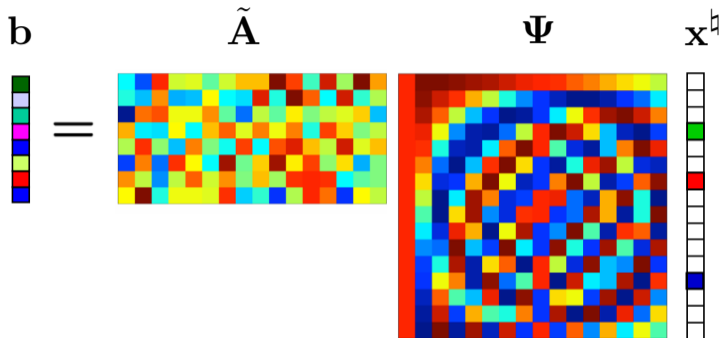


Sparse representations strike back!

$$\mathbf{b} = \tilde{\mathbf{A}} \mathbf{y}^{\natural}$$


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

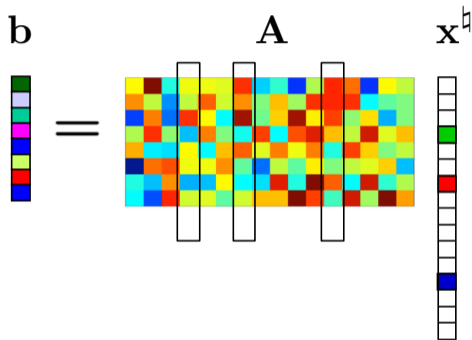
Sparse representations strike back!



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

◦ $\Psi \in \mathbb{R}^{p \times p}$, $\mathbf{x}^\natural \in \mathbb{R}^p$, and $\|\mathbf{x}^\natural\|_0 \leq s < n$

Sparse representations strike back!



◦ $\mathbf{b} \in \mathbb{R}^n$, $\mathbf{A} \in \mathbb{R}^{n \times p}$, and $\mathbf{x}^h \in \mathbb{R}^p$, and $\|\mathbf{x}^h\|_0 \leq s < n < p$

Sparse representations strike back!

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

$n \times 1$ $n \times s$ $s \times 1$

- Observations:**
- The matrix \mathbf{A} effectively becomes *overcomplete*.
 - We could solve for \mathbf{x}^{\natural} if we knew *the location of the non-zero entries of \mathbf{x}^{\natural}* .

Enter sparsity

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

We may consider the estimator with the least number of non-zero entries. That is,

$$\mathbf{x}^{\star} \in \arg \min_{\mathbf{x} \in \mathbb{R}^p} \left\{ \|\mathbf{x}\|_0 : \|\mathbf{b} - \mathbf{A}\mathbf{x}\|_2 \leq \kappa \right\} \quad (\mathcal{P}_0)$$

with some $\kappa \geq 0$. If $\kappa = \|\mathbf{w}\|_2$, then \mathbf{x}^{\natural} is a feasible solution.

Enter sparsity

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

We may consider the estimator with the least number of non-zero entries. That is,

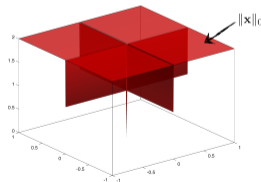
$$\mathbf{x}^{\star} \in \arg \min_{\mathbf{x} \in \mathbb{R}^p} \left\{ \|\mathbf{x}\|_0 : \|\mathbf{b} - \mathbf{A}\mathbf{x}\|_2 \leq \kappa \right\} \quad (\mathcal{P}_0)$$

with some $\kappa \geq 0$. If $\kappa = \|\mathbf{w}\|_2$, then \mathbf{x}^{\natural} is a feasible solution.

o \mathcal{P}_0 has the following characteristics:

- ▶ sample complexity: $\mathcal{O}(s)$
- ▶ computational effort: NP-Hard
- ▶ stability: No

$\|\mathbf{x}\|_0$ over the unit ℓ_{∞} -ball



Enter sparsity

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

We may consider the estimator with the least number of non-zero entries. That is,

$$\mathbf{x}^* \in \arg \min_{\mathbf{x} \in \mathbb{R}^p} \left\{ \|\mathbf{x}\|_0 : \|\mathbf{b} - \mathbf{A}\mathbf{x}\|_2 \leq \kappa \right\} \quad (\mathcal{P}_0)$$

with some $\kappa \geq 0$. If $\kappa = \|\mathbf{w}\|_2$, then \mathbf{x}^{\natural} is a feasible solution.

o \mathcal{P}_0 has the following characteristics:

- ▶ sample complexity: $\mathcal{O}(s)$
- ▶ computational effort: NP-Hard
- ▶ stability: No

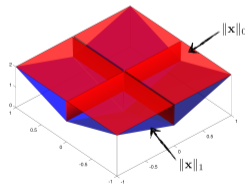
o **Tightest convex relaxation:**

- ▶ $\|\mathbf{x}\|_0^{**}$ is the **biconjugate**
- ▶ i.e., Fenchel conjugate of Fenchel conjugate

o **Fenchel conjugate:**

- ▶ $f^*(\mathbf{y}) := \sup_{\mathbf{x} \in \text{dom}(f)} \mathbf{x}^T \mathbf{y} - f(\mathbf{x})$.

$\|\mathbf{x}\|_1$ is the **convex envelope** of $\|\mathbf{x}\|_0$



A technicality: Restrict $\mathbf{x}^{\natural} \in [-1, 1]^p$.

The role of convexity

A convex candidate solution for $\mathbf{b} = \mathbf{A}\mathbf{x}^\dagger + \mathbf{w}$

$$\mathbf{x}^* \in \arg \min_{\mathbf{x} \in \mathbb{R}^p} \left\{ \|\mathbf{x}\|_1 : \|\mathbf{b} - \mathbf{A}\mathbf{x}\|_2 \leq \|\mathbf{w}\|_2, \|\mathbf{x}\|_\infty \leq 1 \right\}. \quad (\text{SOCP})$$

Theorem (A **model** recovery guarantee [11])

Let $\mathbf{A} \in \mathbb{R}^{n \times p}$ be a matrix of i.i.d. Gaussian random variables with zero mean and variances $1/n$. For any $t > 0$ with probability at least $1 - 6 \exp(-t^2/26)$, we have

$$\|\mathbf{x}^* - \mathbf{x}^\dagger\|_2 \leq \left[\frac{2 \sqrt{2s \log(\frac{p}{s}) + \frac{5}{4}s}}{\sqrt{n} - \sqrt{2s \log(\frac{p}{s}) + \frac{5}{4}s} - t} \right] \|\mathbf{w}\|_2 := \varepsilon, \quad \text{when } \|\mathbf{x}^\dagger\|_0 \leq s.$$

- Observations:**
- o perfect recovery (i.e., $\varepsilon = 0$) with $n \geq 2s \log(\frac{p}{s}) + \frac{5}{4}s$ whp when $\mathbf{w} = 0$.
 - o ε -accurate solution in $k = \mathcal{O}\left(\sqrt{2p+1} \log(\frac{1}{\varepsilon})\right)$ iterations via IPM with a total complexity of $\mathcal{O}(n^2 p^{1.5} \log(\frac{1}{\varepsilon}))$ with each iteration requiring the solution of a structured $n \times 2p$ linear system.
 - o robust to noise.

A Time-Data conundrum — I

A computational dogma

Running time of a learning algorithm increases with the size of the data.

A Time-Data conundrum — I

A computational dogma

Running time of a learning algorithm increases with the size of the data.

