

Big Data Analytics: Optimization and Randomization

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URL

<http://www.cs.uiowa.edu/~tyng/kdd15-tutorial.pdf>

Some Claims

No

- This tutorial is not an exhaustive literature survey
- It is not a survey on different machine learning/data mining algorithms

Yes

- It is about how to **efficiently** solve machine learning/data mining (formulated as optimization) problems for **big data**

Outline

- **Part I: Basics**
- **Part II: Optimization**
- **Part III: Randomization**

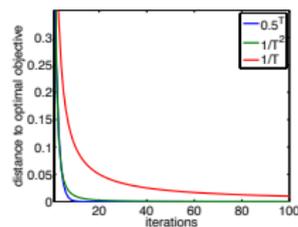
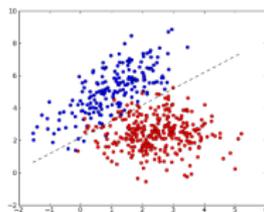
Big Data Analytics: Optimization and Randomization

Part I: Basics

Outline

- 1 Basics
 - Introduction
 - Notations and Definitions

Three Steps for Machine Learning



Data

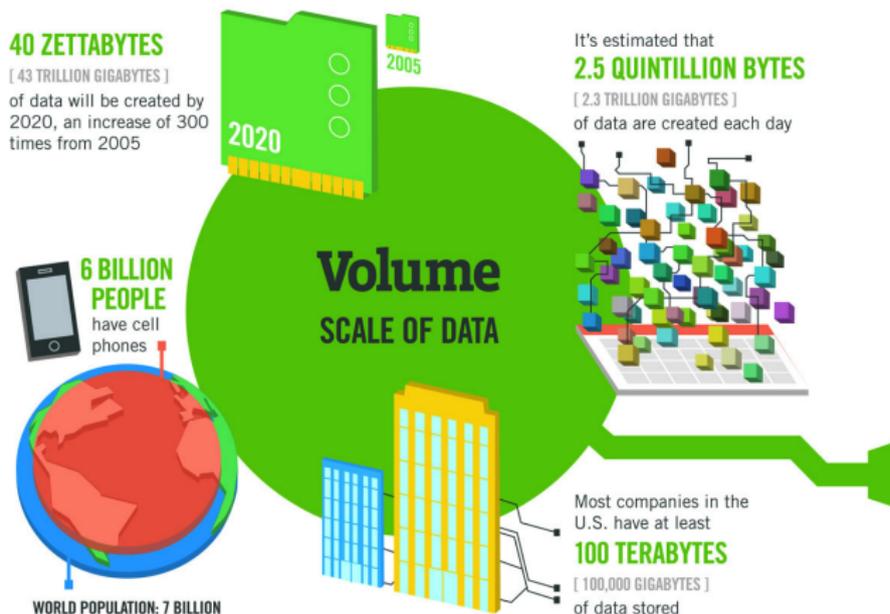
Model

Optimization



Big Data Challenge

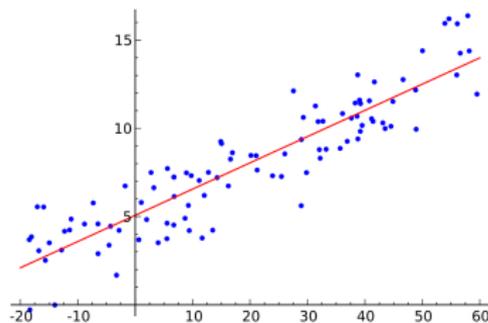
Big Data



Learning as Optimization

Ridge Regression Problem:

$$\min_{\mathbf{w} \in \mathbb{R}^d} \frac{1}{n} \sum_{i=1}^n (y_i - \mathbf{w}^\top \mathbf{x}_i)^2 + \frac{\lambda}{2} \|\mathbf{w}\|_2^2$$

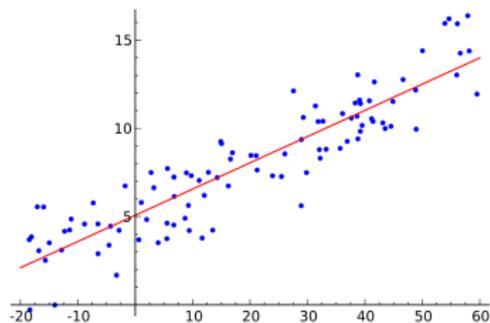


- $\mathbf{x}_i \in \mathbb{R}^d$: d -dimensional feature vector
- $y_i \in \mathbb{R}$: target variable
- $\mathbf{w} \in \mathbb{R}^d$: model parameters
- n : number of data points

Learning as Optimization

Ridge Regression Problem:

$$\min_{\mathbf{w} \in \mathbb{R}^d} \underbrace{\frac{1}{n} \sum_{i=1}^n (y_i - \mathbf{w}^\top \mathbf{x}_i)^2}_{\text{Empirical Loss}} + \frac{\lambda}{2} \|\mathbf{w}\|_2^2$$

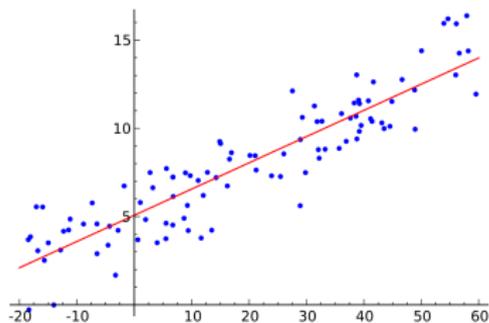


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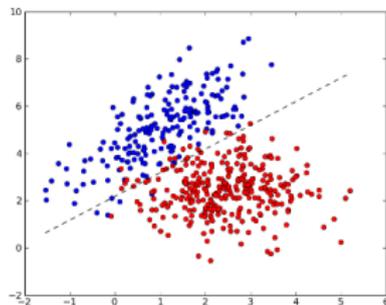


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- n : number of data points

Learning as Optimization

Classification Problems:

$$\min_{\mathbf{w} \in \mathbb{R}^d} \frac{1}{n} \sum_{i=1}^n \ell(y_i \mathbf{w}^\top \mathbf{x}_i) + \frac{\lambda}{2} \|\mathbf{w}\|_2^2$$

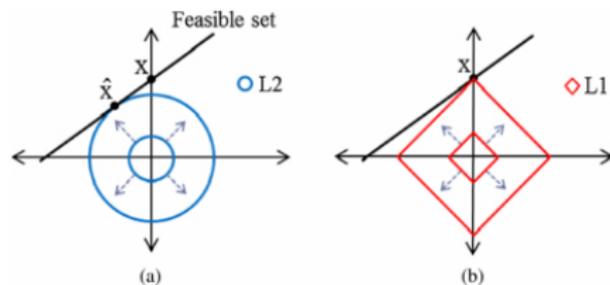


- $y_i \in \{+1, -1\}$: label
- Loss function $\ell(z)$: $z = y\mathbf{w}^\top \mathbf{x}$
 1. **SVMs**: (squared) hinge loss $\ell(z) = \max(0, 1 - z)^p$, where $p = 1, 2$
 2. **Logistic Regression**: $\ell(z) = \log(1 + \exp(-z))$

Learning as Optimization

Feature Selection:

$$\min_{\mathbf{w} \in \mathbb{R}^d} \frac{1}{n} \sum_{i=1}^n \ell(\mathbf{w}^\top \mathbf{x}_i, y_i) + \lambda \|\mathbf{w}\|_1$$

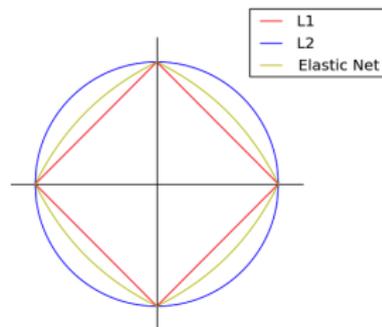


- ℓ_1 regularization $\|\mathbf{w}\|_1 = \sum_{i=1}^d |w_i|$
- λ controls sparsity level

Learning as Optimization

Feature Selection using **Elastic Net**:

$$\min_{\mathbf{w} \in \mathbb{R}^d} \frac{1}{n} \sum_{i=1}^n \ell(\mathbf{w}^\top \mathbf{x}_i, y_i) + \lambda \left(\|\mathbf{w}\|_1 + \gamma \|\mathbf{w}\|_2^2 \right)$$



- Elastic net regularizer, more robust than ℓ_1 regularizer

Learning as Optimization

Multi-class/Multi-task Learning:

$$\min_{\mathbf{W}} \frac{1}{n} \sum_{i=1}^n \ell(\mathbf{W}\mathbf{x}_i, y_i) + \lambda r(\mathbf{W})$$

- $\mathbf{W} \in \mathbb{R}^{K \times d}$
- $r(\mathbf{W}) = \|\mathbf{W}\|_F^2 = \sum_{k=1}^K \sum_{j=1}^d W_{kj}^2$: Frobenius Norm
- $r(\mathbf{W}) = \|\mathbf{W}\|_* = \sum_i \sigma_i$: Nuclear Norm (sum of singular values)
- $r(\mathbf{W}) = \|\mathbf{W}\|_{1,\infty} = \sum_{j=1}^d \|W_{:j}\|_\infty$: $\ell_{1,\infty}$ mixed norm

Learning as Optimization

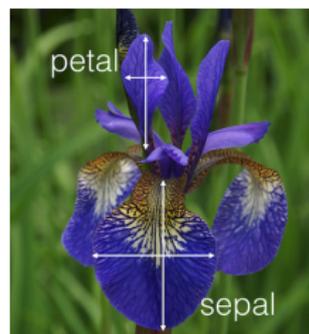
Regularized Empirical Loss Minimization

$$\min_{\mathbf{w} \in \mathbb{R}^d} \frac{1}{n} \sum_{i=1}^n \ell(\mathbf{w}^\top \mathbf{x}_i, y_i) + R(\mathbf{w})$$

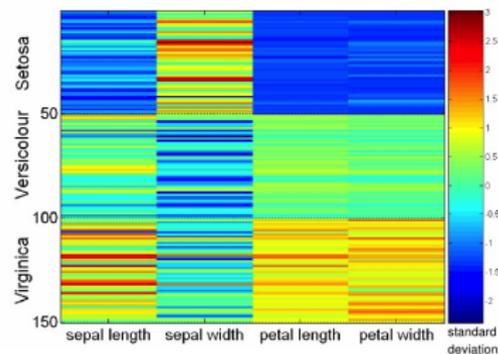
- Both ℓ and R are convex functions
- Extensions to Matrix Cases are possible (sometimes straightforward)
- Extensions to Kernel methods can be combined with randomized approaches
- Extensions to Non-convex (e.g., deep learning) are in progress

Data Matrices and Machine Learning

The Instance-feature Matrix: $X \in \mathbb{R}^{n \times d}$



$$X = \begin{pmatrix} \mathbf{x}_1^T \\ \mathbf{x}_2^T \\ \cdot \\ \cdot \\ \cdot \\ \cdot \\ \mathbf{x}_n^T \end{pmatrix}$$



Data Matrices and Machine Learning

The output vector: $\mathbf{y} = \begin{pmatrix} y_1 \\ y_2 \\ \cdot \\ \cdot \\ \cdot \\ y_n \end{pmatrix} \in \mathbb{R}^{n \times 1}$

- continuous $y_i \in \mathbb{R}$: regression (e.g., house price)
- discrete, e.g., $y_i \in \{1, 2, 3\}$: classification (e.g., species of iris)



Setosa



Versicolour

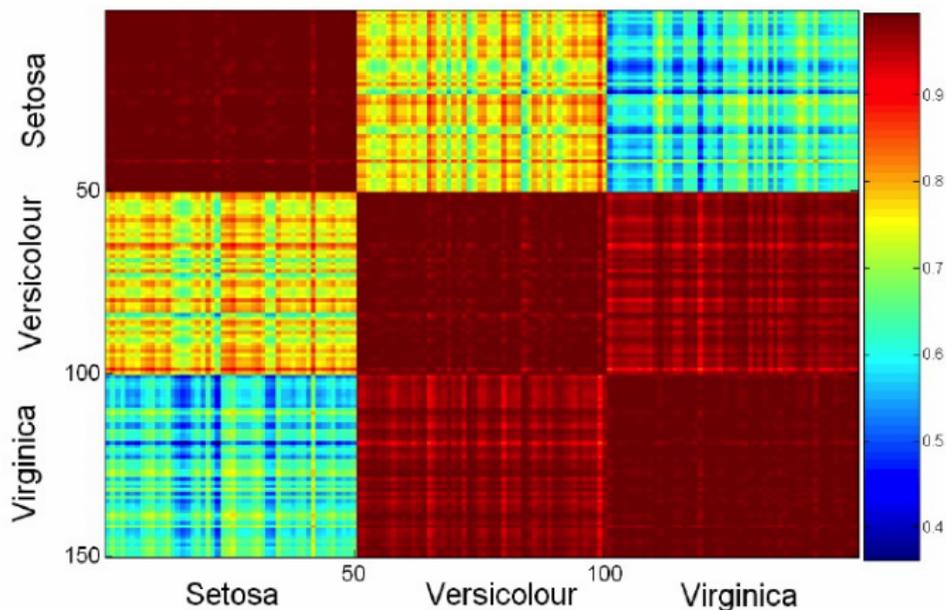


Virginica

Data Matrices and Machine Learning

The Instance-Instance Matrix: $K \in \mathbb{R}^{n \times n}$

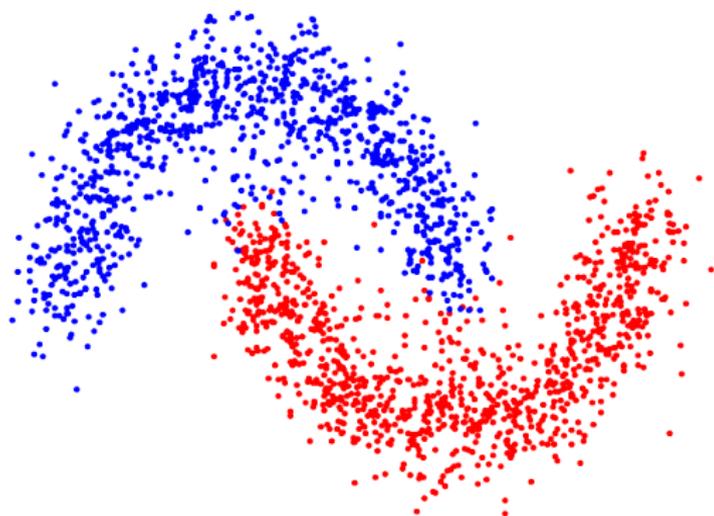
- Similarity Matrix
- Kernel Matrix



Data Matrices and Machine Learning

Some machine learning tasks are formulated on the kernel matrix

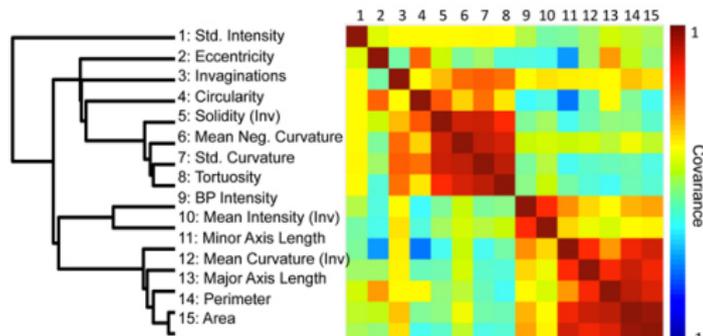
- Clustering
- Kernel Methods



Data Matrices and Machine Learning

The Feature-Feature Matrix: $C \in \mathbb{R}^{d \times d}$

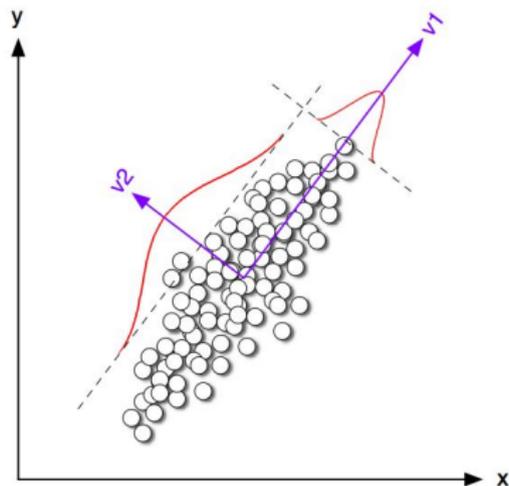
- Covariance Matrix
- Distance Metric Matrix



Data Matrices and Machine Learning

Some machine learning tasks requires **the covariance matrix**

- Principal Component Analysis
- Top-k Singular Value (Eigen-Value) Decomposition of the Covariance Matrix



Why Learning from Big Data is Challenging?