- Misaligned goals in the statistical and optimization disciplines

Discipline	Goal	Metric
Optimization	reaching numerical ϵ -accuracy	$\ \mathbf{x}^k - \mathbf{x}^*\ \leq \epsilon$
Statistics	learning ϵ -accurate model	$\ \mathbf{x}^* - \mathbf{x}^{\natural}\ \leq \epsilon$

- Main issue: ϵ and ϵ are **NOT** the same but should be treated jointly!

A Time-Data conundrum — II

A stylized formalization of the time-data tradeoff

The goals of optimization and statistical modeling are tightly connected:

$$\underbrace{\|\mathbf{x}^k - \mathbf{x}^\dagger\|}_{\text{learning quality}} \leq \underbrace{\|\mathbf{x}^k - \mathbf{x}^*\|}_{\varepsilon: \text{ needs "time" } t(k)} + \underbrace{\|\mathbf{x}^* - \mathbf{x}^\dagger\|}_{\varepsilon: \text{ needs "data" } n},$$

\mathbf{x}^\dagger : true model in \mathbb{R}^p
 \mathbf{x}^* : statistical model estimate
 \mathbf{x}^k : numerical solution at iteration k

o As the number of data samples n increases with a fixed optimization formulation,

$$\mathbf{x}^* \in \arg \min_{\mathbf{x} \in \mathbb{R}^p} \left\{ \|\mathbf{x}\|_1 : \|\mathbf{b} - \mathbf{A}\mathbf{x}\|_2 \leq \|\mathbf{w}\|_2, \|\mathbf{x}\|_\infty \leq 1 \right\}$$

- ▶ numerical methods take longer time t to reach ε -accuracy
 - ▶ e.g., per-iteration time to solve an $n \times 2p$ linear system
- ▶ statistical model estimates ε become more precise when $\|\mathbf{w}\|_2 = \mathcal{O}(\sqrt{n})$

$$\varepsilon = \frac{2 \sqrt{2s \log(\frac{p}{s}) + \frac{5}{4}s}}{\sqrt{n} - \sqrt{2s \log(\frac{p}{s}) + \frac{5}{4}s} - t} \|\mathbf{w}\|_2, \text{ with probability } 1 - 6\exp(-t^2/26).$$

A Time-Data conundrum — II

A stylized formalization of the time-data tradeoff

The goals of optimization and statistical modeling are tightly connected:

$$\underbrace{\|\mathbf{x}^k - \mathbf{x}^\dagger\|}_{\leq \bar{\varepsilon}(t(k), n)} \leq \underbrace{\|\mathbf{x}^k - \mathbf{x}^*\|}_{\varepsilon: \text{ needs "time" } t(k)} + \underbrace{\|\mathbf{x}^* - \mathbf{x}^\dagger\|}_{\varepsilon: \text{ needs "data" } n},$$

\mathbf{x}^\dagger :	true model in \mathbb{R}^p
\mathbf{x}^* :	statistical model estimate
\mathbf{x}^k :	numerical solution at iteration k
$\bar{\varepsilon}(t(k), n)$:	actual learning quality at time $t(k)$ with n samples

o As the number of data samples n increases with a fixed optimization formulation,

$$\mathbf{x}^* \in \arg \min_{\mathbf{x} \in \mathbb{R}^p} \left\{ \|\mathbf{x}\|_1 : \|\mathbf{b} - \mathbf{A}\mathbf{x}\|_2 \leq \|\mathbf{w}\|_2, \|\mathbf{x}\|_\infty \leq 1 \right\}$$

- ▶ numerical methods take longer time t to reach ε -accuracy
 - ▶ e.g., per-iteration time to solve an $n \times 2p$ linear system
- ▶ statistical model estimates ε become more precise when $\|\mathbf{w}\|_2 = \mathcal{O}(\sqrt{n})$

$$\varepsilon = \frac{2 \sqrt{2s \log(\frac{p}{s}) + \frac{5}{4}s}}{\sqrt{n} - \sqrt{2s \log(\frac{p}{s}) + \frac{5}{4}s - t}} \|\mathbf{w}\|_2, \text{ with probability } 1 - 6\exp(-t^2/26).$$

“Time” effort has significant diminishing returns on ε in the underdetermined case* (cf., [6, 3, 12, 5, 4])

* “Data” effort also exhibits a similar behavior in the overdetermined case when a signal prior is used due to noise!

Data as a computational resource

A stylized formalization of the time-data tradeoff

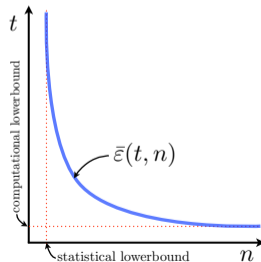
The goals of optimization and statistical modeling are tightly connected:

$$\underbrace{\|\mathbf{x}^{k(t)} - \mathbf{x}^{\natural}\|}_{\leq \bar{\epsilon}(t, n)} \leq \underbrace{\|\mathbf{x}^{k(t)} - \mathbf{x}^{\star}\|}_{\epsilon: \text{ needs "time" } t} + \underbrace{\|\mathbf{x}^{\star} - \mathbf{x}^{\natural}\|}_{\epsilon: \text{ needs "data" } n},$$

\mathbf{x}^{\natural} : true model in \mathbb{R}^p

$\bar{\epsilon}(t, n)$: actual model precision at time t with n samples

- Rest of the lecture:
- o estimator formulation and sample complexity
 - o a “continuous” time-data tradeoff
 - o a different, algorithmic tradeoff with SGD



Sample complexity analysis

Convex optimization formulation for the estimator

$$\mathbf{x}^* \in \arg \min_{\mathbf{x} \in \mathbb{R}^p} \{f(\mathbf{x}) : \mathbf{b} = \mathbf{A}\mathbf{x}\},$$

where $f : \mathbb{R}^p \rightarrow \mathbb{R} \cup \{-\infty, \infty\}$ is a convex function.

Sample complexity

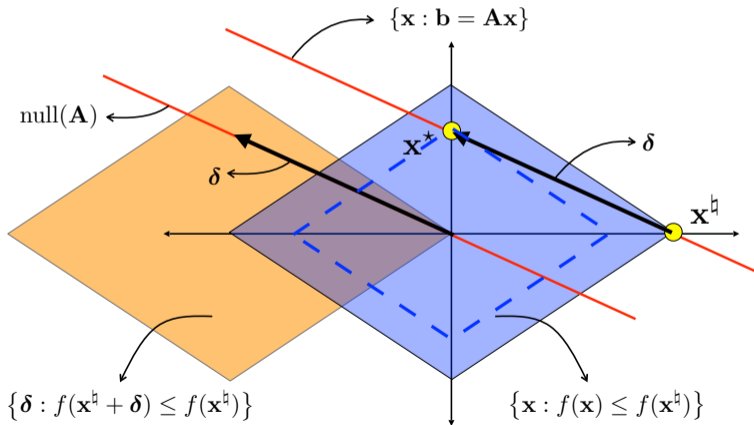
Assume that $A \in \mathbb{R}^{n \times p}$ is a matrix of independent identically distributed (i.i.d.) Gaussian random variables.

What is the minimum number of samples n such that $\mathbf{x}^* = \hat{\mathbf{x}}$ with high probability?

Characterization of the error vector

$$\mathbf{x}^* \in \arg \min_{\mathbf{x} \in \mathbb{R}^p} \{f(\mathbf{x}) : \mathbf{b} = \mathbf{A}\mathbf{x}\}$$

Define the error vector $\delta := \mathbf{x}^* - \mathbf{x}^{\natural}$.