- High per-iteration cost
- High memory cost
- High communication cost
- Large iteration complexity

Outline

- 1 Basics
 - Introduction
 - **Notations and Definitions**

Norms

Vector $\mathbf{x} \in \mathbb{R}^d$

- Euclidean vector norm: $\|\mathbf{x}\|_2 = \sqrt{\mathbf{x}^\top \mathbf{x}} = \sqrt{\sum_{i=1}^d x_i^2}$
- l_p -norm of a vector: $\|\mathbf{x}\|_p = \left(\sum_{i=1}^d |x_i|^p\right)^{1/p}$ where $p \geq 1$
 - 1 l_2 norm $\|\mathbf{x}\|_2 = \sqrt{\sum_{i=1}^d x_i^2}$
 - 2 l_1 norm $\|\mathbf{x}\|_1 = \sum_{i=1}^d |x_i|$
 - 3 l_∞ norm $\|\mathbf{x}\|_\infty = \max_i |x_i|$

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Matrix Factorization

Matrix $X \in \mathbb{R}^{n \times d}$

- Singular Value Decomposition $X = U\Sigma V^T$

- 1 $U \in \mathbb{R}^{n \times r}$: orthonormal columns ($U^T U = I$): span column space
- 2 $\Sigma \in \mathbb{R}^{r \times r}$: diagonal matrix $\Sigma_{ii} = \sigma_i > 0$, $\sigma_1 \geq \sigma_2 \dots \geq \sigma_r$
- 3 $V \in \mathbb{R}^{d \times r}$: orthonormal columns ($V^T V = I$): span row space
- 4 $r \leq \min(n, d)$: max value such that $\sigma_r > 0$: rank of X
- 5 $U_k \Sigma_k V_k^T$: top- k approximation

- Pseudo inverse: $X^\dagger = V\Sigma^{-1}U^T$

- QR factorization: $X = QR$ ($n \geq d$)

- $Q \in \mathbb{R}^{n \times d}$: orthonormal columns
- $R \in \mathbb{R}^{d \times d}$: upper triangular matrix

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- Spectral (induced norm) of a matrix: $\|X\|_2 = \max_{\|u\|_2=1} \|Xu\|_2$
 - $\|A\|_2 = \sigma_1$ (maximum singular value)

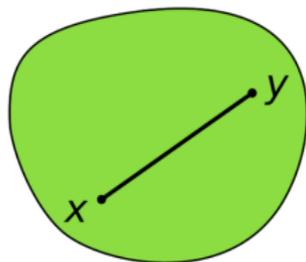
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Convex Optimization

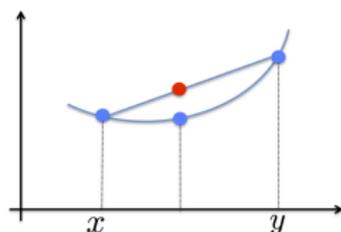
$$\min_{x \in \mathcal{X}} f(x)$$



- \mathcal{X} is a convex domain
 - for any $x, y \in \mathcal{X}$, their convex combination $\alpha x + (1 - \alpha)y \in \mathcal{X}$
- $f(x)$ is a convex function

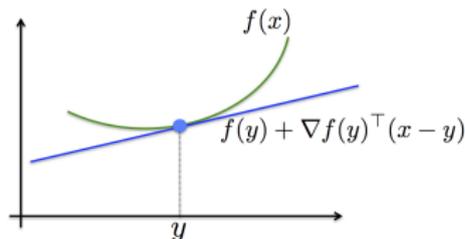
Convex Function

Characterization of Convex Function



$$f(\alpha x + (1 - \alpha)y) \leq \alpha f(x) + (1 - \alpha)f(y),$$

$$\forall x, y \in \mathcal{X}, \alpha \in [0, 1]$$

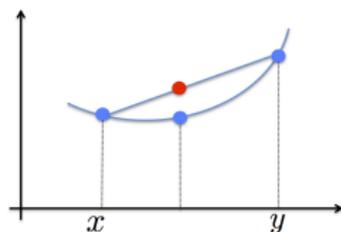


$$f(x) \geq f(y) + \nabla f(y)^\top (x - y) \quad \forall x, y \in \mathcal{X}$$

local optimum is global optimum

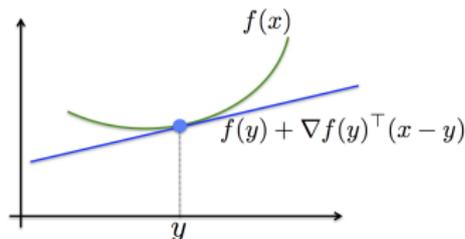
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local optimum is global optimum

Convex vs Strongly Convex

Convex function:

$$f(x) \geq f(y) + \nabla f(y)^\top (x - y) \quad \forall x, y \in \mathcal{X}$$

Strongly Convex function:

$$f(x) \geq f(y) + \nabla f(y)^\top (x - y) + \frac{\lambda}{2} \|x - y\|_2^2 \quad \forall x, y \in \mathcal{X}$$

Global optimum is unique

Convex vs Strongly Convex

Convex function:

$$f(x) \geq f(y) + \nabla f(y)^\top (x - y) \quad \forall x, y \in \mathcal{X}$$

strong convexity
constant

Strongly Convex function:

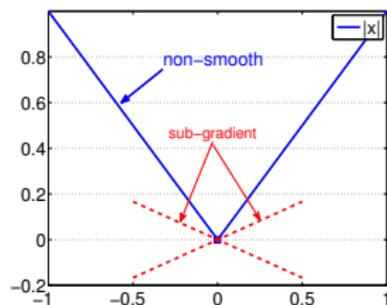
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Non-smooth function vs Smooth function

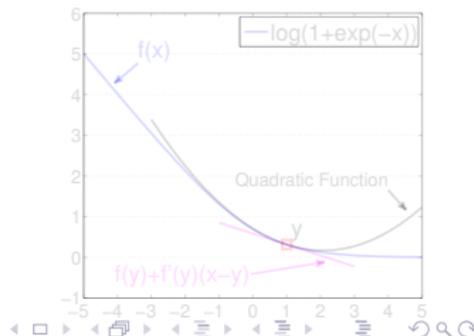
Non-smooth function

- Lipschitz continuous: e.g. **absolute loss**
 $f(x) = |x|$
- $|f(x) - f(y)| \leq G\|x - y\|_2$
- Subgradient: $f(x) \geq f(y) + \partial f(y)^\top (x - y)$



Smooth function

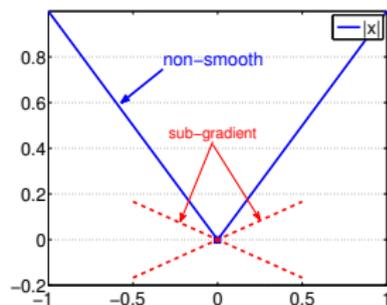
- e.g. **logistic loss** $f(x) = \log(1 + \exp(-x))$
- $\|\nabla f(x) - \nabla f(y)\|_2 \leq L\|x - y\|_2$



Non-smooth function vs Smooth function

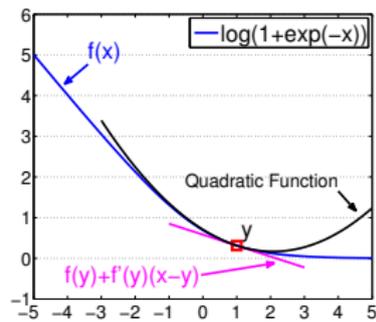
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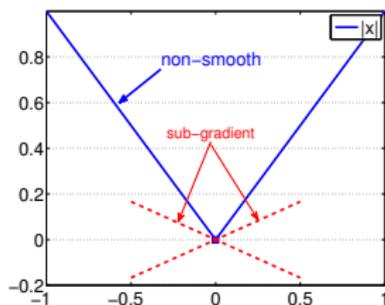


Non-smooth function vs Smooth function

Non-smooth function

Lipschitz
constant

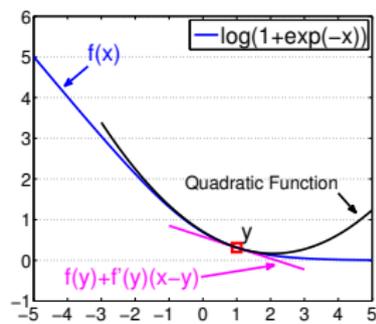
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Smooth function

smoothness
constant

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Next ...

$$\min_{\mathbf{w} \in \mathbb{R}^d} \frac{1}{n} \sum_{i=1}^n \ell(\mathbf{w}^\top \mathbf{x}_i, y_i) + R(\mathbf{w})$$

Part II: Optimization

- stochastic optimization
- distributed optimization

Reduce Iteration Complexity: utilizing properties of functions

Next ...



Part III: Randomization

- Classification, Regression
- SVD, K-means, Kernel methods

Reduce Data Size: utilizing properties of data

Please stay tuned!

Big Data Analytics: Optimization and Randomization

Part II: Optimization

Outline

- 2 Optimization
 - (Sub)Gradient Methods
 - Stochastic Optimization Algorithms for Big Data
 - Stochastic Optimization
 - Distributed Optimization

Learning as Optimization

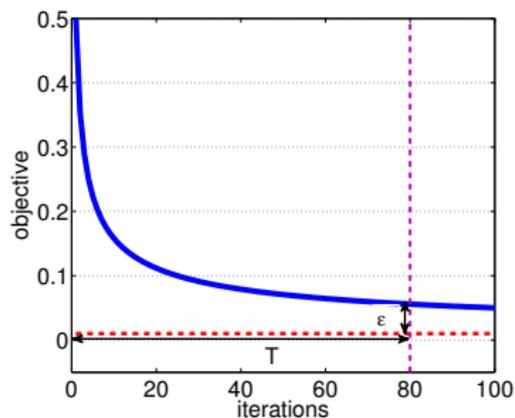
Regularized Empirical Loss Minimization

$$\min_{\mathbf{w} \in \mathbb{R}^d} \underbrace{\frac{1}{n} \sum_{i=1}^n \ell(\mathbf{w}^\top \mathbf{x}_i, y_i) + R(\mathbf{w})}_{F(\mathbf{w})}$$

Convergence Measure

- Most optimization algorithms are iterative

$$\mathbf{w}_{t+1} = \mathbf{w}_t + \Delta \mathbf{w}_t$$



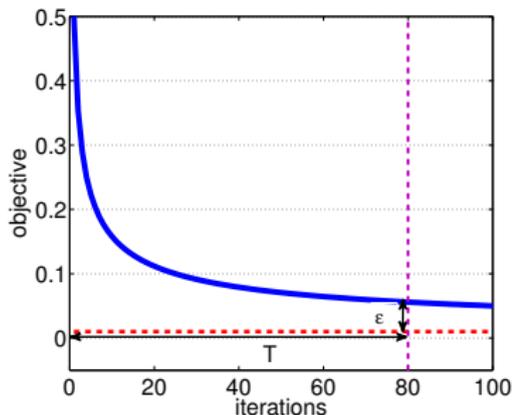
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- Iteration Complexity:** the number of iterations $T(\epsilon)$ needed to have

$$F(\hat{\mathbf{w}}_T) - \min_{\mathbf{w}} F(\mathbf{w}) \leq \epsilon \quad (\epsilon \ll 1)$$



Convergence Measure

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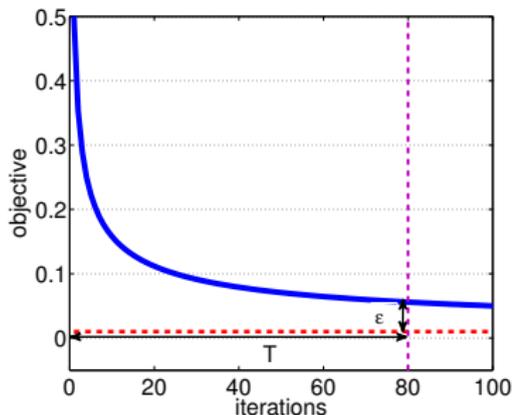
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- Convergence Rate:** after T iterations, how good is the solution

$$F(\hat{\mathbf{w}}_T) - \min_{\mathbf{w}} F(\mathbf{w}) \leq \epsilon(T)$$



Convergence Measure

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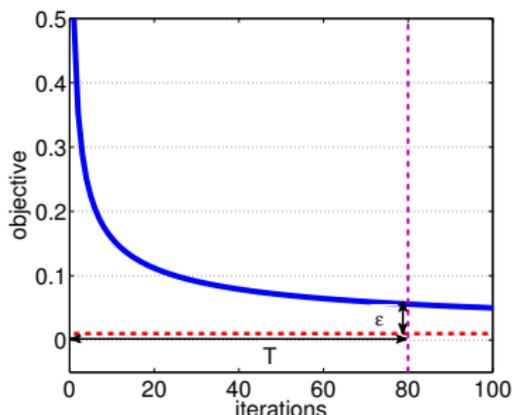
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$$F(\hat{\mathbf{w}}_T) - \min_{\mathbf{w}} F(\mathbf{w}) \leq \epsilon \quad (\epsilon \ll 1)$$

- Convergence Rate:** after T iterations, how good is the solution

$$F(\hat{\mathbf{w}}_T) - \min_{\mathbf{w}} F(\mathbf{w}) \leq \epsilon(T)$$

- Total Runtime** = Per-iteration Cost \times Iteration Complexity



More on Convergence Measure

- Big $O(\cdot)$ notation: explicit dependence on T or ϵ

	Convergence Rate	Iteration Complexity
linear	$O(\mu^T)$ ($\mu < 1$)	$O\left(\log\left(\frac{1}{\epsilon}\right)\right)$
sub-linear	$O\left(\frac{1}{T^\alpha}\right)$ ($\alpha > 0$)	$O\left(\frac{1}{\epsilon^{1/\alpha}}\right)$

Why are we interested in Bounds?

More on Convergence Measure

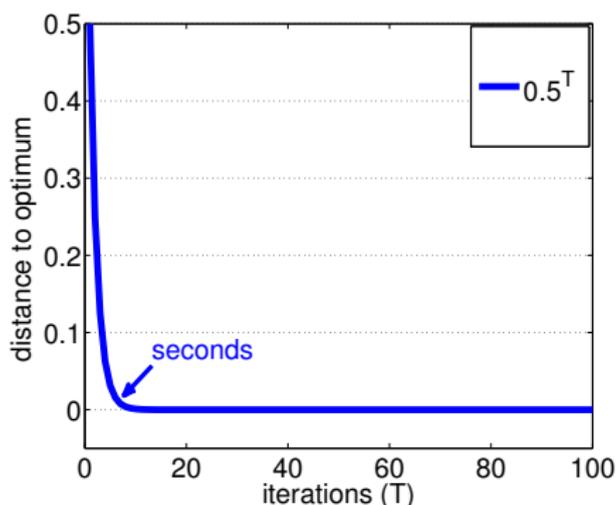
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Why are we interested in Bounds?

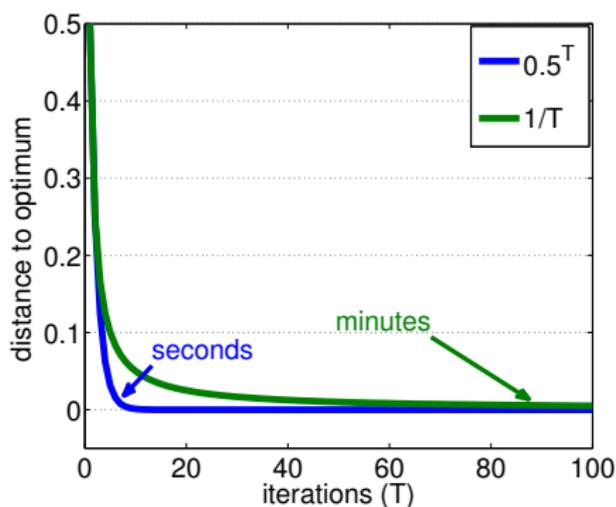
More on Convergence Measure

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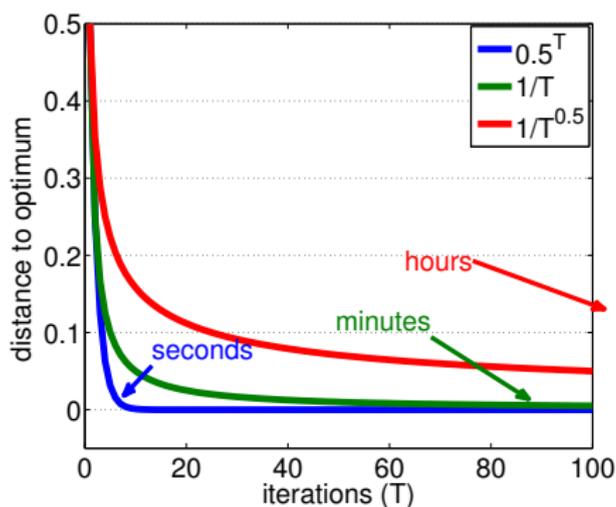
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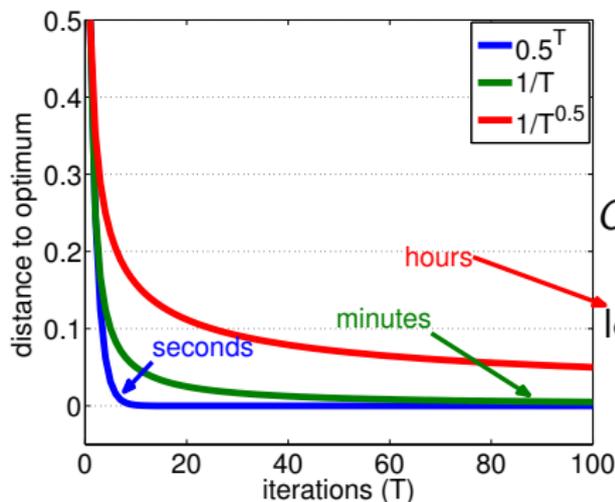
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More on Convergence Measure

	Convergence Rate	Iteration Complexity
linear	$O(\mu^T)$ ($\mu < 1$)	$O\left(\log\left(\frac{1}{\epsilon}\right)\right)$
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Theoretically, we consider

$$O(\mu^T) \prec O\left(\frac{1}{T^2}\right) \prec O\left(\frac{1}{T}\right) \prec O\left(\frac{1}{\sqrt{T}}\right)$$

$$\log\left(\frac{1}{\epsilon}\right) \prec \frac{1}{\sqrt{\epsilon}} \prec \frac{1}{\epsilon} \prec \frac{1}{\epsilon^2}$$

Non-smooth V.S. Smooth

- Non-smooth $\ell(z)$

- **hinge loss**: $\ell(\mathbf{w}^\top \mathbf{x}, y) = \max(0, 1 - y\mathbf{w}^\top \mathbf{x})$
- **absolute loss**: $\ell(\mathbf{w}^\top \mathbf{x}, y) = |\mathbf{w}^\top \mathbf{x} - y|$

- Smooth $\ell(z)$

- **squared hinge loss**: $\ell(\mathbf{w}^\top \mathbf{x}, y) = \max(0, 1 - y\mathbf{w}^\top \mathbf{x})^2$
- **logistic loss**: $\ell(\mathbf{w}^\top \mathbf{x}, y) = \log(1 + \exp(-y\mathbf{w}^\top \mathbf{x}))$
- **square loss**: $\ell(\mathbf{w}^\top \mathbf{x}, y) = (\mathbf{w}^\top \mathbf{x} - y)^2$

Strong convex V.S. Non-strongly convex

- λ -strongly convex $R(\mathbf{w})$
 - l_2 regularizer: $\frac{\lambda}{2} \|\mathbf{w}\|_2^2$
 - Elastic net regularizer: $\tau \|\mathbf{w}\|_1 + \frac{\lambda}{2} \|\mathbf{w}\|_2^2$
- Non-strongly convex $R(\mathbf{w})$
 - unregularized problem: $R(\mathbf{w}) \equiv 0$
 - l_1 regularizer: $\tau \|\mathbf{w}\|_1$

Gradient Method in Machine Learning

$$F(\mathbf{w}) = \frac{1}{n} \sum_{i=1}^n \ell(\mathbf{w}^\top \mathbf{x}_i, y_i) + \frac{\lambda}{2} \|\mathbf{w}\|_2^2$$

- Suppose $\ell(z)$ is smooth
- Full gradient: $\nabla F(\mathbf{w}) = \frac{1}{n} \sum_{i=1}^n \nabla \ell(\mathbf{w}^\top \mathbf{x}_i, y_i) + \lambda \mathbf{w}$
- Per-iteration cost: $O(nd)$

Gradient Descent

$$\mathbf{w}_t = \mathbf{w}_{t-1} - \gamma_t \nabla F(\mathbf{w}_{t-1})$$

Gradient Method in Machine Learning

$$F(\mathbf{w}) = \frac{1}{n} \sum_{i=1}^n \ell(\mathbf{w}^\top \mathbf{x}_i, y_i) + \frac{\lambda}{2} \|\mathbf{w}\|_2^2$$

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- Per-iteration cost: $O(nd)$

Gradient Descent

step size

$$\mathbf{w}_t = \mathbf{w}_{t-1} - \gamma_t \nabla F(\mathbf{w}_{t-1})$$

Gradient Method in Machine Learning

$$F(\mathbf{w}) = \frac{1}{n} \sum_{i=1}^n \ell(\mathbf{w}^\top \mathbf{x}_i, y_i) + \frac{\lambda}{2} \|\mathbf{w}\|_2^2$$

- If $\lambda = 0$: $R(\mathbf{w})$ is non-strongly convex
- Iteration complexity $O(\frac{1}{\epsilon})$

- If $\lambda > 0$: $R(\mathbf{w})$ is λ -strongly convex
- Iteration complexity $O(\frac{1}{\lambda} \log(\frac{1}{\epsilon}))$

Accelerated Gradient Method

Accelerated Gradient Descent

$$\mathbf{w}_t = \mathbf{v}_{t-1} - \gamma_t \nabla F(\mathbf{v}_{t-1})$$

$$\mathbf{v}_t = \mathbf{w}_t + \eta_t (\mathbf{w}_t - \mathbf{w}_{t-1})$$

- \mathbf{w}_t is the output and \mathbf{v}_t is an auxiliary sequence.

Accelerated Gradient Method

Accelerated Gradient Descent

$$\mathbf{w}_t = \mathbf{v}_{t-1} - \gamma_t \nabla F(\mathbf{v}_{t-1})$$

Momentum
Step

$$\mathbf{v}_t = \mathbf{w}_t + \eta_t (\mathbf{w}_t - \mathbf{w}_{t-1})$$

- \mathbf{w}_t is the output and \mathbf{v}_t is an auxiliary sequence.

Accelerated Gradient Method

$$F(\mathbf{w}) = \frac{1}{n} \sum_{i=1}^n \ell(\mathbf{w}^\top \mathbf{x}_i, y_i) + \frac{\lambda}{2} \|\mathbf{w}\|_2^2$$

- If $\lambda = 0$: $R(\mathbf{w})$ is non-strongly convex
- Iteration complexity $O(\frac{1}{\sqrt{\epsilon}})$, better than $O(\frac{1}{\epsilon})$
- If $\lambda > 0$: $R(\mathbf{w})$ is λ -strongly convex
- Iteration complexity $O(\frac{1}{\sqrt{\lambda}} \log(\frac{1}{\epsilon}))$, better than $O(\frac{1}{\lambda} \log(\frac{1}{\epsilon}))$ for small λ

Deal with ℓ_1 regularizer

Consider a more general case

$$\min_{\mathbf{w} \in \mathbb{R}^d} F(\mathbf{w}) = \frac{1}{n} \sum_{i=1}^n \ell(\mathbf{w}^\top \mathbf{x}_i, y_i) + \underbrace{R'(\mathbf{w}) + \tau \|\mathbf{w}\|_1}_{R(\mathbf{w})}$$

- $R(\mathbf{w}) = R'(\mathbf{w}) + \tau \|\mathbf{w}\|_1$
- $R'(\mathbf{w})$: λ -strongly convex and smooth

Deal with ℓ_1 regularizer

Consider a more general case

$$\min_{\mathbf{w} \in \mathbb{R}^d} F(\mathbf{w}) = \underbrace{\frac{1}{n} \sum_{i=1}^n \ell(\mathbf{w}^\top \mathbf{x}_i, y_i) + R'(\mathbf{w})}_{F'(\mathbf{w})} + \tau \|\mathbf{w}\|_1$$

- $R(\mathbf{w}) = R'(\mathbf{w}) + \tau \|\mathbf{w}\|_1$
- $R'(\mathbf{w})$: λ -strongly convex and smooth

Deal with ℓ_1 regularizer

Accelerated Gradient Descent

$$\mathbf{w}_t = \arg \min_{\mathbf{w} \in \mathbb{R}^d} \nabla F'(\mathbf{v}_{t-1})^\top \mathbf{w} + \frac{1}{2\gamma_t} \|\mathbf{w} - \mathbf{v}_{t-1}\|_2^2 + \tau \|\mathbf{w}\|_1$$

$$\mathbf{v}_t = \mathbf{w}_t + \eta_t (\mathbf{w}_t - \mathbf{w}_{t-1})$$

- Proximal mapping has close-form solution: Soft-thresholding
- Iteration complexity and runtime remain unchanged.

Deal with ℓ_1 regularizer

Proximal
mapping

Accelerated Gradient Descent

$$\mathbf{w}_t = \arg \min_{\mathbf{w} \in \mathbb{R}^d} \nabla F'(\mathbf{v}_{t-1})^\top \mathbf{w} + \frac{1}{2\gamma_t} \|\mathbf{w} - \mathbf{v}_{t-1}\|_2^2 + \tau \|\mathbf{w}\|_1$$

$$\mathbf{v}_t = \mathbf{w}_t + \eta_t (\mathbf{w}_t - \mathbf{w}_{t-1})$$

- Proximal mapping has close-form solution: Soft-thresholding
- Iteration complexity and runtime remain unchanged.

Sub-Gradient Method in Machine Learning

$$F(\mathbf{w}) = \frac{1}{n} \sum_{i=1}^n \ell(\mathbf{w}^\top \mathbf{x}_i, y_i) + \frac{\lambda}{2} \|\mathbf{w}\|_2^2$$

- Suppose $\ell(z)$ is non-smooth
- Full sub-gradient: $\partial F(\mathbf{w}) = \frac{1}{n} \sum_{i=1}^n \partial \ell(\mathbf{w}^\top \mathbf{x}_i, y_i) + \lambda \mathbf{w}$

Sub-Gradient Descent

$$\mathbf{w}_t = \mathbf{w}_{t-1} - \gamma_t \partial F(\mathbf{w}_{t-1})$$

Sub-Gradient Method in Machine Learning

$$F(\mathbf{w}) = \frac{1}{n} \sum_{i=1}^n \ell(\mathbf{w}^\top \mathbf{x}_i, y_i) + \frac{\lambda}{2} \|\mathbf{w}\|_2^2$$

- Suppose $\ell(z)$ is non-smooth
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Sub-Gradient Descent

$$\mathbf{w}_t = \mathbf{w}_{t-1} - \gamma_t \partial F(\mathbf{w}_{t-1})$$

Sub-Gradient Method

$$F(\mathbf{w}) = \frac{1}{n} \sum_{i=1}^n \ell(\mathbf{w}^\top \mathbf{x}_i, y_i) + \frac{\lambda}{2} \|\mathbf{w}\|_2^2$$

- If $\lambda = 0$: $R(\mathbf{w})$ is non-strongly convex
- Iteration complexity $O\left(\frac{1}{\epsilon^2}\right)$
- If $\lambda > 0$: $R(\mathbf{w})$ is λ -strongly convex
- Iteration complexity $O\left(\frac{1}{\lambda\epsilon}\right)$
- No efficient acceleration scheme in general

Problem Classes and Iteration Complexity

$$\min_{\mathbf{w} \in \mathbb{R}^d} \frac{1}{n} \sum_{i=1}^n \ell(\mathbf{w}^\top \mathbf{x}_i, y_i) + R(\mathbf{w})$$

- Iteration complexity

		$\ell(z) \equiv \ell(z, y)$	
		Non-smooth	Smooth
$R(\mathbf{w})$	Non-strongly convex	$O\left(\frac{1}{\epsilon^2}\right)$	$O\left(\frac{1}{\sqrt{\epsilon}}\right)$
	λ -strongly convex	$O\left(\frac{1}{\lambda\epsilon}\right)$	$O\left(\frac{1}{\sqrt{\lambda}} \log\left(\frac{1}{\epsilon}\right)\right)$

- Per-iteration cost: $O(nd)$, too high if n or d are large.

Outline

- 2 Optimization
 - (Sub)Gradient Methods
 - Stochastic Optimization Algorithms for Big Data
 - Stochastic Optimization
 - Distributed Optimization

Stochastic First-Order Method by Data Sampling

- Stochastic Gradient Descent (SGD)
- Stochastic Variance Reduced Gradient (SVRG)
- Stochastic Average Gradient Algorithm (SAGA)
- Stochastic Dual Coordinate Ascent (SDCA)
- Accelerated Proximal Coordinate Gradient (APCG)

Assumption: $\|x_i\| \leq 1$ for any i

Basic SGD (Nemirovski & Yudin (1978))

$$F(\mathbf{w}) = \frac{1}{n} \sum_{i=1}^n \ell(\mathbf{w}^\top \mathbf{x}_i, y_i) + \frac{\lambda}{2} \|\mathbf{w}\|_2^2$$

- **Full** sub-gradient: $\partial F(\mathbf{w}) = \frac{1}{n} \sum_{i=1}^n \partial \ell(\mathbf{w}^\top \mathbf{x}_i, y_i) + \lambda \mathbf{w}$
- Randomly sample $i \in \{1, \dots, n\}$
- **Stochastic** sub-gradient: $\partial \ell(\mathbf{w}^\top \mathbf{x}_i, y_i) + \lambda \mathbf{w}$

$$\mathbb{E}_i[\partial \ell(\mathbf{w}^\top \mathbf{x}_i, y_i) + \lambda \mathbf{w}] = \partial F(\mathbf{w})$$

Basic SGD (Nemirovski & Yudin (1978))

Applicable in all settings!

$$\min_{\mathbf{w} \in \mathbb{R}^d} F(\mathbf{w}) = \frac{1}{n} \sum_{i=1}^n \ell(\mathbf{w}^\top \mathbf{x}_i, y_i) + \frac{\lambda}{2} \|\mathbf{w}\|_2^2$$

sample: $i_t \in \{1, \dots, n\}$

update: $\mathbf{w}_t = \mathbf{w}_{t-1} - \gamma_t \left(\partial \ell(\mathbf{w}_{t-1}^\top \mathbf{x}_{i_t}, y_{i_t}) + \lambda \mathbf{w}_{t-1} \right)$

output: $\bar{\mathbf{w}}_T = \frac{1}{T} \sum_{t=1}^T \mathbf{w}_t$

Basic SGD (Nemirovski & Yudin (1978))

Applicable in all settings!

$$\min_{\mathbf{w} \in \mathbb{R}^d} F(\mathbf{w}) = \frac{1}{n} \sum_{i=1}^n \ell(\mathbf{w}^\top \mathbf{x}_i, y_i) + \frac{\lambda}{2} \|\mathbf{w}\|_2^2$$

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Basic SGD (Nemirovski & Yudin (1978))

$$F(\mathbf{w}) = \frac{1}{n} \sum_{i=1}^n \ell(\mathbf{w}^\top \mathbf{x}_i, y_i) + \frac{\lambda}{2} \|\mathbf{w}\|_2^2$$

- If $\lambda = 0$: $R(\mathbf{w})$ is non-strongly convex
- Iteration complexity $O\left(\frac{1}{\epsilon^2}\right)$
- If $\lambda > 0$: $R(\mathbf{w})$ is λ -strongly convex
- Iteration complexity $O\left(\frac{1}{\lambda\epsilon}\right)$
- Exactly the same as sub-gradient descent!

Total Runtime

- Per-iteration cost: $O(d)$
- Much lower than full gradient method
- e.g. hinge loss (SVM)

$$\text{stochastic gradient: } \partial \ell(\mathbf{w}^\top \mathbf{x}_{i_t}, y_{i_t}) = \begin{cases} -y_{i_t} \mathbf{x}_{i_t}, & 1 - y_{i_t} \mathbf{w}^\top \mathbf{x}_{i_t} > 0 \\ 0, & \text{otherwise} \end{cases}$$

Total Runtime

$$\min_{\mathbf{w} \in \mathbb{R}^d} \frac{1}{n} \sum_{i=1}^n \ell(\mathbf{w}^\top \mathbf{x}_i, y_i) + R(\mathbf{w})$$

- Iteration complexity

		$\ell(z) \equiv \ell(z, y)$	
		Non-smooth	Smooth
$R(\mathbf{w})$	Non-strongly convex	$O\left(\frac{1}{\epsilon^2}\right)$	$O\left(\frac{1}{\epsilon^2}\right)$
	λ -strongly convex	$O\left(\frac{1}{\lambda\epsilon}\right)$	$O\left(\frac{1}{\lambda\epsilon}\right)$

- For SGD, only strongly convexity helps but the smoothness does not make any difference!