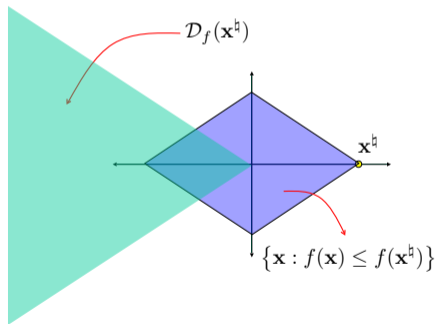


Descent cone

Definition (Descent cone)

Let $f : \mathbb{R}^p \rightarrow \mathbb{R} \cup \{-\infty, \infty\}$ be a proper lower-semicontinuous function. The **descent cone** of f at \mathbf{x}^h is defined as

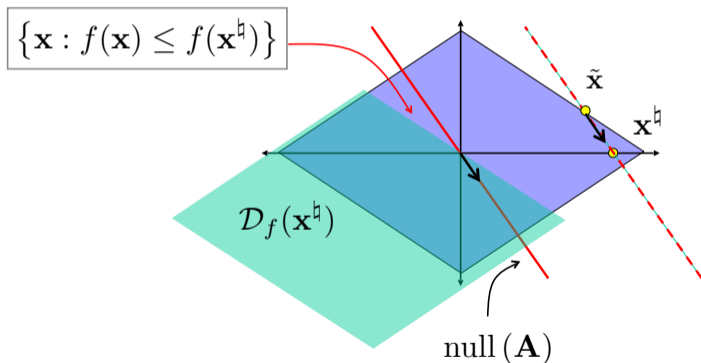
$$\mathcal{D}_f(\mathbf{x}^h) := \text{cone} \left(\left\{ \mathbf{x} : f(\mathbf{x}^h + \mathbf{x}) \leq f(\mathbf{x}^h) \right\} \right).$$



Condition for exact recovery in the *noiseless* case

Proposition (Condition for exact recovery)

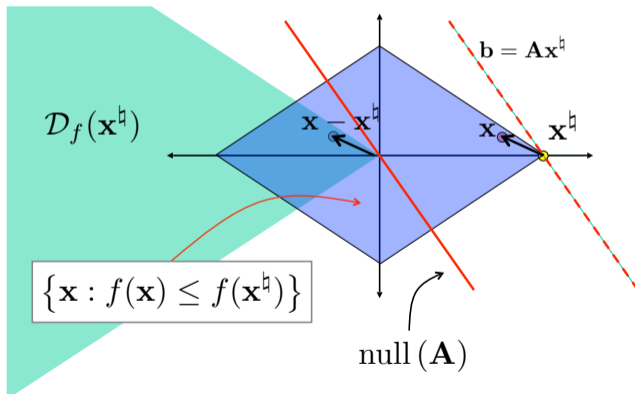
We have successful recovery, i.e., $\delta := \mathbf{x}^* - \mathbf{x}^{\natural} = 0$ with $\mathbf{x}^* \in \arg \min_{\mathbf{x} \in \mathbb{R}^p} \{f(\mathbf{x}) : \mathbf{b} = \mathbf{A}\mathbf{x}\}$, if and only if $\text{null}(\mathbf{A}) \cap \mathcal{D}_f(\mathbf{x}^{\natural}) = \{0\}$.



Condition for exact recovery in the *noiseless* case

Proposition (Condition for exact recovery)

We have successful recovery, i.e., $\delta := \mathbf{x}^* - \mathbf{x}^{\natural} = 0$ with $\mathbf{x}^* \in \arg \min_{\mathbf{x} \in \mathbb{R}^p} \{f(\mathbf{x}) : \mathbf{b} = \mathbf{A}\mathbf{x}\}$, if and only if $\text{null}(\mathbf{A}) \cap \mathcal{D}_f(\mathbf{x}^{\natural}) = \{0\}$.



Statistical dimension and approximate kinematic formula

Now we have

$$\mathbb{P} \{ \mathbf{x}^* = \mathbf{x}^{\natural} \} = \mathbb{P} \{ \text{null}(\mathbf{A}) \cap \mathcal{D}_f(\mathbf{x}^{\natural}) = \{0\} \}.$$

Definition (Statistical dimension [1]¹)

Let $\mathcal{C} \subseteq \mathbb{R}^p$ be a closed convex cone. The *statistical dimension* of \mathcal{C} is defined as

$$d(\mathcal{C}) := \mathbb{E} \left[\|\text{proj}_{\mathcal{C}}(\mathbf{g})\|_2^2 \right].$$

Theorem (Approximate kinematic formula [1])

Let $A \in \mathbb{R}^{n \times p}$, $n < p$, be a matrix of i.i.d. standard Gaussian random variables, and let $\mathcal{C} \subseteq \mathbb{R}^p$ be a closed convex cone. Let $\eta \in (0, 1)$. Then

$$\begin{aligned} n \geq d(\mathcal{C}) + c_{\eta} \sqrt{p} &\Rightarrow \mathbb{P} \{ \text{null}(\mathbf{A}) \cap \mathcal{C} = \{0\} \} \geq 1 - \eta; \\ n \leq d(\mathcal{C}) - c_{\eta} \sqrt{p} &\Rightarrow \mathbb{P} \{ \text{null}(\mathbf{A}) \cap \mathcal{C} = \{0\} \} \leq \eta, \end{aligned}$$

where $c_{\eta} := \sqrt{8 \log(4/\eta)}$.

¹The statistical dimension is closely related to the Gaussian complexity [2], Gaussian width [7], and Gaussian squared complexity [6].

Probability of exact recovery

Corollary

For any $\eta \in (0, 1)$,

$$n \geq d(\mathcal{D}_f(\mathbf{x}^\natural)) + c_\eta \sqrt{p} \quad \Rightarrow \quad \mathbb{P} \{ \mathbf{x}^* = \mathbf{x}^\natural \} \geq 1 - \eta;$$

$$n \leq d(\mathcal{D}_f(\mathbf{x}^\natural)) - c_\eta \sqrt{p} \quad \Rightarrow \quad \mathbb{P} \{ \mathbf{x}^* = \mathbf{x}^\natural \} \leq \eta,$$

where $c_\eta := \sqrt{8 \log(4/\eta)}$.

- There is a *phase transition* at $n \approx d(\mathcal{D}_f(\mathbf{x}^\natural))$.

Examples ([1])

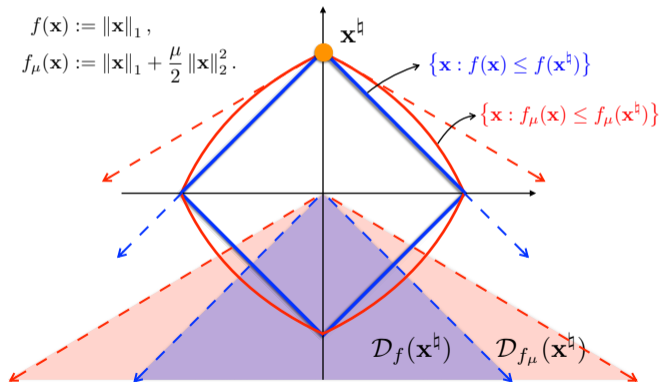
- Let $f(\mathbf{x}) := \|\mathbf{x}\|_1$, and let $\mathbf{x}^\natural \in \mathbb{R}^p$ be s -sparse. Then $d(\mathcal{D}_f(\mathbf{x}^\natural)) \leq 2s \log(p/s) + (5/4)s$.
- Let $f(\mathbf{x}) := \|\mathbf{X}\|_*$, and let $\mathbf{X}^\natural \in \mathbb{R}^{p \times p}$ of rank r . Then $d(\mathcal{D}_f(\mathbf{x}^\natural)) \leq 3r(2p - r)$.