Full Gradient V.S. Stochastic Gradient

- Full gradient method needs fewer iterations
- Stochastic gradient method has lower cost per iteration

- For small ϵ , use full gradient
- Satisfied with large ϵ , use stochastic gradient

- Full gradient can be accelerated
- Stochastic gradient cannot

- Full gradient's iterations complexity depends on smoothness and strong convexity
- Stochastic gradient's iteration complexity only depends on strong convexity

SVRG (Johnson & Zhang, 2013; Zhang et al., 2013; Xiao & Zhang, 2014)

$$\min_{\mathbf{w} \in \mathbb{R}^d} F(\mathbf{w}) = \frac{1}{n} \sum_{i=1}^n \ell(\mathbf{w}^\top \mathbf{x}_i, y_i) + \frac{\lambda}{2} \|\mathbf{w}\|_2^2$$

- Applicable when $\ell(z)$ is smooth and $R(\mathbf{w})$ is λ -strongly convex
- Stochastic gradient:

$$g_{i_t}(\mathbf{w}) = \nabla \ell(\mathbf{w}^\top \mathbf{x}_{i_t}, y_{i_t}) + \lambda \mathbf{w}$$

- $\mathbb{E}_{i_t} [g_{i_t}(\mathbf{w})] = \nabla F(\mathbf{w})$ but...
- $\text{Var} [g_{i_t}(\mathbf{w})] \neq 0$ even if $\mathbf{w} = \mathbf{w}^*$

SVRG (Johnson & Zhang, 2013; Zhang et al., 2013; Xiao & Zhang, 2014)

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- $\text{Var} [g_{i_t}(\mathbf{w})] \neq 0$ even if $\mathbf{w} = \mathbf{w}^*$

SVRG (Johnson & Zhang, 2013; Zhang et al., 2013; Xiao & Zhang, 2014)

- Compute the full gradient at a **reference point** $\tilde{\mathbf{w}}$

$$\nabla F(\tilde{\mathbf{w}}) = \frac{1}{n} \sum_{i=1}^n \nabla \ell(\tilde{\mathbf{w}}^T \mathbf{x}_i, y_i) + \lambda \tilde{\mathbf{w}}$$

- **Stochastic variance reduced gradient:**

$$\tilde{g}_{i_t}(\mathbf{w}) = \nabla F(\tilde{\mathbf{w}}) - g_{i_t}(\tilde{\mathbf{w}}) + g_{i_t}(\mathbf{w})$$

- $\mathbb{E}_{i_t} [\tilde{g}_{i_t}(\mathbf{w})] = \nabla F(\mathbf{w})$
- $\text{Var} [\tilde{g}_{i_t}(\mathbf{w})] \rightarrow 0$ as $\tilde{\mathbf{w}}, \mathbf{w} \rightarrow \mathbf{w}^*$

SVRG (Johnson & Zhang, 2013; Zhang et al., 2013; Xiao & Zhang, 2014)

- At optimal solution \mathbf{w}^* : $\nabla F(\mathbf{w}^*) = \mathbf{0}$
- It does not mean

$$g_{i_t}(\mathbf{w}) \longrightarrow \mathbf{0}$$

as $\mathbf{w} \rightarrow \mathbf{w}^*$

- However, we have

$$\tilde{g}_{i_t}(\mathbf{w}) = \nabla F(\tilde{\mathbf{w}}) - g_{i_t}(\tilde{\mathbf{w}}) + g_{i_t}(\mathbf{w}) \longrightarrow \mathbf{0}$$

as $\tilde{\mathbf{w}}, \mathbf{w} \rightarrow \mathbf{w}^*$

SVRG (Johnson & Zhang, 2013; Zhang et al., 2013; Xiao & Zhang, 2014)

Iterate $s = 1, \dots, T - 1$

Let $\mathbf{w}_0 = \tilde{\mathbf{w}}_s$ and compute $\nabla F(\tilde{\mathbf{w}}_s)$

Iterate $t = 1, \dots, K$

$$\tilde{g}_{i_t}(\mathbf{w}_{t-1}) = \nabla F(\tilde{\mathbf{w}}_s) - g_{i_t}(\tilde{\mathbf{w}}_s) + g_{i_t}(\mathbf{w}_{t-1})$$

$$\mathbf{w}_t = \mathbf{w}_{t-1} - \gamma_t \tilde{g}_{i_t}(\mathbf{w}_{t-1})$$

$$\tilde{\mathbf{w}}_{s+1} = \frac{1}{K} \sum_{t=1}^K \mathbf{w}_t$$

output: $\tilde{\mathbf{w}}_T$

- $K = O\left(\frac{1}{\lambda}\right)$

SVRG (Johnson & Zhang, 2013; Zhang et al., 2013; Xiao & Zhang, 2014)

- Per-iteration cost: $O\left(d\left(n + \frac{1}{\lambda}\right)\right)$
- Iteration complexity

		$\ell(z) \equiv \ell(z, y)$	
		Non-smooth	Smooth
$R(\mathbf{w})$	Non-strongly convex	N.A.	N.A.
	λ -strongly convex	N.A.	$O\left(\log\left(\frac{1}{\epsilon}\right)\right)$

- Total Runtime: $O\left(d\left(n + \frac{1}{\lambda}\right) \log\left(\frac{1}{\epsilon}\right)\right)$
- Use proximal mapping for ℓ_1 regularizer

SVRG (Johnson & Zhang, 2013; Zhang et al., 2013; Xiao & Zhang, 2014)

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- Use proximal mapping for ℓ_1 regularizer

SAGA (Defazio et al. (2014))

$$\min_{\mathbf{w} \in \mathbb{R}^d} F(\mathbf{w}) = \frac{1}{n} \sum_{i=1}^n \ell(\mathbf{w}^\top \mathbf{x}_i, y_i) + \frac{\lambda}{2} \|\mathbf{w}\|_2^2$$

- A new version of SAG (Roux et al. (2012))
- Applicable when $\ell(z)$ is smooth
- Strong convexity is not required.

SAGA (Defazio et al. (2014))

- SAGA also reduces the variance of stochastic gradient but with a different technique
- SVRG uses gradients at the same point $\tilde{\mathbf{w}}$

$$\begin{aligned}\tilde{g}_{i_t}(\mathbf{w}) &= \nabla F(\tilde{\mathbf{w}}) - g_{i_t}(\tilde{\mathbf{w}}) + g_{i_t}(\mathbf{w}) \\ \nabla F(\tilde{\mathbf{w}}) &= \frac{1}{n} \sum_{i=1}^n \nabla \ell(\tilde{\mathbf{w}}^T \mathbf{x}_i, y_i) + \lambda \tilde{\mathbf{w}}\end{aligned}$$

- SAGA uses gradients at different point $\{\tilde{\mathbf{w}}_1, \tilde{\mathbf{w}}_2, \dots, \tilde{\mathbf{w}}_n\}$

$$\begin{aligned}\tilde{g}_{i_t}(\mathbf{w}) &= G - g_{i_t}(\tilde{\mathbf{w}}_{i_t}) + g_{i_t}(\mathbf{w}) \\ G &= \frac{1}{n} \sum_{i=1}^n \nabla \ell(\tilde{\mathbf{w}}_i^T \mathbf{x}_i, y_i) + \lambda \tilde{\mathbf{w}}_{i_t}\end{aligned}$$

SAGA (Defazio et al. (2014))

- SAGA also reduces the variance of stochastic gradient but with a different technique
- SVRG uses gradients at the same point $\tilde{\mathbf{w}}$

$$\tilde{g}_{it}(\mathbf{w}) = \nabla F(\tilde{\mathbf{w}}) - g_{it}(\tilde{\mathbf{w}}) + g_{it}(\mathbf{w})$$

$$\nabla F(\tilde{\mathbf{w}}) = \frac{1}{n} \sum_{i=1}^n \nabla \ell(\tilde{\mathbf{w}}^T \mathbf{x}_i, y_i) + \lambda \tilde{\mathbf{w}}$$

- SAGA uses gradients at different point $\{\tilde{\mathbf{w}}_1, \tilde{\mathbf{w}}_2, \dots, \tilde{\mathbf{w}}_n\}$

Average Gradient

$$\tilde{g}_{it}(\mathbf{w}) = G - g_{it}(\tilde{\mathbf{w}}_{it}) + g_{it}(\mathbf{w})$$

$$G = \frac{1}{n} \sum_{i=1}^n \nabla \ell(\tilde{\mathbf{w}}_i^T \mathbf{x}_i, y_i) + \lambda \tilde{\mathbf{w}}_{it}$$

SAGA (Defazio et al. (2014))

- Initialize average gradient G_0 :

$$G_0 = \frac{1}{n} \sum_{i=1}^n g_i, \quad g_i = \nabla \ell(\mathbf{w}_0^\top \mathbf{x}_i, y_i) + \lambda \mathbf{w}_0$$

- stochastic variance reduced gradient:

$$\begin{aligned} \tilde{g}_{i_t}(\mathbf{w}_{t-1}) &= G_{t-1} - g_{i_t} + \left(\nabla \ell(\mathbf{w}_{t-1}^\top \mathbf{x}_{i_t}, y_{i_t}) + \lambda \mathbf{w}_{t-1} \right) \\ \mathbf{w}_t &= \mathbf{w}_{t-1} - \gamma_t \tilde{g}_{i_t}(\mathbf{w}_{t-1}) \end{aligned}$$

- Update average gradient

$$G_t = \frac{1}{n} \sum_{i=1}^n g_i, \quad g_{i_t} = \nabla \ell(\mathbf{w}_{t-1}^\top \mathbf{x}_{i_t}, y_{i_t}) + \lambda \mathbf{w}_{t-1}$$

SAGA (Defazio et al. (2014))

- Initialize average gradient G_0 :

$$G_0 = \frac{1}{n} \sum_{i=1}^n g_i, \quad g_i = \nabla \ell(\mathbf{w}_0^\top \mathbf{x}_i, y_i) + \lambda \mathbf{w}_0$$

- stochastic variance reduced gradient:

$$\begin{aligned} \tilde{g}_{i_t}(\mathbf{w}_{t-1}) &= G_{t-1} - g_{i_t} + \left(\nabla \ell(\mathbf{w}_{t-1}^\top \mathbf{x}_{i_t}, y_{i_t}) + \lambda \mathbf{w}_{t-1} \right) \\ \mathbf{w}_t &= \mathbf{w}_{t-1} - \gamma_t \tilde{g}_{i_t}(\mathbf{w}_{t-1}) \end{aligned}$$

- Update average gradient

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SAGA: efficient update of averaged gradient

- G_t and G_{t-1} only differs in g_i for $i = i_t$
- Before we update g_i , we update

$$G_t = \frac{1}{n} \sum_{i=1}^n g_i = G_{t-1} - \frac{1}{n} g_{i_t} + \frac{1}{n} \left(\nabla \ell(\mathbf{w}_{t-1}^\top \mathbf{x}_{i_t}, y_{i_t}) + \lambda \mathbf{w}_{t-1} \right)$$

- computation cost: $O(d)$
- To implemente SAGA, we have to store and update all: g_1, g_2, \dots, g_n
- Require extra memory space $O(nd)$

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SAGA (Defazio et al. (2014))

- Per-iteration cost: $O(d)$
- Iteration complexity

		$\ell(z) \equiv \ell(z, y)$	
		Non-smooth	Smooth
$R(\mathbf{w})$	Non-strongly convex	N.A.	$O\left(\frac{n}{\epsilon}\right)$
	λ -strongly convex	N.A.	$O\left(\left(n + \frac{1}{\lambda}\right) \log\left(\frac{1}{\epsilon}\right)\right)$

- Total Runtime (strongly convex): $O\left(d\left(n + \frac{1}{\lambda}\right) \log\left(\frac{1}{\epsilon}\right)\right)$. Same as SVRG!
- Use proximal mapping for ℓ_1 regularizer

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Compare the Runtime of SGD and SVRG/SAGA

- Smooth but non-strongly convex:
 - SGD: $O\left(\frac{d}{\epsilon^2}\right)$
 - SAGA: $O\left(\frac{dn}{\epsilon}\right)$
- Smooth and strongly convex:
 - SGD: $O\left(\frac{d}{\lambda\epsilon}\right)$
 - SVRG/SAGA: $O\left(d\left(n + \frac{1}{\lambda}\right)\log\left(\frac{1}{\epsilon}\right)\right)$
- For small ϵ , use SVRG/SAGA
- Satisfied with large ϵ , use SGD

Conjugate Duality

- Define $\ell_i(z) \equiv \ell(z, y_i)$
- Conjugate function: $\ell_i^*(\alpha) \iff \ell_i(z)$

$$\ell_i(z) = \max_{\alpha \in \mathbb{R}} [\alpha z - \ell^*(\alpha)], \quad \ell_i^*(\alpha) = \max_{z \in \mathbb{R}} [\alpha z - \ell(z)]$$

- E.g. hinge loss: $\ell_i(z) = \max(0, 1 - y_i z)$

$$\ell_i^*(\alpha) = \begin{cases} \alpha y_i & \text{if } -1 \leq \alpha y_i \leq 0 \\ +\infty & \text{otherwise} \end{cases}$$

- E.g. square hinge loss: $\ell_i(z) = \max(0, 1 - y_i z)^2$

$$\ell_i^*(\alpha) = \begin{cases} \frac{\alpha^2}{4} + \alpha y_i & \text{if } \alpha y_i \leq 0 \\ +\infty & \text{otherwise} \end{cases}$$

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SDCA (Shalev-Shwartz & Zhang (2013))

- Stochastic Dual Coordinate Ascent (liblinear (Hsieh et al., 2008))
- Applicable when $R(\mathbf{w})$ is λ -strongly convex
- Smoothness is not required
- From Primal problem to Dual problem:

$$\begin{aligned}
 & \min_{\mathbf{w}} \frac{1}{n} \sum_{i=1}^n \ell(\underbrace{\mathbf{w}^\top \mathbf{x}_i}_z, y_i) + \frac{\lambda}{2} \|\mathbf{w}\|_2^2 \\
 &= \min_{\mathbf{w}} \frac{1}{n} \sum_{i=1}^n \max_{\alpha_i \in \mathbb{R}} \left[\alpha_i (\mathbf{w}^\top \mathbf{x}_i) - \ell_i^*(\alpha_i) \right] + \frac{\lambda}{2} \|\mathbf{w}\|_2^2 \\
 &= \max_{\alpha \in \mathbb{R}^n} \frac{1}{n} \sum_{i=1}^n -\ell_i^*(\alpha_i) - \frac{\lambda}{2} \left\| \frac{1}{\lambda n} \sum_{i=1}^n \alpha_i \mathbf{x}_i \right\|_2^2
 \end{aligned}$$

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 \end{aligned}$$

SDCA (Shalev-Shwartz & Zhang (2013))

- Solve **Dual Problem**:

$$\max_{\alpha \in \mathbb{R}^n} \frac{1}{n} \sum_{i=1}^n -\ell_i^*(\alpha_i) - \frac{\lambda}{2} \left\| \frac{1}{\lambda n} \sum_{i=1}^n \alpha_i \mathbf{x}_i \right\|_2^2$$

- Sample $i_t \in \{1, \dots, n\}$. Optimize α_{i_t} while fixing others

SDCA (Shalev-Shwartz & Zhang (2013))

- Maintain a **primal solution**: $\mathbf{w}_t = \frac{1}{\lambda n} \sum_{i=1}^n \alpha_i^t \mathbf{x}_i$
- Change variable $\alpha_i \rightarrow \Delta \alpha_i$

$$\begin{aligned} & \max_{\Delta \alpha \in \mathbb{R}^n} \frac{1}{n} \sum_{i=1}^n -\ell_i^*(\alpha_i^t + \Delta \alpha_i) - \frac{\lambda}{2} \left\| \frac{1}{\lambda n} \left(\sum_{i=1}^n \alpha_i^t \mathbf{x}_i + \sum_{i=1}^n \Delta \alpha_i \mathbf{x}_i \right) \right\|_2^2 \\ \iff & \max_{\Delta \alpha \in \mathbb{R}^n} \frac{1}{n} \sum_{i=1}^n -\ell_i^*(\alpha_i^t + \Delta \alpha_i) - \frac{\lambda}{2} \left\| \mathbf{w}_t + \frac{1}{\lambda n} \sum_{i=1}^n \Delta \alpha_i \mathbf{x}_i \right\|_2^2 \end{aligned}$$

SDCA (Shalev-Shwartz & Zhang (2013))

Dual Coordinate Updates

$$\begin{aligned}\Delta\alpha_{i_t} &= \max_{\Delta\alpha_{i_t} \in \mathbb{R}^n} -\frac{1}{n} \ell_{i_t}^*(-\alpha_{i_t}^t - \Delta\alpha_{i_t}) - \frac{\lambda}{2} \left\| \mathbf{w}_t + \frac{1}{\lambda n} \Delta\alpha_{i_t} \mathbf{x}_{i_t} \right\|_2^2 \\ \alpha_{i_t}^{t+1} &= \alpha_{i_t}^t + \Delta\alpha_{i_t} \\ \mathbf{w}_{t+1} &= \mathbf{w}_t + \frac{1}{\lambda n} \Delta\alpha_{i_t} \mathbf{x}_{i_t}\end{aligned}$$

SDCA updates

- Close-form solution for $\Delta\alpha_j$: hinge loss, squared hinge loss, absolute loss and square loss (Shalev-Shwartz & Zhang (2013))
- e.g. square loss

$$\Delta\alpha_j = \frac{y_i - \mathbf{w}_t^\top \mathbf{x}_i - \alpha_j^t}{1 + \|\mathbf{x}_i\|_2^2 / (\lambda n)}$$

- Per-iteration cost: $O(d)$
- **Approximate solution**: logistic loss (Shalev-Shwartz & Zhang (2013))

SDCA

- Iteration complexity

		$\ell(z) \equiv \ell(z, y)$	
		Non-smooth	Smooth
$R(\mathbf{w})$	Non-strongly convex	N.A.	N.A.
	λ -strongly convex	$O\left(n + \frac{1}{\lambda\epsilon}\right)$	$O\left(\left(n + \frac{1}{\lambda}\right) \log\left(\frac{1}{\epsilon}\right)\right)$

- Total Runtime (smooth loss): $O\left(d\left(n + \frac{1}{\lambda}\right) \log\left(\frac{1}{\epsilon}\right)\right)$. The same as SVRG and SAGA!

SDCA

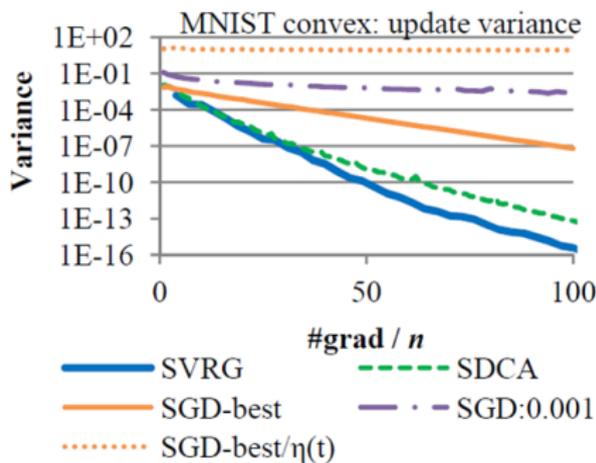
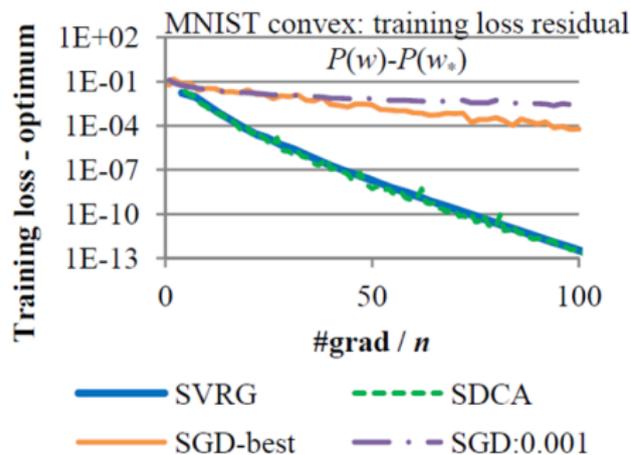
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- Total Runtime (smooth loss): $O\left(d\left(n + \frac{1}{\lambda}\right) \log\left(\frac{1}{\epsilon}\right)\right)$. **The same as SVRG and SAGA!**

SVRG V.S. SDCA V.S. SGD

- ℓ_2 -regularized logistic regression with $\lambda = 10^{-4}$
- MNIST data
- Johnson & Zhang (2013)



APCG (Lin et al. (2014))

- Recall the acceleration scheme for full gradient method
 - Auxiliary sequence (β^t)
 - Momentum step
- Maintain a **primal solution**: $\mathbf{w}_t = \frac{1}{\lambda n} \sum_{i=1}^n \beta_i^t \mathbf{x}_i$

Dual Coordinate Updates

$$\Delta \beta_{i_t} = \max_{\Delta \beta_{i_t} \in \mathbb{R}^n} -\frac{1}{n} \ell_{i_t}^*(-\beta_{i_t}^t - \Delta \beta_{i_t}) - \frac{\lambda}{2} \left\| \mathbf{w}_t + \frac{1}{\lambda n} \Delta \beta_{i_t} \mathbf{x}_{i_t} \right\|_2^2$$

$$\alpha_{i_t}^{t+1} = \beta_{i_t}^t + \Delta \beta_{i_t}$$

$$\beta^{t+1} = \alpha^{t+1} + \eta_t (\alpha^{t+1} - \alpha^t)$$

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Momentum Step

$$\alpha_{i_t}^{t+1} = \beta_{i_t}^t + \Delta \beta_{i_t}$$

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- Per-iteration cost: $O(d)$
- Iteration complexity

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		Non-smooth	Smooth
$R(\mathbf{w})$	Non-strongly convex	N.A.	N.A.
	λ -strongly convex	$O\left(n + \sqrt{\frac{n}{\lambda\epsilon}}\right)$	$O\left(\left(n + \sqrt{\frac{n}{\lambda}}\right) \log\left(\frac{1}{\epsilon}\right)\right)$

- Compared to SDCA, APCG has shorter runtime when λ is very small.

APCG V.S. SDCA

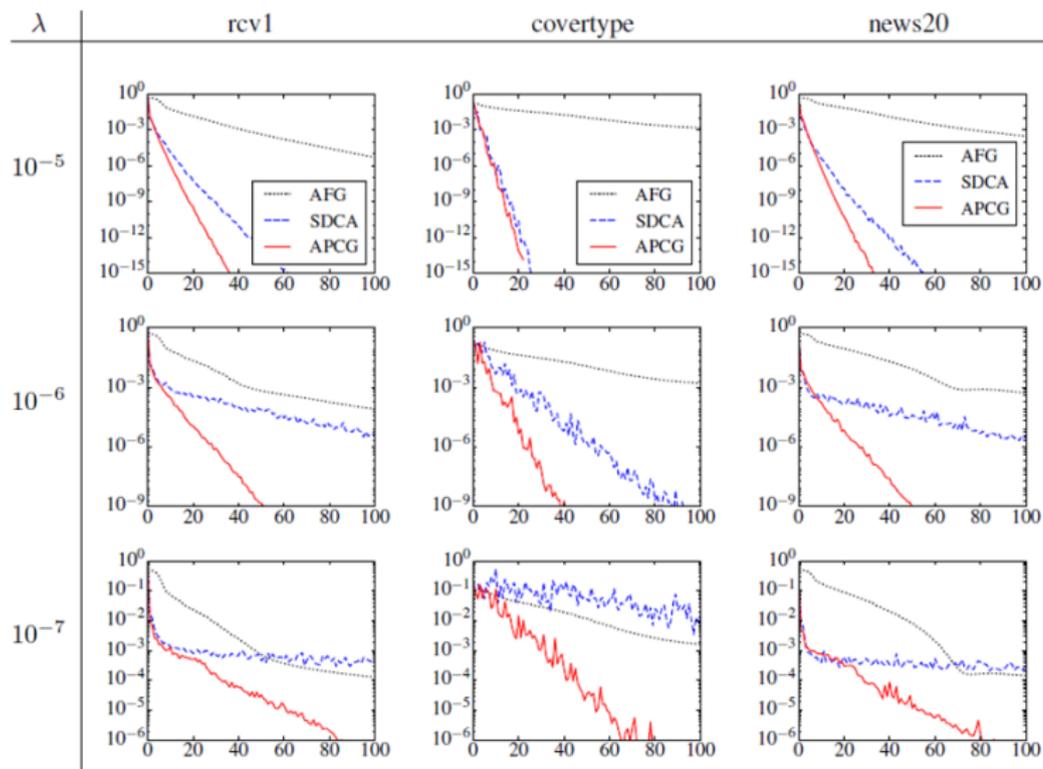
- squared hinge loss SVM
- real data

datasets	number of samples n	number of features d	sparsity
rcv1	20,242	47,236	0.16%
covtype	581,012	54	22%
news20	19,996	1,355,191	0.04%

- $F(\mathbf{w}_t) - F(\mathbf{w}^*)$ V.S. the number of passes of data

APCG V.S. SDCA

Lin et al. (2014)



For general $R(\mathbf{w})$

- Dual Problem:

$$\max_{\alpha \in \mathbb{R}^n} \frac{1}{n} \sum_{i=1}^n -\ell_i^*(\alpha_i) - R^* \left(\frac{1}{\lambda n} \sum_{i=1}^n \alpha_i \mathbf{x}_i \right)$$

- R^* is the conjugate of R
- Sample $i_t \in \{1, \dots, n\}$. Optimize α_{i_t} while fixing others
- Can be still updated in $O(d)$ in many cases ([Shalev-Shwartz & Zhang \(2013\)](#))
- Iteration complexity and runtime of SDCA and APCG remain unchanged.

APCG for primal problem

$$\min_{\mathbf{w} \in \mathbb{R}^d} F(\mathbf{w}) = \frac{1}{n} \sum_{i=1}^n \ell(\mathbf{w}^\top \mathbf{x}_i, y_i) + \frac{\lambda}{2} \|\mathbf{w}\|_2^2 + \tau \|\mathbf{w}\|_1$$

- Suppose $d \gg n$. Per-iteration cost $O(d)$ is too high
- Apply APCG to the primal instead of dual problem
- Sample over features instead of data
- Per-iteration cost becomes $O(n)$

APCG for primal problem

$$\min_{\mathbf{w} \in \mathbb{R}^d} F(\mathbf{w}) = \frac{1}{2} \|\mathbf{X}\mathbf{w} - \mathbf{y}\|_2^2 + \frac{\lambda}{2} \|\mathbf{w}\|_2^2 + \tau \|\mathbf{w}\|_1$$

$$\mathbf{X} = [\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_n]$$

- Full gradient: $\nabla F(\mathbf{w}) = \mathbf{X}^T(\mathbf{X}\mathbf{w} - \mathbf{y}) + \lambda\mathbf{w}$
- Partial gradient: $\nabla_i F(\mathbf{w}) = \mathbf{x}_i^T(\mathbf{X}\mathbf{w} - \mathbf{y}) + \lambda w_i$

Proximal Coordinate Gradient (PCG) (Nesterov (2012))

$$\mathbf{w}_i^t = \begin{cases} \arg \min_{w \in \mathbb{R}} \nabla_i F(\mathbf{w}^{t-1}) w_i + \frac{1}{2\gamma_t} (w_i - \mathbf{w}_i^{t-1})^2 + \tau |w_i| & \text{if } i = t_i \\ \mathbf{w}_i^{t-1} & \text{otherwise} \end{cases}$$

- $\nabla_i F(\mathbf{w}^t)$ can be updated in $O(n)$

APCG for primal problem

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Proximal
mapping

- $\nabla_i F(\mathbf{w}^t)$ can be updated in $O(n)$

APCG for primal problem

- APCG accelerates PCG using
 - Auxiliary sequence (\mathbf{v}^t)
 - Momentum step

APCG

$$\mathbf{w}_i^t = \begin{cases} \arg \min_{w_i \in \mathbb{R}} \nabla_i F(\mathbf{v}^{t-1}) w_i + \frac{1}{2\gamma_t} (w_i - \mathbf{v}_i^{t-1})^2 + \tau |w_i| & \text{if } i = t_i \\ \mathbf{w}_i^{t-1} & \text{otherwise} \end{cases}$$

$$\mathbf{v}^t = \mathbf{w}^t + \eta_t (\mathbf{w}^t - \mathbf{w}^{t-1})$$

APCG for primal problem

- Per-iteration cost: $O(n)$
- Iteration complexity

		$\ell(z) \equiv \ell(z, y)$	
		Non-smooth	Smooth
$R(\mathbf{w})$	Non-strongly convex	N.A.	$O\left(\frac{d}{\sqrt{\epsilon}}\right)$
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- $n \gg d$: Apply APCG to the dual problem.
- $d \gg n$: Apply APCG to the primal problem.

Which Algorithm to Use

- Satisfied with large ϵ : SGD
- For small ϵ :

		$\ell(z) \equiv \ell(z, y)$	
		Non-smooth	Smooth
$R(\mathbf{w})$	Non-strongly convex	SGD	SAGA
	λ -strongly convex	APCG	APCG

Summary

smooth	str-cvx	SGD	SAGA	SDCA	APCG
No	No	$\frac{1}{\epsilon^2}$	N.A.	N.A.	N.A.
Yes	No	$\frac{1}{\epsilon^2}$	$\frac{n}{\epsilon}$	N.A.	N.A.
No	Yes	$\frac{1}{\lambda\epsilon}$	N.A.	$n + \frac{1}{\epsilon}$	$n + \sqrt{\frac{n}{\lambda\epsilon}}$
Yes	Yes	$\frac{1}{\lambda\epsilon}$	$(n + \frac{1}{\lambda}) \log(\frac{1}{\epsilon})$	$(n + \frac{1}{\lambda}) \log(\frac{1}{\epsilon})$	$(n + \frac{1}{\sqrt{\lambda}}) \log(\frac{1}{\epsilon})$

Table : Per-iteration cost: $O(d)$

smooth	str-cvx	SVRG
No	No	N.A.
Yes	No	N.A.
No	Yes	N.A.
Yes	Yes	$\log(\frac{1}{\epsilon})$

Table : Per-iteration cost: $O(d(n + \frac{1}{\epsilon}))$

Summary

smooth	str-cvx	SGD	SAGA	SDCA	APCG
No	No	$\frac{1}{\epsilon^2}$	N.A.	N.A.	N.A.
Yes	No	$\frac{1}{\epsilon^2}$	$\frac{n}{\epsilon}$	N.A.	N.A.
No	Yes	$\frac{1}{\lambda\epsilon}$	N.A.	$n + \frac{1}{\epsilon}$	$n + \sqrt{\frac{n}{\lambda\epsilon}}$
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Summary

	SGD	SVRG	SAGA	SDCA	APCG
Memory	$O(d)$	$O(d)$	$O(dn)$	$O(d)$	$O(d)$
Parameters	γ_t	γ_t, K	γ_t	None	η_t
absolute					
hinge					
square					
squared hinge					
logistic					
$\lambda > 0$					
$\lambda = 0$					
Primal					
Dual					

Summary

	SGD	SVRG	SAGA	SDCA	APCG
Memory	$O(d)$	$O(d)$	$O(dn)$	$O(d)$	$O(d)$
Parameters	γ_t	γ_t, K	γ_t	None	η_t
absolute	✓	✗	✗	✓	✓
hinge	✓	✗	✗	✓	✓
square	✓	✓	✓	✓	✓
squared hinge	✓	✓	✓	✓	✓
logistic	✓	✓	✓	✓	✓
$\lambda > 0$					
$\lambda = 0$					
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Memory	$O(d)$	$O(d)$	$O(dn)$	$O(d)$	$O(d)$
Parameters	γ_t	γ_t, K	γ_t	None	η_t
absolute	✓	✗	✗	✓	✓
hinge	✓	✗	✗	✓	✓
square	✓	✓	✓	✓	✓
squared hinge	✓	✓	✓	✓	✓
logistic	✓	✓	✓	✓	✓
$\lambda > 0$	✓	✓	✓	✓	✓
$\lambda = 0$	✓	✓	✓	✗	✗
Primal					
Dual					

Summary

	SGD	SVRG	SAGA	SDCA	APCG
Memory	$O(d)$	$O(d)$	$O(dn)$	$O(d)$	$O(d)$
Parameters	γ_t	γ_t, K	γ_t	None	η_t
absolute	✓	✗	✗	✓	✓
hinge	✓	✗	✗	✓	✓
square	✓	✓	✓	✓	✓
squared hinge	✓	✓	✓	✓	✓
logistic	✓	✓	✓	✓	✓
$\lambda > 0$	✓	✓	✓	✓	✓
$\lambda = 0$	✓	✓	✓	✗	✗
Primal	✓	✓	✓	✗	✓
Dual	✗	✗	✗	✓	✓

Outline

- 2 Optimization
 - (Sub)Gradient Methods
 - Stochastic Optimization Algorithms for Big Data
 - Stochastic Optimization
 - Distributed Optimization

Big Data and Distributed Optimization

Distributed Optimization



- data distributed over a cluster of multiple machines
- moving to single machine suffers
 - **low** network bandwidth
 - **limited** disk or memory
- communication V.S. computation
 - **RAM** 100 nanoseconds
 - **standard network connection** 250,000 nanoseconds

Distributed Data

- N data points are partitioned and distributed to m machines
- $[\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_N] = S_1 \cup S_2 \cup \dots \cup S_m$
- Machine j only has access to S_j .
- W.L.O.G: $|S_j| = n = \frac{N}{m}$



A simple solution: Average Solution

- Global problem

$$\mathbf{w}^* = \arg \min_{\mathbf{w} \in \mathbb{R}^d} \left\{ F(\mathbf{w}) = \frac{1}{N} \sum_{i=1}^N \ell(\mathbf{w}^\top \mathbf{x}_i, y_i) + R(\mathbf{w}) \right\}$$

- Machine j solves a local problem

$$\mathbf{w}_j = \arg \min_{\mathbf{w} \in \mathbb{R}^d} \left\{ f_j(\mathbf{w}) = \frac{1}{n} \sum_{i \in S_j} \ell(\mathbf{w}^\top \mathbf{x}_i, y_i) + R(\mathbf{w}) \right\}$$



Center computes: $\hat{\mathbf{w}} = \frac{1}{m} \sum_{j=1}^m \mathbf{w}_j$, Issue: Will not converge to \mathbf{w}^*

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\mathbf{w}_1



\mathbf{w}_2



\mathbf{w}_3



\mathbf{w}_4



\mathbf{w}_5



\mathbf{w}_6

Center computes: $\hat{\mathbf{w}} = \frac{1}{m} \sum_{j=1}^m \mathbf{w}_j$, Issue: Will not converge to \mathbf{w}^*

Mini-Batch SGD: Average Stochastic Gradient

- Machine j sample $i_t \in S_j$ and construct a stochastic gradient

$$g_j(\mathbf{w}_{t-1}) = \partial \ell(\mathbf{w}_{t-1}^\top \mathbf{x}_{i_t}, y_{i_t}) + \partial R(\mathbf{w}_{t-1})$$



$$g_1(\mathbf{w}_{t-1}) \quad g_2(\mathbf{w}_{t-1}) \quad g_3(\mathbf{w}_{t-1}) \quad g_4(\mathbf{w}_{t-1}) \quad g_5(\mathbf{w}_{t-1}) \quad g_6(\mathbf{w}_{t-1})$$

Center computes: $\mathbf{w}_t = \mathbf{w}_{t-1} - \gamma_t \underbrace{\frac{1}{m} \sum_{j=1}^m g_j(\mathbf{w}_{t-1})}_{\text{Mini-batch SG}}$

Total Runtime

Single machine

- Total Runtime
= Per-iteration Cost \times Iteration Complexity

Distributed optimization

- Total Runtime
= (Communication Time Per-round + Local Runtime Per-round)
 \times Rounds of Communication

Mini-Batch SGD

Applicable in all settings!