Smoothing increases the statistical dimension

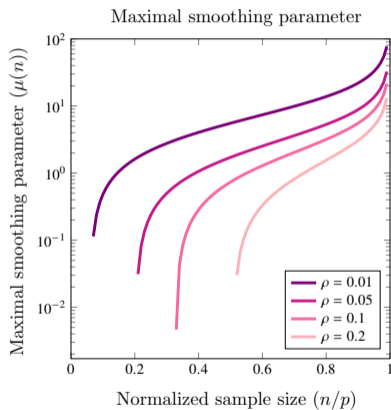
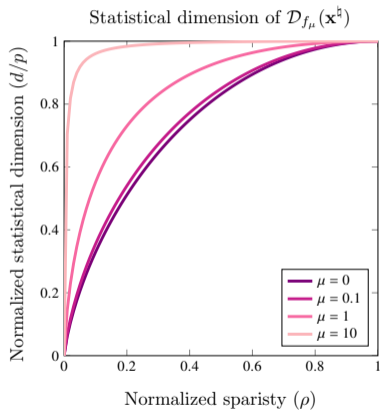
Key properties of the statistical dimension [1]

- The statistical dimension is invariant under unitary transformations (rotations).
- Let \mathcal{C}_1 and \mathcal{C}_2 be closed convex cones. If $\mathcal{C}_1 \subseteq \mathcal{C}_2$, then $d(\mathcal{C}_1) \leq d(\mathcal{C}_2)$.

The larger the statistical dimension is, the more number of observations is required.



Numerical results for the statistical dimension and $\mu(n)$



Smoothing decreases the computational cost

- Consider the estimator,

$$\mathbf{x}^* \in \arg \min_{\mathbf{x} \in \mathbb{R}^p} \left\{ f_\mu(\mathbf{x}) : \mathbf{b} = \mathbf{A}\mathbf{x}, \|\mathbf{x}\|_\infty \leq \|\mathbf{x}^*\|_\infty \right\}, \quad \mu \in [0, \infty).$$

Proposition

Let $\mu > 0$ and $f(\mathbf{x}) = \|\mathbf{x}\|_1$. Consider solving (1) with a primal-dual method as in [4, 5]. The output after the k -th iteration, \mathbf{x}^k , satisfies

$$\|\mathbf{x}^* - \mathbf{x}^k\|_2 \leq \frac{4p\kappa(\mathbf{A}) \left[\rho(1 + \mu \|\mathbf{x}^*\|_\infty)^2 + (1 - \rho) \right]}{\mu k} \propto \frac{1}{\mu k} \Big|_{\rho \ll 1},$$

where $\rho := s/p$, s being the number of non-zero entries in \mathbf{x}^* , and $\kappa(\mathbf{A})$ denotes the restricted condition number of \mathbf{A} .

- Observations:**
- When $\rho \ll 1$, the number of iterations k to achieve the required precision decreases.
 - In fact, we need $1/(\mu\epsilon)$ iterations to have an error bound $\|\mathbf{x}^* - \mathbf{x}^k\|_2 \leq \epsilon$ for a fixed $\epsilon > 0$.

Time-data tradeoff

- Define the maximal smoothing parameter

$$\mu(n) := \arg \max_{\mu > 0} \left\{ \mu : d \left(\mathcal{D}_{f_\mu}(\mathbf{x}^{\natural}) \right) \leq n \right\}.$$

- Consider the “conservative” estimator in probability,

$$\mathbf{x}^* \in \arg \min_{\mathbf{x} \in \mathbb{R}^p} \left\{ f_\mu(\mathbf{x}) \Big|_{\mu = \frac{1}{4} \mu(n)} : \mathbf{b} = \mathbf{A}\mathbf{x} \right\}.$$

Corollary

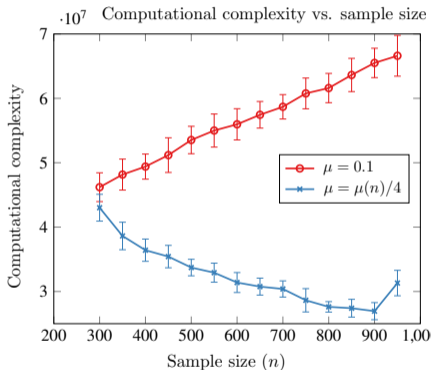
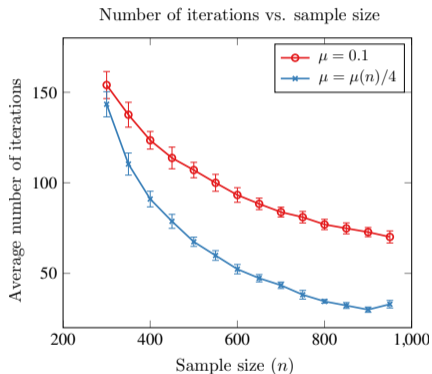
Let $\rho := s/p \ll 1$. Then we have, with high probability, $\mathbf{x}^* = \mathbf{x}^{\natural}$, and

$$\left\| \mathbf{x}^{\natural} - \mathbf{x}^k \right\|_2 \propto \frac{1}{\mu(n)k}.$$

Therefore, to achieve the error bound, $\left\| \mathbf{x}^{\natural} - \mathbf{x}^k \right\|_2 \leq \varepsilon$ for a fixed $\varepsilon > 0$, it suffices to choose

$$k = O \left(\frac{1}{\mu(n)} \right).$$

A numerical result for the time-data tradeoff



Another trade-off in optimization

- o Statistics vs Optimization:

Discipline	Goal	Metric
Optimization	reaching numerical ϵ -accuracy	$\ \mathbf{x}^k - \mathbf{x}^*\ \leq \epsilon$
Statistics	learning ϵ -accurate model	$\ \mathbf{x}^* - \hat{\mathbf{x}}\ \leq \epsilon$

Remarks: *As data sample size gets larger we have seen that:*

- o Algorithms take **longer to reach ϵ** accuracy.
- o However, **statistical error ϵ decreases** as the estimation is more precise.

Another trade-off in optimization

- Statistics vs Optimization:

Discipline	Goal	Metric
Optimization	reaching numerical ϵ -accuracy	$\ \mathbf{x}^k - \mathbf{x}^*\ \leq \epsilon$
Statistics	learning ϵ -accurate model	$\ \mathbf{x}^* - \hat{\mathbf{x}}\ \leq \epsilon$

Remarks: *As data sample size gets larger we have seen that:*

- Algorithms take **longer to reach ϵ** accuracy.
- However, **statistical error ϵ decreases** as the estimation is more precise.

Similar analogy exists between **per-iteration cost** and **convergence rate** for optimization algorithms

Another trade-off in optimization

- Statistics vs Optimization:

Discipline	Goal	Metric
Optimization	reaching numerical ϵ -accuracy	$\ \mathbf{x}^k - \mathbf{x}^*\ \leq \epsilon$
Statistics	learning ϵ -accurate model	$\ \mathbf{x}^* - \hat{\mathbf{x}}\ \leq \epsilon$

Remarks: *As data sample size gets larger we have seen that:*

- Algorithms take **longer to reach ϵ** accuracy.
- However, **statistical error ϵ decreases** as the estimation is more precise.

Similar analogy exists between **per-iteration cost** and **convergence rate** for optimization algorithms

Understanding this trade-off helps us reduce total complexity!

Recall: GD vs. SGD

Problem (Unconstrained convex minimization)

Deterministic setting

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

- $f(\mathbf{x})$ is a *proper, closed, convex and smooth*.
- The solution set
 $\mathcal{S}^* := \{\mathbf{x}^* \in \text{dom}(f) : f(\mathbf{x}^*) = f^*\} \neq \emptyset$.

Stochastic programming

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

- $f(\mathbf{x})$ is *proper, closed, convex and smooth*.
- The solution set
 $\mathcal{S}^* := \{\mathbf{x}^* \in \text{dom}(f) : f(\mathbf{x}^*) = f^*\} \neq \emptyset$.
- θ is a random vector, supported on set Θ .

Algorithms

Gradient Descent

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

- $\alpha_k < 2/L$.

Stochastic Gradient Descent

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

- $\alpha_k = \mathcal{O}(1/\sqrt{k})$
- $\mathbb{E}[G(\mathbf{x}^k, \theta_k)] = \nabla f(\mathbf{x}^k)$

Example: Convex optimization with finite sum

- Consider the finite sum (e.g., ERM) setting

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

Algorithms in the finite sum setting

Gradient Descent

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

- $\nabla f(\mathbf{x}^k) = \frac{1}{n} \sum_{j=1}^n \nabla f_j(\mathbf{x}^k)$

Stochastic Gradient Descent

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

- $G(\mathbf{x}^k, \theta_k) = \nabla f_j(\mathbf{x}^k), j \sim \text{Uniform}(\{1, \dots, n\})$

Example: Convex optimization with finite sum

- Consider the finite sum (e.g., ERM) setting

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

Algorithms in the finite sum setting

Gradient Descent

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

- $\nabla f(\mathbf{x}^k) = \frac{1}{n} \sum_{j=1}^n \nabla f_j(\mathbf{x}^k)$

Stochastic Gradient Descent

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

- $G(\mathbf{x}^k, \theta_k) = \nabla f_j(\mathbf{x}^k), j \sim \text{Uniform}(\{1, \dots, n\})$

- $f(\mathbf{x})$: convex and L -Lipschitz gradient

	rate	cost per iteration	iteration complexity	total complexity
GD	$1/k$	n	$1/\epsilon$	n/ϵ
SGD	$1/\sqrt{k}$	1	$1/\epsilon^2$	$1/\epsilon^2$

Example: Convex optimization with finite sum

- Consider the finite sum (e.g., ERM) setting

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

Algorithms in the finite sum setting

Gradient Descent

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

- $\nabla f(\mathbf{x}^k) = \frac{1}{n} \sum_{j=1}^n \nabla f_j(\mathbf{x}^k)$

Stochastic Gradient Descent

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

- $G(\mathbf{x}^k, \theta_k) = \nabla f_j(\mathbf{x}^k), j \sim \text{Uniform}(\{1, \dots, n\})$

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

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

When f is μ -strongly convex and L -Lipschitz gradient

Finite sums

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

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

- Remarks:**
- o SGD trades off **convergence rate** with **low per-iteration cost**.
 - o When n is large, SGD proves to be effective.
 - o To **control variance** of the stochastic gradient estimate, SGD **decreases step size** at a certain rate.
 - o In turn, convergence deteriorates from **linear** to **sublinear**.

An observation of GD vs. SGD step

$$\mathbf{x}^{k+1} = \mathbf{x}^k - \gamma_k \nabla f(\mathbf{x}^k) \quad (\text{GD})$$

Lemma

Assume f is Lipschitz smooth with constant L . Then,

$$f(\mathbf{x}^{k+1}) - f(\mathbf{x}^k) \leq (\gamma_k^2 L - \gamma_k) \|\nabla f(\mathbf{x}^k)\|^2.$$

An observation of GD vs. SGD step

$$\mathbf{x}^{k+1} = \mathbf{x}^k - \gamma_k G(\mathbf{x}^k, \theta_k) \quad (\text{SGD})$$

Lemma

Assume f is Lipschitz smooth with constant L . Then,

$$\mathbb{E}[f(\mathbf{x}^{k+1}) - f(\mathbf{x}^k)] \leq (\gamma_k^2 L - \gamma_k) \mathbb{E}[\|\nabla f(\mathbf{x}^k)\|^2] + L\gamma_k^2 \mathbb{E}[\|G(\mathbf{x}^k, \theta_k) - \nabla f(\mathbf{x}^k)\|^2]$$

An observation of GD vs. SGD step

$$\mathbf{x}^{k+1} = \mathbf{x}^k - \gamma_k G(\mathbf{x}^k, \theta_k) \quad (\text{SGD})$$

Lemma

Assume f is Lipschitz smooth with constant L . Then,

$$\mathbb{E}[f(\mathbf{x}^{k+1}) - f(\mathbf{x}^k)] \leq (\gamma_k^2 L - \gamma_k) \mathbb{E}[\|\nabla f(\mathbf{x}^k)\|^2] + L\gamma_k^2 \mathbb{E}[\|G(\mathbf{x}^k, \theta_k) - \nabla f(\mathbf{x}^k)\|^2]$$

- The variance of gradient estimate dominates as $\nabla f(\mathbf{x}^k) \rightarrow 0$.
- To ensure convergence we need to control variance.

$\gamma_k \rightarrow 0 \implies$ Slow convergence!

Can we decrease the variance while using a constant step-size?

An observation of GD vs. SGD step

$$\mathbf{x}^{k+1} = \mathbf{x}^k - \gamma_k G(\mathbf{x}^k, \theta_k) \quad (\text{SGD})$$

Lemma

Assume f is Lipschitz smooth with constant L . Then,

$$\mathbb{E}[f(\mathbf{x}^{k+1}) - f(\mathbf{x}^k)] \leq (\gamma_k^2 L - \gamma_k) \mathbb{E}[\|\nabla f(\mathbf{x}^k)\|^2] + L\gamma_k^2 \mathbb{E}[\|G(\mathbf{x}^k, \theta_k) - \nabla f(\mathbf{x}^k)\|^2]$$

- The variance of gradient estimate dominates as $\nabla f(\mathbf{x}^k) \rightarrow 0$.
- To ensure convergence we need to control variance.

$\gamma_k \rightarrow 0 \implies$ Slow convergence!

Can we decrease the variance while using a constant step-size?

Choose a stochastic gradient, s.t. $\mathbb{E}[\|G(\mathbf{x}^k; \theta_k)\|^2] \rightarrow 0$.

A simple approach: Mini-batch SGD

- More samples \rightarrow better estimate for full gradient.

SGD with mini batches

Let $G(\mathbf{x}, \theta)$ be an unbiased gradient estimate ($\mathbb{E}[G(\mathbf{x}, \theta)] = \nabla f(\mathbf{x})$) and B_k be the batch size. Then,

$$\mathbf{x}^{k+1} = \mathbf{x}^k - \alpha_k \frac{1}{B_k} \sum_{j=1}^{B_k} G(\mathbf{x}^k, \theta_{k,j})$$

Theorem

Let $B_k > 0$ be the batch size and $G(\mathbf{x}, \theta)$ be an unbiased gradient estimate with bounded variance, i.e., $\mathbb{E}[\|G(\mathbf{x}, \theta) - \nabla f(\mathbf{x})\|^2 | \mathbf{x}] \leq \sigma^2$. Then, the mini-batch estimate has the following properties:

$$\mathbb{E} \left[\frac{1}{B_k} \sum_{j=1}^{B_k} G(\mathbf{x}, \theta_{k,j}) \right] = \nabla f(\mathbf{x}) \quad \text{and} \quad \mathbb{E} \left[\left\| \frac{1}{B_k} \sum_{j=1}^{B_k} G(\mathbf{x}, \theta_{k,j}) - \nabla f(\mathbf{x}) \right\|^2 \mid \mathbf{x} \right] \leq \frac{\sigma^2}{B_k}$$

- Remarks:**
- We might need to increase the batch size over time to take variance to 0.
 - We can come up with a “smarter” estimate for $\nabla f(\mathbf{x})$.