- **Communication Time Per-round**: increase in m in a complicated way.
- **Local Runtime Per-round**: $O(1)$

Suppose $R(\mathbf{w})$ is λ -strongly convex

- **Rounds of Communication**: $O\left(\frac{1}{m\lambda\epsilon}\right)$

Suppose $R(\mathbf{w})$ is non-strongly convex

- **Rounds of Communication**: $O\left(\frac{1}{m\epsilon^2}\right)$

More machines reduce the rounds of communication but increase communication time per-round.

Mini-Batch SGD

Applicable in all settings!

- **Communication Time Per-round**: increase in m in a complicated way.
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More machines reduce the rounds of communication but increase communication time per-round.

Distributed SDCA (Yang, 2013; Ma et al., 2015)

- Only works when $R(\mathbf{w}) = \frac{\lambda}{2} \|\mathbf{w}\|_2^2$ with $\lambda > 0$. (No ℓ_1)
- Global dual problem

$$\max_{\alpha \in \mathbb{R}^N} \frac{1}{N} \sum_{i=1}^N -\ell_i^*(\alpha_i) - \frac{\lambda}{2} \left\| \frac{1}{\lambda N} \sum_{i=1}^N \alpha_i \mathbf{x}_i \right\|_2^2$$

- $\alpha = [\alpha_{S_1}, \alpha_{S_2}, \dots, \alpha_{S_m}]$
- Machine j solves a local dual problem only over α_{S_j}

$$\max_{\alpha_{S_j} \in \mathbb{R}^n} \frac{1}{N} \sum_{i \in S_j} -\ell_i^*(\alpha_i) - \frac{\lambda}{2} \left\| \frac{1}{\lambda N} \sum_{i=1}^N \alpha_i \mathbf{x}_i \right\|_2^2$$

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DisDCA (Yang, 2013), CoCoA+ (Ma et al., 2015)

- Center maintains a **primal solution**: $\mathbf{w}^t = \frac{1}{\lambda N} \sum_{i=1}^N \alpha_i^t \mathbf{x}_i$
- Change variable $\alpha_i \rightarrow \Delta \alpha_i$

$$\begin{aligned} & \max_{\Delta \alpha_{S_j} \in \mathbb{R}^n} \frac{1}{N} \sum_{i \in S_j} -\ell_i^*(\alpha_i^t + \Delta \alpha_i) - \frac{\lambda}{2} \left\| \frac{1}{\lambda N} \left(\sum_{i=1}^N \alpha_i^t \mathbf{x}_i + \sum_{i \in S_j} \Delta \alpha_i \mathbf{x}_i \right) \right\|_2^2 \\ \iff & \max_{\Delta \alpha_{S_j} \in \mathbb{R}^n} \frac{1}{N} \sum_{i \in S_j} -\ell_i^*(\alpha_i^t + \Delta \alpha_i) - \frac{\lambda}{2} \left\| \mathbf{w}^t + \frac{1}{\lambda N} \sum_{i \in S_j} \Delta \alpha_i \mathbf{x}_i \right\|_2^2 \end{aligned}$$

DisDCA (Yang, 2013), CoCoA+ (Ma et al., 2015)

- Machine j approximately solves

$$\Delta\alpha_{S_j}^t \approx \arg \max_{\Delta\alpha_{S_j} \in \mathbb{R}^n} \frac{1}{N} \sum_{i \in S_j} -\ell_i^*(\alpha_i^t + \Delta\alpha_j) - \frac{\lambda}{2} \left\| \mathbf{w}^t + \frac{1}{\lambda N} \sum_{i \in S_j} \Delta\alpha_j \mathbf{x}_i \right\|_2^2$$

$$\alpha_{S_j}^{t+1} = \alpha_{S_j}^t + \Delta\alpha_{S_j}^t, \quad \Delta\mathbf{w}_j^t = \frac{1}{\lambda N} \sum_{i \in S_j} \Delta\alpha_{S_j}^t \mathbf{x}_i$$



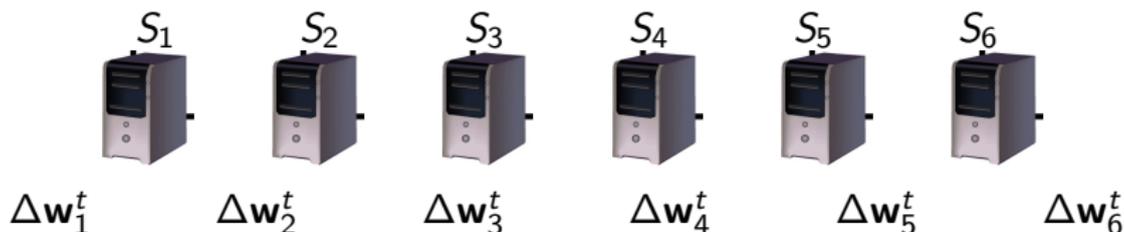
$$\text{Center computes: } \mathbf{w}^{t+1} = \mathbf{w}^t + \sum_{j=1}^m \Delta\mathbf{w}_j^t$$

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$$\Delta\alpha_{S_j}^t \approx \arg \max_{\Delta\alpha_{S_j} \in \mathbb{R}^n} \frac{1}{N} \sum_{i \in S_j} -\ell_i^*(\alpha_i^t + \Delta\alpha_j) - \frac{\lambda}{2} \left\| \mathbf{w}^t + \frac{1}{\lambda N} \sum_{i \in S_j} \Delta\alpha_j \mathbf{x}_i \right\|_2^2$$

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$$\text{Center computes: } \mathbf{w}^{t+1} = \mathbf{w}^t + \sum_{j=1}^m \Delta\mathbf{w}_j^t$$

CoCoA+ (Ma et al., 2015)

- Local objective value

$$\mathcal{G}_j(\Delta\alpha_{S_j}, \mathbf{w}^t) = \frac{1}{N} \sum_{i \in S_j} -\ell_i^*(\alpha_i^t + \Delta\alpha_i) - \frac{\lambda}{2} \left\| \mathbf{w}^t + \frac{1}{\lambda N} \sum_{i \in S_j} \Delta\alpha_i \mathbf{x}_i \right\|_2^2$$

- Solve $\Delta\alpha_{S_j}^t$ by **any local solver** as long as

$$\left(\max_{\Delta\alpha_{S_j}} \mathcal{G}_j(\Delta\alpha_{S_j}, \mathbf{w}^t) - \mathcal{G}_j(\Delta\alpha_{S_j}^t, \mathbf{w}^t) \right) \leq \Theta \left(\max_{\Delta\alpha_{S_j}} \mathcal{G}_j(\Delta\alpha_{S_j}, \mathbf{w}^t) - \mathcal{G}_j(\mathbf{0}, \mathbf{w}^t) \right)$$

$$0 < \Theta < 1$$

CoCoA+ (Ma et al., 2015)

Suppose $\ell(z)$ is smooth, $R(\mathbf{w})$ is λ -strongly convex and SDCA is the local solver

- Local Runtime Per-round: $O((\frac{1}{\lambda} + \frac{N}{m}) \log(\frac{1}{\Theta}))$
- Rounds of Communication: $O(\frac{1}{1-\Theta} \frac{1}{\lambda} \log(\frac{1}{\epsilon}))$

Suppose $\ell(z)$ is non-smooth, $R(\mathbf{w})$ is λ -strongly convex and SDCA is the local solver

- Local Runtime Per-round: $O((\frac{1}{\lambda} + \frac{N}{m}) \frac{1}{\Theta})$
- Rounds of Communication: $O(\frac{1}{1-\Theta} \frac{1}{\lambda \epsilon})$

CoCoA+ (Ma et al., 2015)

Suppose $\ell(z)$ is smooth, $R(\mathbf{w})$ is λ -strongly convex and SDCA is the local solver

- **Local Runtime Per-round:** $O\left(\left(\frac{1}{\lambda} + \frac{N}{m}\right) \log\left(\frac{1}{\Theta}\right)\right)$
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Suppose $\ell(z)$ is non-smooth, $R(\mathbf{w})$ is λ -strongly convex and SDCA is the local solver

- **Local Runtime Per-round:** $O\left(\left(\frac{1}{\lambda} + \frac{N}{m}\right) \frac{1}{\Theta}\right)$
- **Rounds of Communication:** $O\left(\frac{1}{1-\Theta} \frac{1}{\lambda\epsilon}\right)$

Distributed SDCA in Practice

- Choice of Θ (how long we run the local solver?)
- Choice of m (how many machines to use?)

- Fast machines but slow network: Use small Θ and small m
- Fast network but slow machines: Use large Θ and large m

Distributed SDCA in Practice

- Choice of Θ (how long we run the local solver?)
- Choice of m (how many machines to use?)

- Fast machines but slow network: Use small Θ and small m
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DiSCO (Zhang & Xiao, 2015)

- The rounds of communication of Dual SDCA does not depends on m .
- **DiSCO: Distributed Second-Order method** (Zhang & Xiao, 2015)
- The rounds of communication of DiSCO depends on m .

DiSCO (Zhang & Xiao, 2015)

- Global problem

$$\min_{\mathbf{w} \in \mathbb{R}^d} \left\{ F(\mathbf{w}) = \frac{1}{N} \sum_{i=1}^N \ell(\mathbf{w}^\top \mathbf{x}_i, y_i) + R(\mathbf{w}) \right\}$$

- Local problem

$$\min_{\mathbf{w} \in \mathbb{R}^d} \left\{ f_j(\mathbf{w}) = \frac{1}{n} \sum_{i \in S_j} \ell(\mathbf{w}^\top \mathbf{x}_i, y_i) + R(\mathbf{w}) \right\}$$

- Global problem can be written as

$$\min_{\mathbf{w} \in \mathbb{R}^d} \left\{ F(\mathbf{w}) = \frac{1}{m} \sum_{j=1}^m f_j(\mathbf{w}) \right\}$$

- Applicable when $f_j(\mathbf{w})$ is smooth, λ -strongly convex and **self-concordant**

Newton Direction

- At optimal solution w^* :

$$\nabla F(\mathbf{w}^*) = \mathbf{0}$$

- We hope moving \mathbf{w}^t along $-\mathbf{v}^t$ leads to $\nabla F(\mathbf{w}^t - \mathbf{v}^t) = \mathbf{0}$
- Taylor expansion:

$$F(\mathbf{w}^t - \mathbf{v}^t) \approx \nabla F(\mathbf{w}^t) - \nabla^2 F(\mathbf{w}^t)\mathbf{v}^t = \mathbf{0}$$

- Such \mathbf{v}^t is called a Newton's direction

Newton Method

Newton Method

Find a Newton direction \mathbf{v}_t by solving

$$\nabla^2 F(\mathbf{w}_t) \mathbf{v}_t = -\nabla F(\mathbf{w}_t)$$

Then update

$$\mathbf{w}_{t+1} = \mathbf{w}_t - \gamma_t \mathbf{v}_t$$

Require solving a linear $d \times d$ equation system. Costly when $d > 1000$.

DiSCO (Zhang & Xiao, 2015)

Inexact Newton Method

Find an inexact Newton direction \mathbf{v}_t using Preconditioned Conjugate Gradient (PCG) (Golub & Ye, 1997)

$$\|\nabla^2 F(\mathbf{w}_t)\mathbf{v}_t - \nabla F(\mathbf{w}_t)\|_2 \leq \epsilon_t$$

Then update

$$\mathbf{w}_{t+1} = \mathbf{w}_t - \gamma_t \mathbf{v}_t$$

DiSCO (Zhang & Xiao, 2015)

PCG

Keep computing

$$\mathbf{v} \leftarrow P^{-1} \times \nabla^2 F(\mathbf{w}_t) \times \mathbf{v}$$

iteratively until \mathbf{v} becomes an inexact Newton direction.

- **Preconditioner:** $P = \nabla^2 f_1(\mathbf{w}_t) + \mu I$
- μ : a tuning parameter such that

$$\|\nabla^2 f_1(\mathbf{w}_t) - \nabla^2 F(\mathbf{w}_t)\|_2 \leq \mu$$

- f_1 is “similar” to F so that P is a good **local** preconditioner.
- $\mu = O(\frac{1}{\sqrt{n}}) = O(\sqrt{\frac{m}{N}})$

DiSCO (Zhang & Xiao, 2015)

PCG

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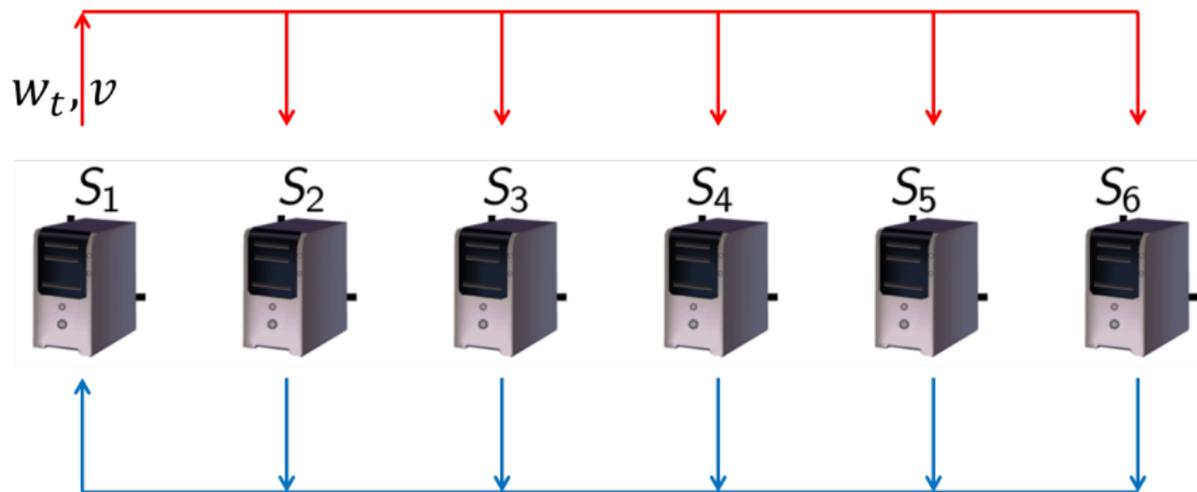
DiSCO (Zhang & Xiao, 2015)

DiSCO compute $\nabla^2 F(\mathbf{w}_t) \times \mathbf{v}$ distributedly:

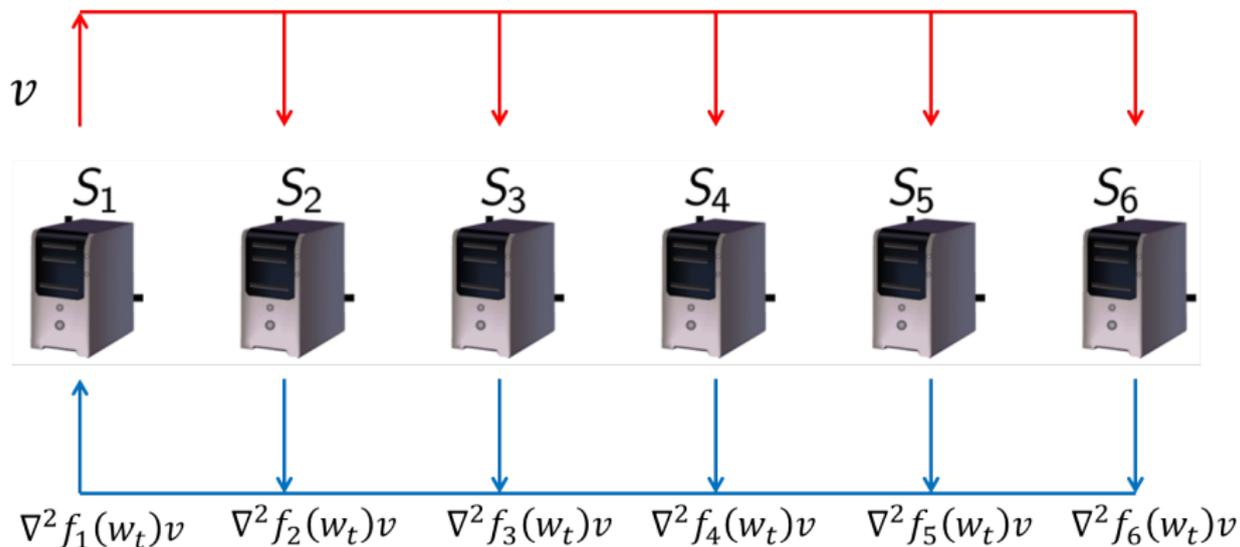
$$\begin{aligned} & \nabla^2 F(\mathbf{w}_t) \times \mathbf{v} \\ = & \underbrace{\nabla^2 f_1(\mathbf{w}_t) \times \mathbf{v}}_{\text{machine 1}} + \underbrace{\nabla^2 f_2(\mathbf{w}_t) \times \mathbf{v}}_{\text{machine 2}} + \cdots + \underbrace{\nabla^2 f_m(\mathbf{w}_t) \times \mathbf{v}}_{\text{machine } m} \end{aligned}$$

Then, compute $P^{-1} \times \nabla^2 F(\mathbf{w}_t) \times \mathbf{v}$ only in machine 1

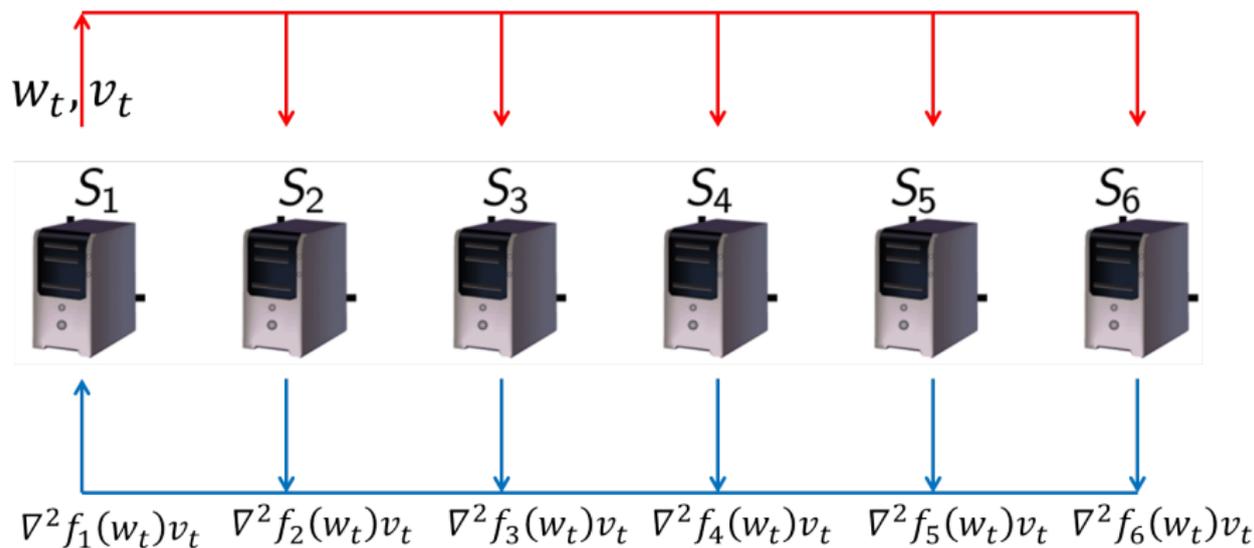
DiSCO (Zhang & Xiao, 2015)



DiSCO (Zhang & Xiao, 2015)

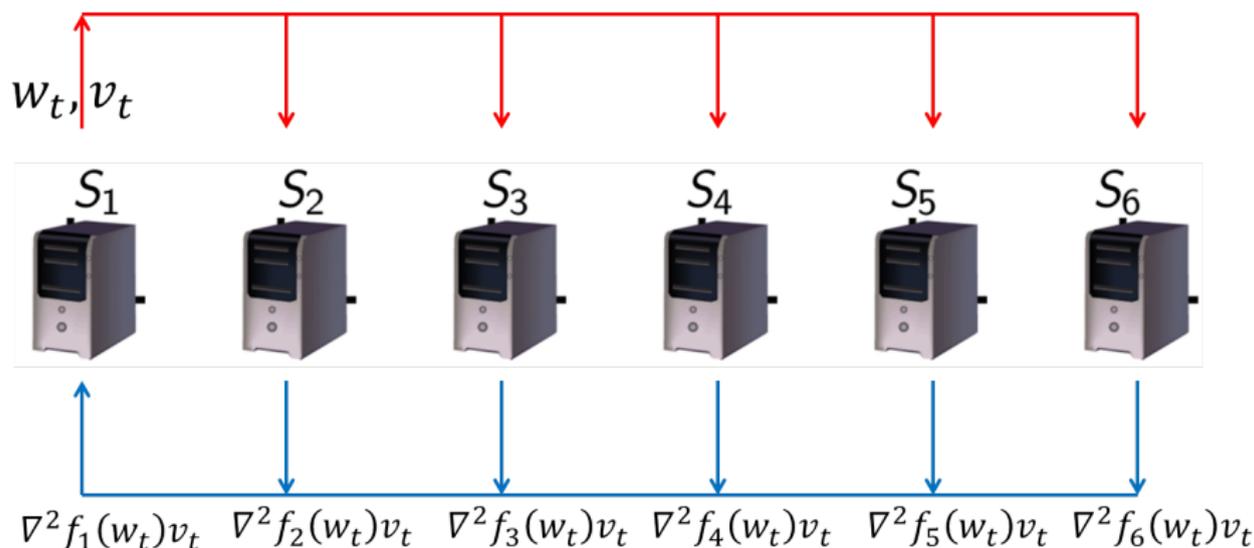


DiSCO (Zhang & Xiao, 2015)



$$\text{Machine 1: } P^{-1}(\nabla^2 F(w_t) v_t) = P^{-1} \left(\frac{1}{m} \sum_{j=1}^m \nabla^2 f_j(w_t) v_t \right)$$

DiSCO (Zhang & Xiao, 2015)



Machine 1:
$$P^{-1}(\nabla^2 F(w_t)v_t) = P^{-1}\left(\frac{1}{m}\sum_{j=1}^m \nabla^2 f_j(w_t)v_t\right)$$

Run PCG until $\|\nabla^2 F(w_t)v_t - \nabla F(w_t)\|_2 \leq \epsilon_t$

DiSCO (Zhang & Xiao, 2015)

- For high-dimensional data (e.g. $d \geq 1000$), computing $P^{-1} \times \nabla^2 F(\mathbf{w}_t) \times \mathbf{v}$ is time costly.
- Instead, use SDCA in machine 1 to solve

$$P^{-1} \times \nabla^2 F(\mathbf{w}_t) \times \mathbf{v} \approx \arg \min_{\mathbf{u} \in \mathbb{R}^d} \frac{1}{2} \mathbf{u}^\top P \mathbf{u} - \mathbf{u}^\top F(\mathbf{w}_t) \mathbf{v}$$

- Local runtime: $O\left(\frac{N}{m} + \frac{1+\mu}{\lambda+\mu}\right)$

DiSCO (Zhang & Xiao, 2015)

Suppose SDCA is the local solver

- **Local Runtime Per-round:** $O\left(\frac{N}{m} + \frac{1+\mu}{\lambda+\mu}\right)$
- **Rounds of Communication:** $O\left(\sqrt{\frac{\mu}{\lambda}} \log\left(\frac{1}{\epsilon}\right)\right)$

Choice of m (how many machines to use?). ($\mu = O\left(\sqrt{\frac{m}{N}}\right)$)

- Fast machines but slow network: Use small m
- Fast network but slow machine: Use large m

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DSVRG (Lee et al., 2015)

- A distributed version of SVRG using a “round-robin” scheme
- Assume the user can control the distribution of data before algorithm.
- Applicable when $f_j(\mathbf{w})$ is smooth and λ -strongly convex

DSVRG (Lee et al., 2015)

Iterate $s = 1, \dots, T - 1$

Let $\mathbf{w}_0 = \tilde{\mathbf{w}}_s$ and compute $\nabla F(\tilde{\mathbf{w}}_s)$

Iterate $t = 1, \dots, K$

$$\tilde{g}_{i_t}(\mathbf{w}_{t-1}) = \nabla F(\tilde{\mathbf{w}}_s) - g_{i_t}(\tilde{\mathbf{w}}_s) + g_{i_t}(\mathbf{w}_{t-1})$$

$$\mathbf{w}_t = \mathbf{w}_{t-1} - \gamma_t \tilde{g}_{i_t}(\mathbf{w}_{t-1})$$

$$\tilde{\mathbf{w}}_{s+1} = \frac{1}{K} \sum_{t=1}^K \mathbf{w}_t$$

output: $\tilde{\mathbf{w}}_T$

- Each machine can only sample from its own data. However,
- $\mathbb{E}_{i_t \in S_j}[\tilde{g}_{i_t}(\mathbf{w}_{t-1})] \neq \nabla F(\mathbf{w}_{t-1})$

DSVRG (Lee et al., 2015)

Easy to
distribute

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DSVRG (Lee et al., 2015)

Iterate $s = 1, \dots, T - 1$

Let $\mathbf{w}_0 = \tilde{\mathbf{w}}_s$ and compute $\nabla F(\tilde{\mathbf{w}}_s)$

Hard to
distribute

Iterate $t = 1, \dots, K$

$$\tilde{g}_{i_t}(\mathbf{w}_{t-1}) = \nabla F(\tilde{\mathbf{w}}_s) - g_{i_t}(\tilde{\mathbf{w}}_s) + g_{i_t}(\mathbf{w}_{t-1})$$

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Iterate $t = 1, \dots, K$

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DSVRG (Lee et al., 2015)

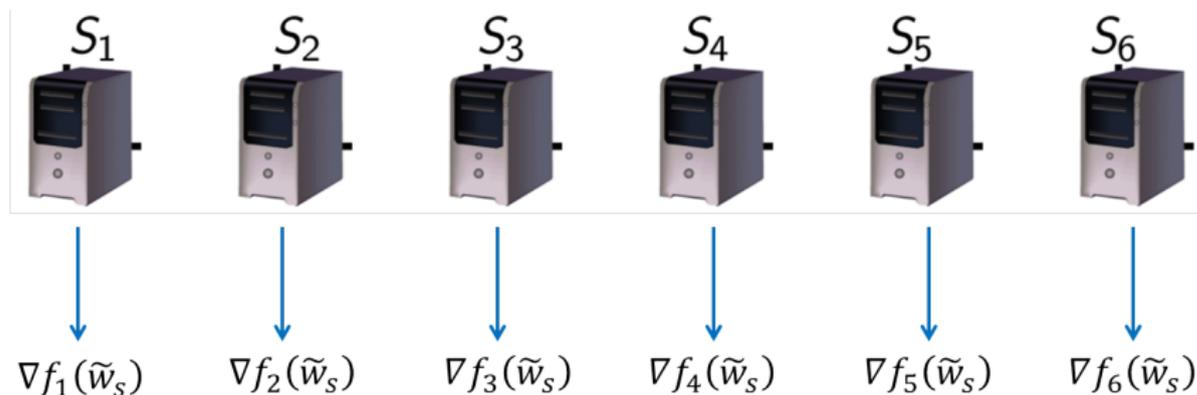
Solution:

- Store a second set of data R_j in machine j , which are sampled with replacement from $\{x_1, x_2, \dots, x_n\}$ before the algorithm starts.
- Construct the stochastic gradient $\tilde{g}_{i_t}(\mathbf{w}_{t-1})$ by sampling $i_t \in R_j$ and removing i_t from R_j after.

$$\mathbb{E}_{i_t \in R_j}[\tilde{g}_{i_t}(\mathbf{w}_{t-1})] = \nabla F(\mathbf{w}_{t-1})$$

- When $R_j = \emptyset$, pass \mathbf{w}_t to next machine.

Full Gradient Step



Center:
$$\nabla F(\tilde{w}_s) = \frac{1}{m} \sum_{j=1}^m \nabla f_j(\tilde{w}_s)$$

Full Gradient Step



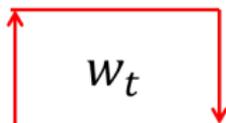
Center:
$$\nabla F(\tilde{w}_s) = \frac{1}{m} \sum_{j=1}^m \nabla f_j(\tilde{w}_s)$$

Stochastic Gradient Step

Iterate $t = 1, \dots, m$

$$\tilde{g}_t(\mathbf{w}_{t-1}) = \nabla F(\tilde{\mathbf{w}}_s) - g_{i_t}(\tilde{\mathbf{w}}_s) + g_{i_t}(\mathbf{w}_{t-1})$$

$$\mathbf{w}_t = \mathbf{w}_{t-1} - \gamma_t \tilde{g}_t(\mathbf{w}_{t-1})$$

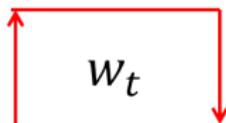


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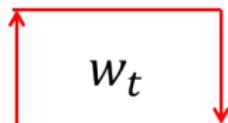


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DSVRG (Lee et al., 2015)

Suppose $|R_j| = r$ for all j .

- Local Runtime Per-round: $O(\frac{N}{m} + r)$
- Rounds of Communication: $O(\frac{1}{r\lambda} \log(\frac{1}{\epsilon}))$

DSVRG (Lee et al., 2015)

Choice of m (how many machines to use?).

- Fast machines but slow network: Use small m
- Fast network but slow machine: Use large m

Choice of r (how many data points to pre-sample in R_j ?).

- The larger, the better
- Required machine memory space: $|S_j| + |R_j| = \frac{N}{m} + r$

Other Distributed Optimization Methods

- ADMM (Boyd et al., 2011; Ozdaglar, 2015)
 - **Rounds of Communication:**
 $O(\text{Network Graph Dependency Term} \times \frac{1}{\sqrt{\lambda}} \log(\frac{1}{\epsilon}))$
- DANE (Shamir et al., 2014)
 - Approximate Newton direction with a difference approach from DISCO

Summary

$\ell(z)$ is smooth and $R(\mathbf{w})$ is λ -strongly convex.

alg.	Mini-SGD	Dist-SDCA	DiSCO
Runtime Per-round	$O(1)$	$O(\frac{1}{\lambda} + \frac{N}{m})$	$O(\frac{N}{m})$
Round of Comm.	$O(\frac{1}{\lambda m \epsilon})$	$O(\frac{1}{\lambda} \log(\frac{1}{\epsilon}))$	$O(\frac{m^{1/4}}{\sqrt{\lambda} N^{1/4}} \log(\frac{1}{\epsilon}))$

Table : Assume $\mu = O(\sqrt{\frac{m}{N}})$

alg.	DSVRG	
	Full Grad.	Stoch. Grad.
Runtime Per-round	$O(\frac{N}{m})$	$O(r)$
Round of Comm.	$O(\log(\frac{1}{\epsilon}))$	$O(\frac{1}{r\lambda} \log(\frac{1}{\epsilon}))$

Summary

$\ell(z)$ is non-smooth and $g(\mathbf{w})$ is λ -strongly convex.

alg.	Mini-SGD	Dist-SDCA	DiSCO	DSVRG
Runtime Per-round	$O(1)$	$O(\frac{1}{\lambda} + \frac{N}{m})$	N.A.	N.A.
Round of Comm.	$O(\frac{1}{\lambda m \epsilon})$	$O(\frac{1}{\lambda \epsilon})$	N.A.	N.A.

Summary

$g(\mathbf{w})$ is non-strongly convex.

alg.	Mini-SGD	Dist-SDCA	DiSCO	DSVRG
Runtime Per-round	$O(1)$	N.A.	N.A.	N.A.
Round of Comm.	$O(\frac{1}{m\epsilon^2})$	N.A.	N.A.	N.A.

Which Algorithm to Use

- Algorithm to use

		$\ell(z) \equiv \ell(z, y)$	
		Non-smooth	Smooth
$R(\mathbf{w})$	Non-strongly convex	Mini-SGD	DSVRG
	λ -strongly convex	Dist-SDCA	DiSCO/DSVRG

- Between DiSCO/DSVRG
 - Use DiSCO for small λ , e.g., $\lambda < 10^{-5}$
 - Use DSVRG for large λ , e.g., $\lambda > 10^{-5}$

Distributed Machine Learning Systems and Library

- Petuum: <http://petuum.github.io>
- Apache Spark: <http://spark.apache.org/>
- Parameter Server: <http://parameterserver.org/>
- Birds: <http://cs.uiowa.edu/~tyng/software.html>

THANK YOU! QUESTIONS?