How to construct a new estimate $G(\mathbf{x}^k; \theta_k)$? [8]

Finite sum structure:	SGD update rule:
$f^* := \min_{\mathbf{x} \in \mathbb{R}^p} \left\{ f(\mathbf{x}) := \frac{1}{n} \sum_{j=1}^n f_j(\mathbf{x}) \right\}$	$\mathbf{x}^{k+1} = \mathbf{x}^k - \gamma_k \nabla f_j(\mathbf{x}^k)$

- Let $X = \nabla f_j(\mathbf{x}^k)$ be a random variable (due to $j \sim \text{Uniform}(\{1, \dots, n\})$).
- Let $Y = \nabla f_j(\tilde{\mathbf{x}})$ be another random variable, and $\tilde{\mathbf{x}}$ is a particularly selected point.

Remarks:

- We want X and Y to be correlated (we will see why!).
- Given Y , we should be able to estimate $\mathbb{E}[X]$ with more confidence.

Observations:

- Choice of $\tilde{\mathbf{x}}$ affects how correlated X and Y are.
- We can compute $\mathbb{E}[Y] = \frac{1}{n} \sum_{j=1}^n \nabla f_j(\tilde{\mathbf{x}}) = \nabla f(\tilde{\mathbf{x}})$.

Goal:

- Find a **good** estimate of $\mathbb{E}[X] = \frac{1}{n} \sum_{j=1}^n \nabla f_j(\mathbf{x}^k) = \nabla f(\mathbf{x}^k)$.

How to construct a new estimate $G(\mathbf{x}^k; \theta_k)$? [8]

Finite sum structure:	SGD update rule:
$f^* := \min_{\mathbf{x} \in \mathbb{R}^p} \left\{ f(\mathbf{x}) := \frac{1}{n} \sum_{j=1}^n f_j(\mathbf{x}) \right\}$	$\mathbf{x}^{k+1} = \mathbf{x}^k - \gamma_k \nabla f_j(\mathbf{x}^k)$

- Let $X = \nabla f_j(\mathbf{x}^k)$ be a random variable (due to $j \sim \text{Uniform}(\{1, \dots, n\})$).
- Let $Y = \nabla f_j(\tilde{\mathbf{x}})$ be another random variable, and $\tilde{\mathbf{x}}$ is a particularly selected point.

A generalized estimator: $R_\alpha = \alpha(X - Y) + \mathbb{E}[Y]$

- $\mathbb{E}[R_\alpha] = \alpha\mathbb{E}[X] + (1 - \alpha)\mathbb{E}[Y]$
- $\text{Var}(R_\alpha) = \alpha^2(\text{Var}(X) + \text{Var}(Y) - 2\text{Cov}(X, Y))$

- Observations:**
- When $\alpha = 1$, R_α becomes unbiased, i.e., $\mathbb{E}[R_\alpha] = \mathbb{E}[X]$.
 - If $\text{Cov}(X, Y)$ is large enough (X and Y are correlated enough), $\text{Var}(R_\alpha) \leq \text{Var}(X)$.

How could we use this information to construct our estimate?

Variance reduction techniques: SVRG

- Select the stochastic gradient ∇f_{i_k} , and compute a gradient estimate

$$\mathbf{r}_k = \nabla f_{i_k}(\mathbf{x}^k) - \nabla f_{i_k}(\tilde{\mathbf{x}}) + \nabla f(\tilde{\mathbf{x}}).$$

- As $\tilde{\mathbf{x}} \rightarrow \mathbf{x}^*$ and $\mathbf{x}^k \rightarrow \mathbf{x}^*$,

$$\nabla f_{i_k}(\mathbf{x}^k) - \nabla f_{i_k}(\tilde{\mathbf{x}}) + \nabla f(\tilde{\mathbf{x}}) \rightarrow 0.$$

- Therefore,

$$\mathbb{E}[\|\nabla f_{i_k}(\mathbf{x}^k) - \nabla f_{i_k}(\tilde{\mathbf{x}}) + \nabla f(\tilde{\mathbf{x}})\|^2] \rightarrow 0.$$

Remarks:

- Remember the generalized estimator: $R_\alpha = \alpha(X - Y) + \mathbb{E}[Y]$.
- For SVRG, $\alpha = 1$, $X = \nabla f_{i_k}(\mathbf{x}^k)$ and $Y = \nabla f_{i_k}(\tilde{\mathbf{x}})$.
- We will see how $\tilde{\mathbf{x}}$ is computed!

Stochastic gradient algorithm with variance reduction

Stochastic gradient with variance reduction (SVRG) [9, 13]

1. Choose $\tilde{\mathbf{x}}^0 \in \mathbb{R}^p$ as a starting point and $\gamma > 0$ and $q \in \mathbb{N}_+$.

2. For $s = 0, 1, 2, \dots$, perform:

2a. $\tilde{\mathbf{x}} = \tilde{\mathbf{x}}^s$, $\tilde{\mathbf{v}} = \nabla f(\tilde{\mathbf{x}})$, $\mathbf{x}^0 = \tilde{\mathbf{x}}$.

2b. For $k = 0, 1, \dots, q-1$, perform:

$$\begin{cases} \text{Pick } i_k \in \{1, \dots, n\} \text{ uniformly at random} \\ \mathbf{r}_k = \nabla f_{i_k}(\mathbf{x}^k) - \nabla f_{i_k}(\tilde{\mathbf{x}}) + \tilde{\mathbf{v}} \\ \mathbf{x}^{k+1} := \mathbf{x}^k - \gamma \mathbf{r}_k, \end{cases} \quad (1)$$

2c. Update $\tilde{\mathbf{x}}^{s+1} = \frac{1}{m} \sum_{j=0}^{q-1} \mathbf{x}^j$.

Features

- The SVRG method uses a multistage scheme to reduce the **variance** of the **stochastic gradient** \mathbf{r}_k .
- **Learning rate** γ does not necessarily tend to 0 while \mathbf{x}^k and $\tilde{\mathbf{x}}^s$ tend to \mathbf{x}_* .
- Each stage, SVRG uses $n + 2q$ component **gradient** evaluations.
- n for the **full gradient** at the beginning of each stage, and $2q$ for each of the q **stochastic gradient steps**.

Convergence analysis

Assumption A5.

- (i) f is μ -strongly convex
- (ii) The learning rate $0 < \gamma < 1/(4L_{\max})$, where $L_{\max} = \max_{1 \leq j \leq n} L_j$.
- (iii) q is large enough such that

$$\kappa = \frac{1}{\mu\gamma(1 - 4\gamma L_{\max})q} + \frac{4\gamma L_{\max}(q + 1)}{(1 - 4\gamma L_{\max})q} < 1.$$

Theorem

Assumptions:

- The sequence $\{\tilde{\mathbf{x}}^s\}_{k \geq 0}$ is generated by SVRG.
- Assumption A5 is satisfied.

Conclusion: Linear convergence is obtained:

$$\mathbb{E}f(\tilde{\mathbf{x}}^s) - f(\mathbf{x}^*) \leq \kappa^s (f(\tilde{\mathbf{x}}^0) - f(\mathbf{x}^*)).$$

Choice of γ and q , and complexity

Chose γ and q such that $\kappa \in (0, 1)$:

For example

$$\gamma = 0.1/L_{\max}, q = 100(L_{\max}/\mu) \implies \kappa \approx 5/6.$$

Complexity

$$\mathbb{E}f(\tilde{\mathbf{x}}^s) - f(\mathbf{x}^*) \leq \epsilon, \quad \text{when } s \geq \log((f(\tilde{\mathbf{x}}^0) - f(\mathbf{x}^*))/\epsilon) / \log(\kappa^{-1})$$

- o Each stage needs $n + 2q$ **component gradient evaluations**
- o With $q = \mathcal{O}(L_{\max}/\mu)$, we obtain an **overall complexity** of

$$\mathcal{O}\left((n + L_{\max}/\mu) \log(1/\epsilon)\right).$$

Comparison: GD vs. SGD vs. SVRG

- GD update:

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

- SGD update:

$$\{ \mathbf{x}^{k+1} := \mathbf{x}^k - \gamma \nabla f_{i_k}(\mathbf{x}^k),$$

- SVRG update:

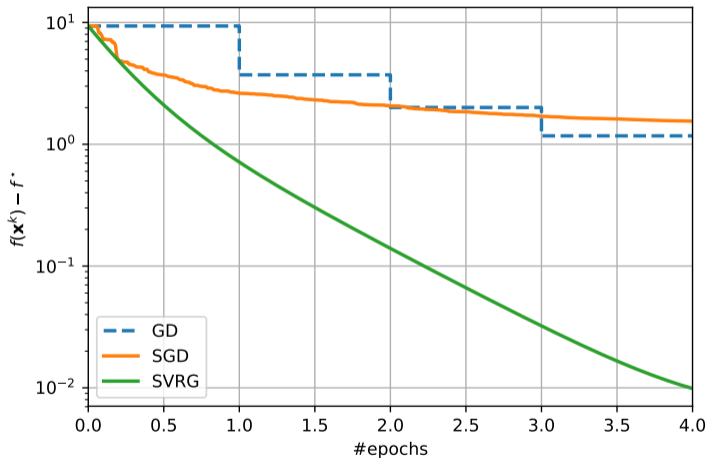
$$\begin{cases} \mathbf{r}_k = \nabla f_{i_k}(\mathbf{x}^k) - \nabla f_{i_k}(\tilde{\mathbf{x}}) + \nabla f(\tilde{\mathbf{x}}) \\ \mathbf{x}^{k+1} := \mathbf{x}^k - \gamma \mathbf{r}_k, \end{cases}$$

	SGD	SVRG	GD
Requires gradient storage?	no	no	no
Epoch-based	no	yes	no
Parameters	stepsize	stepsize & epoch length	stepsize
Gradient evaluations	1 per iteration	$n + 2q$ per epoch	n per iteration

Table: Comparisons of SGD, SVRG and GD [8]

- Recall that $q = \mathcal{O}(L_{\max}/\mu)$ is the epoch length for SVRG.

Example: ℓ_2 -regularized least squares with synthetic data



Taxonomy of algorithms

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

- $f(\mathbf{x}) = \frac{1}{n} \sum_{j=1}^n f_j(\mathbf{x})$: μ -strongly convex with L -Lipschitz continuous gradient.

SVRG	GD	SGD
Linear	Linear	Sublinear

Table: Rate of convergence.

- $\kappa = L/\mu$.

SVRG	AGD	SGD
$\mathcal{O}((n + \kappa) \log(1/\varepsilon))$	$\mathcal{O}(n\kappa \log(1/\varepsilon))$	$1/\varepsilon$

Table: Complexity to obtain ε -solution.

Wrap up!

- Please check Homework 1 on Friday!
- Logistics on remote “lab hours” will be announced on moodle.

* Calculation of $d(\mathcal{D}_f(\mathbf{x}^{\natural}))$ and $d(\mathcal{D}_{f_\mu}(\mathbf{x}^{\natural}))$

Lemma ([1])

Let f be a proper lower-semicontinuous convex function, and let $\mathbf{x} \in \text{dom}(f)$. We have

$$d(\mathcal{D}_f(\mathbf{x})) \leq \inf_{\tau > 0} \mathbb{E} \left[\text{dist}^2(\mathbf{g}, \tau \partial f(\mathbf{x})) \right],$$

where \mathbf{g} is a vector of i.i.d. standard Gaussian random variables.

The upper bounds on $d(\mathcal{D}_f(\mathbf{x}^{\natural}))$ and $d(\mathcal{D}_{f_\mu}(\mathbf{x}^{\natural}))$ can be derived based on above.

Proposition

Let \mathbf{x}^{\natural} be an s -sparse vector. We have

$$d(\mathcal{D}_{f_\mu}(\mathbf{x}^{\natural})) \leq \inf_{\tau > 0} \left\{ s(1 + \tau^2) + 2\mu f_\mu(\mathbf{x}^{\natural})\tau^2 + (p - s) \sqrt{\frac{2}{\pi}} \int_{\tau}^{\infty} (u - \tau)^2 e^{-u^2/2} du \right\}.$$

Note that $f = f_\mu|_{\mu=0}$.

*Variance reduction techniques: SAGA

- Select the stochastic gradient \mathbf{r}_k as

$$\mathbf{r}_k = \nabla f_{i_k}(\mathbf{x}^k) - \nabla f_{i_k}(\tilde{\mathbf{x}}_{i_k}^k) + \frac{1}{n} \sum_{j=1}^n \nabla f_j(\tilde{\mathbf{x}}_j^k),$$

where, at each iteration, $\tilde{\mathbf{x}}$ is updated as $\tilde{\mathbf{x}}_{i_k}^k = \mathbf{x}^k$ and $\tilde{\mathbf{x}}_j^k$ stays the same for $j \neq i_k$.

- As $\tilde{\mathbf{x}}_j^k \rightarrow \mathbf{x}^*$ and $\mathbf{x}^k \rightarrow \mathbf{x}^*$,

$$\nabla f_{i_k}(\mathbf{x}^k) - \nabla f_{i_k}(\tilde{\mathbf{x}}_{i_k}^k) + \frac{1}{n} \sum_{j=1}^n \nabla f_j(\tilde{\mathbf{x}}_j^k) \rightarrow 0.$$

- Therefore,

$$\mathbb{E} \left[\left\| \nabla f_{i_k}(\mathbf{x}^k) - \nabla f_{i_k}(\tilde{\mathbf{x}}_{i_k}^k) + \frac{1}{n} \sum_{j=1}^n \nabla f_j(\tilde{\mathbf{x}}_j^k) \right\|^2 \right] \rightarrow 0.$$

*Variance reduction techniques: SAGA

Stochastic Average Gradient (SAGA) [8]

- 1a.** Choose $\tilde{\mathbf{x}}_i^0 = \mathbf{x}^0 \in \mathbb{R}^p, \forall i, q \in \mathbb{N}_+$ and stepsize $\gamma > 0$.
- 1b.** Store $\nabla f_i(\tilde{\mathbf{x}}_i^0)$ in a table data-structure with length n .
- 2.** For $k = 0, 1 \dots$ perform:
 - 2a.** Pick $i_k \in \{1, \dots, n\}$ uniformly at random
 - 2b.** Take $\tilde{\mathbf{x}}_{i_k}^{k+1} = \mathbf{x}^k$, store $\nabla f_{i_k}(\tilde{\mathbf{x}}_{i_k}^{k+1})$ in the table and leave other entries the same.
 - 2c.** $\mathbf{r}_k = \nabla f_{i_k}(\mathbf{x}^k) - \nabla f_{i_k}(\tilde{\mathbf{x}}_{i_k}^k) + \frac{1}{n} \sum_{j=1}^n \nabla f_j(\tilde{\mathbf{x}}_j^k)$
- 3.** $\mathbf{x}^{k+1} = \mathbf{x}^k - \gamma \mathbf{r}_k$

Recipe:

In each iteration:

- ▶ Store last gradient evaluated at each datapoint.
- ▶ Previous gradient for datapoint j is $\nabla f_j(\tilde{\mathbf{x}}_j^k)$.
- ▶ Perform SG-iterations with the following stochastic gradient

$$\mathbf{r}_k = \nabla f_{i_k}(\mathbf{x}^k) - \nabla f_{i_k}(\tilde{\mathbf{x}}_{i_k}^k) + \frac{1}{n} \sum_{j=1}^n \nabla f_j(\tilde{\mathbf{x}}_j^k).$$

*Convergence of SAGA

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

Theorem (Convergence of SAGA [8])

Suppose that f is μ -strongly convex and that the stepsize is $\gamma = \frac{1}{2(\mu n + L)}$ with

$$\rho = 1 - \frac{\mu}{2(\mu n + L)} < 1,$$

$$C = \|\mathbf{x}^0 - \mathbf{x}^*\|^2 + \frac{n}{\mu n + L} [f(\mathbf{x}^0) - \langle \nabla f(\mathbf{x}^*), \mathbf{x}^0 - \mathbf{x}^* \rangle - f(\mathbf{x}^*)]$$

Then

$$\mathbb{E}[\|\mathbf{x}^k - \mathbf{x}^*\|^2] \leq \rho^k C.$$

- Allows the constant step-size.
- Obtains linear rate convergence.

*Variance reduction techniques: SARAH

- o Select the stochastic gradient \mathbf{r}_k

$$\mathbf{r}_k = \nabla f_{i_k}(\mathbf{x}^k) - \nabla f_{i_k}(\mathbf{x}^{k-1}) + \mathbf{r}_{k-1},$$

- o The variance reduction in SARAH can be characterized as

$$\mathbb{E}[\|\mathbf{r}_k\|^2] \leq \left[1 - \left(\frac{2}{\gamma L} - 1\right)\mu^2\gamma^2\right]^k \mathbb{E}[\|\nabla f(\mathbf{x}^0)\|^2].$$

*Variance reduction techniques: SARAH

Stochastic Recursive Gradient Algorithm (SARAH) [10]

1. Choose $\bar{\mathbf{x}}^0 \in \mathbb{R}^p$, $q \in \mathbb{N}_+$ and stepsize $\gamma > 0$.
2. For $k = 0, 1 \dots$ perform:
 2. $\mathbf{x}^0 = \bar{\mathbf{x}}^k$, $\mathbf{r}_0 = \frac{1}{n} \sum_{j=1}^n f_j(\bar{\mathbf{x}}^0)$
 - 2a. $\mathbf{x}^1 = \mathbf{x}^0 - \gamma \mathbf{r}_0$
 - 2b. For $l = 1 \dots, q - 1$, perform:
$$\begin{cases} \text{pick } i_l \in \{1, \dots, n\} \text{ uniformly at random,} \\ \mathbf{r}_l = \nabla f_{i_l}(\mathbf{x}^l) - \nabla f_{i_l}(\mathbf{x}^{l-1}) + \mathbf{r}_{l-1}, \\ \mathbf{x}^{l+1} = \mathbf{x}^l - \gamma \mathbf{r}_l. \end{cases}$$
- 3 Update $\bar{\mathbf{x}}^{k+1} = \mathbf{x}^l$ where l is chosen uniformly at random from $\{0, \dots, q\}$.

Recipe: *In a cycle of q inner iterations:*

- o Compute stochastic step direction by recursively adding and subtracting component gradients.

$$\mathbf{r}_l = \nabla f_{i_l}(\mathbf{x}^l) - \nabla f_{i_l}(\mathbf{x}^{l-1}) + \mathbf{r}_{l-1}.$$

- o Perform q SG-iterations with \mathbf{r}_l .
- o Update next iteration by picking uniformly at random from q previous iterations.

*Convergence of SARAH

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

Theorem (Convergence of SARAH [10])

Suppose that f is μ -strongly convex and that the stepsize γ and number of inner iterations q satisfies

$$\rho_q = \frac{1}{\mu\gamma(1+q)} + \frac{L_{\max}\gamma}{2 - L_{\max}\gamma} < 1.$$

Then

$$\mathbb{E}[\|\nabla f(\bar{\mathbf{x}}^k)\|^2] \leq \rho_q^k \|\nabla f(\bar{\mathbf{x}}^0)\|^2.$$

References I

- [1] Dennis Amelunxen, Martin Lotz, Michael B. McCoy, and Joel A. Tropp.
Living on the edge: Phase transitions in convex programs with random data.
2014.
[arXiv:1303.6672v2 \[cs.IT\]](#).
- [2] Peter L. Barlett and Shahar Mendelson.
Rademacher and Gaussian complexities: Risk bounds and structural results.
J. Mach. Learn. Res., 3, 2002.
- [3] Léon Bottou and Oliver Bousquet.
The tradeoffs of large scale learning.
In Advances in Neural Information Processing Systems, 2007.
- [4] John J Bruer, Joel A Tropp, Volkan Cevher, and Stephen Becker.
Time–data tradeoffs by aggressive smoothing.
In Advances in Neural Information Processing Systems, pages 1664–1672, 2014.
- [5] John J Bruer, Joel A Tropp, Volkan Cevher, and Stephen R Becker.
Designing statistical estimators that balance sample size, risk, and computational cost.
IEEE Journal of Selected Topics in Signal Processing, 9(4):612–624, 2015.

References II

- [6] Venkat Chandrasekaran and Michael I. Jordan.
Computational and statistical tradeoffs via convex relaxation.
Proc. Natl. Acad. Sci., 110(13):E1181–E1190, 2013.
- [7] Venkat Chandrasekaran, Benjamin Recht, Pablo A. Parrilo, and Alan S. Willsky.
The convex geometry of linear inverse problems.
Found. Comput. Math., 12:805–849, 2012.
- [8] Aaron Defazio, Francis Bach, and Simon Lacoste-Julien.
Saga: A fast incremental gradient method with support for non-strongly convex composite objectives.
In Z. Ghahramani, M. Welling, C. Cortes, N. D. Lawrence, and K. Q. Weinberger, editors, *Advances in Neural Information Processing Systems 27*, pages 1646–1654. Curran Associates, Inc., 2014.
- [9] Rie Johnson and Tong Zhang.
Accelerating stochastic gradient descent using predictive variance reduction.
In C. J. C. Burges, L. Bottou, M. Welling, Z. Ghahramani, and K. Q. Weinberger, editors, *Advances in Neural Information Processing Systems 26*, pages 315–323. Curran Associates, Inc., 2013.
- [10] Lam M. Nguyen, Jie Liu, Katya Scheinberg, and Martin Takac.
Sarah: A novel method for machine learning problems using stochastic recursive gradient, 2017.

References III

- [11] Samet Oymak, Christos Thrampoulidis, and Babak Hassibi.
Simple bounds for noisy linear inverse problems with exact side information.
2013.
[arXiv:1312.0641v2 \[cs.IT\]](#).
- [12] Shai Shalev-Shwartz and Nathan Srebro.
Svm optimization: inverse dependence on training set size.
In Proceedings of the 25th international conference on Machine learning, pages 928–935, 2008.
- [13] Lin Xiao and Tong Zhang.
A proximal stochastic gradient method with progressive variance reduction.
SIAM Journal on Optimization, 24, 03 2014.