Big Data Analytics: Optimization and Randomization

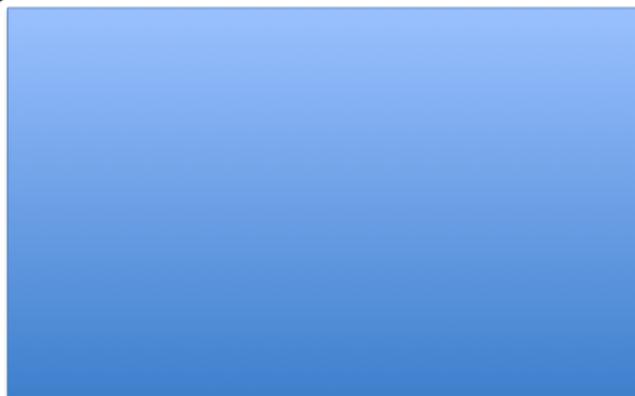
Part III: Randomization

Outline

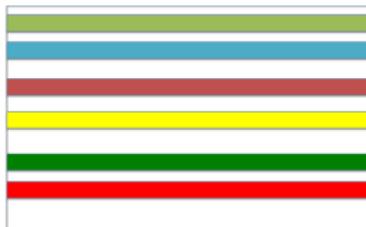
- 1 Basics
- 2 Optimization
- 3 Randomized Dimension Reduction
- 4 Randomized Algorithms
- 5 Concluding Remarks

Random Sketch

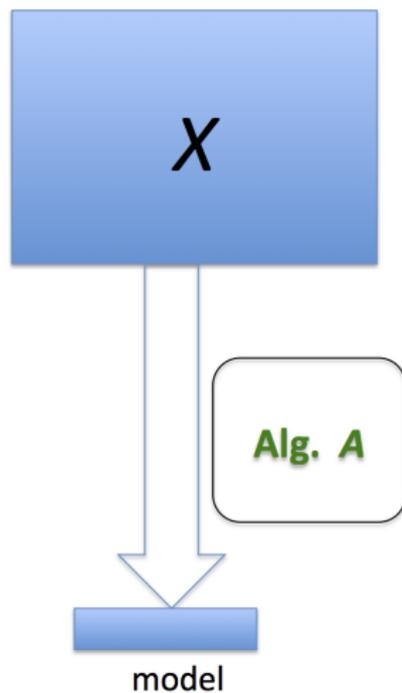
Approximate a large data matrix



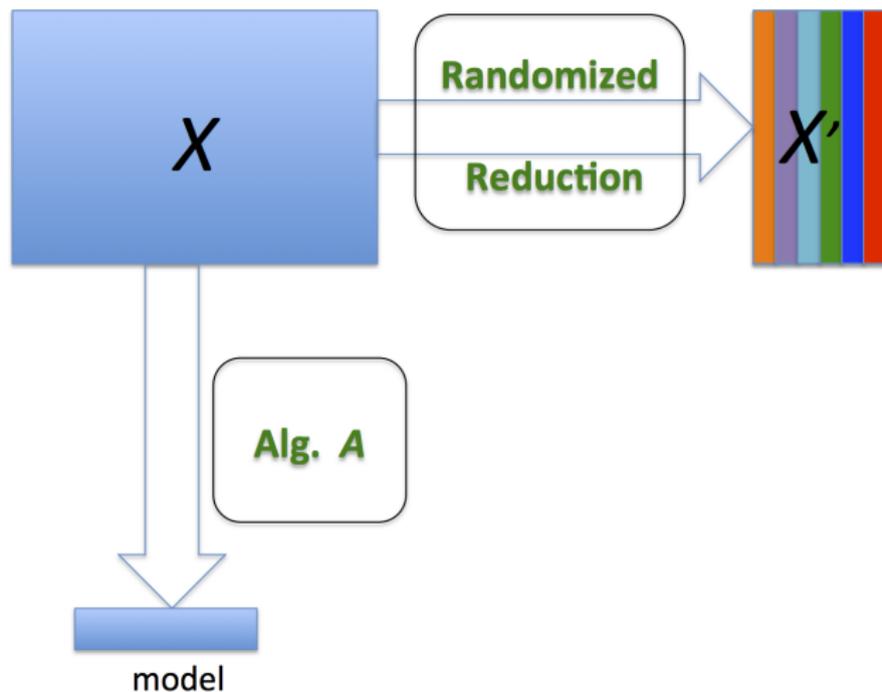
by a much smaller sketch



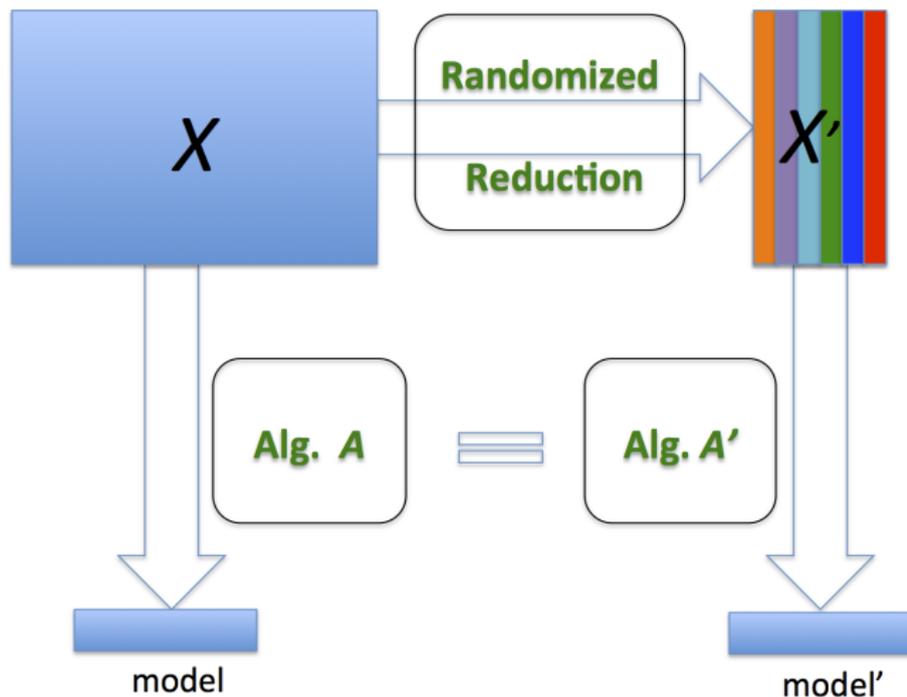
The Framework of Randomized Algorithms



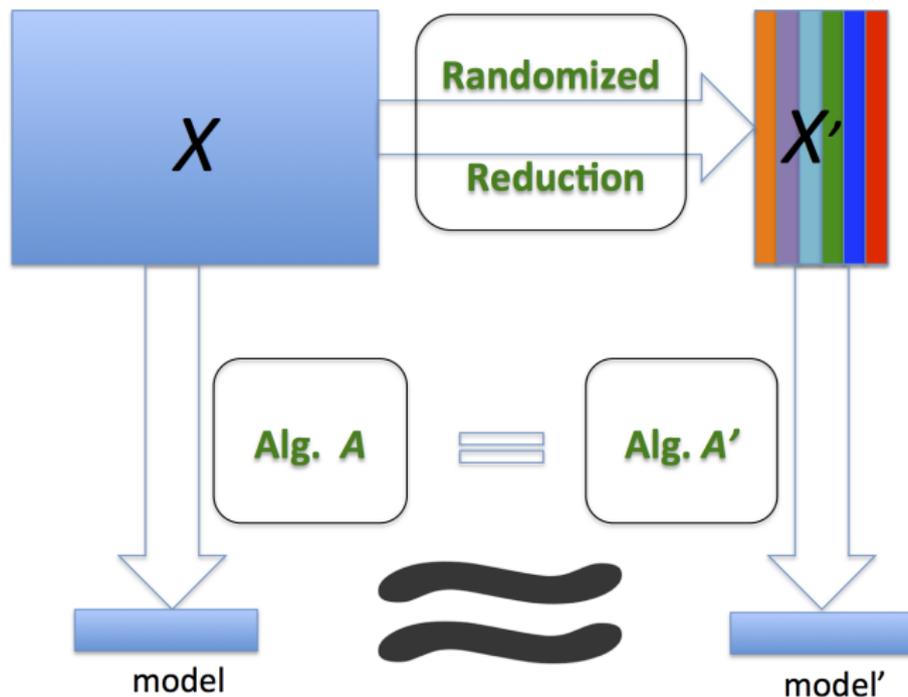
The Framework of Randomized Algorithms



The Framework of Randomized Algorithms



The Framework of Randomized Algorithms



Why randomized dimension reduction?

- Efficient
- Robust (e.g., dropout)
- Formal Guarantees
- Can explore parallel algorithms

Randomized Dimension Reduction

- Johnson-Lindenstauss (JL) transforms
- Subspace embeddings
- Column sampling

JL Lemma

JL Lemma (Johnson & Lindenstrauss, 1984)

For any $0 < \epsilon, \delta < 1/2$, there exists a probability distribution on $m \times d$ real matrices A such that there exists a small universal constant $c > 0$ and for any fixed $\mathbf{x} \in \mathbb{R}^d$ with a probability at least $1 - \delta$, we have

$$\left| \|A\mathbf{x}\|_2^2 - \|\mathbf{x}\|_2^2 \right| \leq c \sqrt{\frac{\log(1/\delta)}{m}} \|\mathbf{x}\|_2^2$$

or for $m = \Theta(\epsilon^{-2} \log(1/\delta))$, then with a probability at least $1 - \delta$

$$\left| \|A\mathbf{x}\|_2^2 - \|\mathbf{x}\|_2^2 \right| \leq \epsilon \|\mathbf{x}\|_2^2$$

Embedding a set of points into low dimensional space

Given a set of points $\mathbf{x}_1, \dots, \mathbf{x}_n \in \mathbb{R}^d$, we can embed them into a low dimensional space $A\mathbf{x}_1, \dots, A\mathbf{x}_n \in \mathbb{R}^m$ such that

the pairwise distance between any two points are well preserved in the low dimensional space

$$\|A\mathbf{x}_i - A\mathbf{x}_j\|_2^2 = \|A(\mathbf{x}_i - \mathbf{x}_j)\|_2^2 \leq (1 + \epsilon) \|\mathbf{x}_i - \mathbf{x}_j\|_2^2$$

$$\|A\mathbf{x}_i - A\mathbf{x}_j\|_2^2 = \|A(\mathbf{x}_i - \mathbf{x}_j)\|_2^2 \geq (1 - \epsilon) \|\mathbf{x}_i - \mathbf{x}_j\|_2^2$$

In other words, in order to have all pairwise Euclidean distances preserved up to $1 \pm \epsilon$, only $m = \Theta(\epsilon^{-2} \log(n^2/\delta))$ dimensions are necessary

JL transforms: Gaussian Random Projection

Gaussian Random Projection (Dasgupta & Gupta, 2003): $A \in \mathbb{R}^{m \times d}$

- $A_{ij} \sim \mathcal{N}(0, 1/m)$
- $m = \Theta(\epsilon^{-2} \log(1/\delta))$
- Computational cost of AX : where $X \in \mathbb{R}^{d \times n}$
 - mnd for dense matrices
 - $\text{nnz}(X)m$ for sparse matrices

Computational Cost is very High (could be as high as solving many problems)

Accelerate JL transforms: using discrete distributions

Using Discrete Distributions (Achlioptas, 2003):

- $\Pr(A_{ij} = \pm \frac{1}{\sqrt{m}}) = 0.5$
- $\Pr(A_{ij} = \pm \sqrt{\frac{3}{m}}) = \frac{1}{6}, \Pr(A_{ij} = 0) = \frac{2}{3}$
- Database friendly
- Replace multiplications by additions and subtractions

Accelerate JL transforms: using Hadmard transform (I)

Fast JL transform based on randomized Hadmard transform:

Motivation: Can we simply use random sampling matrix $P \in \mathbb{R}^{m \times d}$ that randomly selects m coordinates out of d coordinates (scaled by $\sqrt{d/m}$)?

Unfortunately: by Chernoff bound

$$| \|P\mathbf{x}\|_2^2 - \|\mathbf{x}\|_2^2 | \leq \frac{\sqrt{d}\|\mathbf{x}\|_\infty}{\|\mathbf{x}\|_2} \sqrt{\frac{3 \log(2/\delta)}{m}} \|\mathbf{x}\|_2^2$$

Unless $\frac{\sqrt{d}\|\mathbf{x}\|_\infty}{\|\mathbf{x}\|_2} \leq c$, the random sampling does not work

Remedy is given by randomized Hadmard transform

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Randomized Hadamard transform

Hadamard transform:

- $H \in \mathbb{R}^{d \times d}$: $H = \sqrt{\frac{1}{d}} H_{2^k}$

$$H_1 = [1], \quad H_2 = \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}, \quad H_{2^k} = \begin{bmatrix} H_{2^{k-1}} & H_{2^{k-1}} \\ H_{2^{k-1}} & -H_{2^{k-1}} \end{bmatrix}$$

- $\|H\mathbf{x}\|_2 = \|\mathbf{x}\|_2$ and H is orthogonal
- Computational costs of $H\mathbf{x}$: $d \log(d)$

randomized Hadamard transform: HD

- $D \in \mathbb{R}^{d \times d}$: a diagonal matrix $\Pr(D_{ii} = \pm 1) = 0.5$
- HD is orthogonal and $\|HD\mathbf{x}\|_2 = \|\mathbf{x}\|_2$

Key property: $\frac{\sqrt{d} \|HD\mathbf{x}\|_\infty}{\|HD\mathbf{x}\|_2} \leq \sqrt{\log(d/\delta)}$ w.h.p $1 - \delta$

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Accelerate JL transforms: using Hadmard transform (I)

Fast JL transform based on randomized Hadmard transform (Tropp, 2011):

$$A = \sqrt{\frac{d}{m}} PHD$$

yields

$$|\|A\mathbf{x}\|_2^2 - \|\mathbf{x}\|_2^2| \leq \sqrt{\frac{3 \log(2/\delta) \log(d/\delta)}{m}} \|\mathbf{x}\|_2^2$$

- $m = \Theta(\epsilon^{-2} \log(1/\delta) \log(d/\delta))$ suffice for $1 \pm \epsilon$
- additional factor $\log(d/\delta)$ can be removed
- Computational cost of AX : $O(nd \log(m))$

Accelerate JL transforms: using a sparse matrix (I)

Random hashing (Dasgupta et al., 2010)

$$A = HD$$

where $D \in \mathbb{R}^{d \times d}$ and $H \in \mathbb{R}^{m \times d}$

- random hashing: $h(j) : \{1, \dots, d\} \rightarrow \{1, \dots, m\}$
- $H_{ij} = 1$ if $h(j) = i$: sparse matrix (each column has only one non-zero entry)
- $D \in \mathbb{R}^{d \times d}$: a diagonal matrix $\Pr(D_{ii} = \pm 1) = 0.5$
- $[A\mathbf{x}]_j = \sum_{i:h(i)=j} x_i D_{ii}$

Technically speaking, random hashing does not satisfy JL lemma

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Accelerate JL transforms: using a sparse matrix (I)

- key properties:

- $E[\langle HD\mathbf{x}_1, HD\mathbf{x}_2 \rangle] = \langle \mathbf{x}_1, \mathbf{x}_2 \rangle$
- and norm perserving $|\|HD\mathbf{x}\|_2^2 - \|\mathbf{x}\|_2^2| \leq \epsilon \|\mathbf{x}\|_2^2$, only when

$$\frac{\|\mathbf{x}\|_\infty}{\|\mathbf{x}\|_2} \leq \frac{1}{\sqrt{c}}$$

Apply randomized Hadmard transform P first: $\Theta(c \log(c/\delta))$ blocks of randomized Hadmard transform

$$\frac{\|P\mathbf{x}\|_\infty}{\|P\mathbf{x}\|_2} \leq \frac{1}{\sqrt{c}}$$

Accelerate JL transforms: using a sparse matrix (II)

Sparse JL transform based on block random hashing (Kane & Nelson, 2014)

$$A = \begin{bmatrix} \frac{1}{\sqrt{s}} Q_1 \\ \dots \\ \frac{1}{\sqrt{s}} Q_s \end{bmatrix}$$

- Each $Q_s \in \mathbb{R}^{v \times d}$ is an independent random hashing (*HD*) matrix
- Set $v = \Theta(\epsilon^{-1})$ and $s = \Theta(\epsilon^{-1} \log(1/\delta))$
- Computational Cost of AX : $O\left(\frac{\text{nnz}(X)}{\epsilon} \log\left[\frac{1}{\delta}\right]\right)$

Randomized Dimension Reduction

- Johnson-Lindenstaus (JL) transforms
- Subspace embeddings
- Column sampling

Subspace Embeddings

Definition: a subspace embedding given some parameters $0 < \epsilon, \delta < 1, k \leq d$ is a distribution \mathcal{D} over matrices $A \in \mathbb{R}^{m \times d}$ such that for **any fixed linear subspace** $W \in \mathbb{R}^d$ with $\dim(W) = k$ it holds that

$$\Pr_{A \sim \mathcal{D}}(\forall \mathbf{x} \in W, \|A\mathbf{x}\|_2 \in (1 \pm \epsilon)\|\mathbf{x}\|_2) \geq 1 - \delta$$

It implies

- If $U \in \mathbb{R}^{d \times k}$ is orthogonal matrix (contains the orthonormal bases)
 - $AU \in \mathbb{R}^{m \times k}$ is of full column rank
 - $\|AU\|_2 \in (1 \pm \epsilon)$
 - $(1 - \epsilon)^2 \leq \|U^T A^T AU\|_2 \leq (1 + \epsilon)^2$
- These are **key properties** in the theoretical analysis of many algorithms (e.g., low-rank matrix approximation, randomized least-squares regression, randomized classification)

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Subspace Embeddings

From a JL transform to a Subspace Embedding (Sarlós, 2006).

Let $A \in \mathbb{R}^{m \times d}$ be a JL transform. If

$$m = O\left(\frac{k \log \left\lceil \frac{k}{\delta \epsilon} \right\rceil}{\epsilon^2}\right)$$

Then w.h.p $1 - \delta^k$, $A \in \mathbb{R}^{m \times d}$ is a subspace embedding w.r.t a k -dimensional space in \mathbb{R}^d

Subspace Embeddings

Making block random hashing a Subspace Embedding (Nelson & Nguyen, 2013).

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- Set $v = \Theta(k\epsilon^{-1} \log^5(k/\delta))$ and $s = \Theta(\epsilon^{-1} \log^3(k/\delta))$
- w.h.p $1 - \delta$, $A \in \mathbb{R}^{m \times d}$ with $m = \Theta\left(\frac{k \log^8(k/\delta)}{\epsilon^2}\right)$ is a subspace embedding w.r.t a k -dimensional space in \mathbb{R}^d
- Computational Cost of AX : $O\left(\frac{\text{nnz}(X)}{\epsilon} \log^3\left[\frac{k}{\delta}\right]\right)$

Sparse Subspace Embedding (SSE)

Random hashing is SSE with a Constant Probability (Nelson & Nguyen, 2013)

$$A = HD$$

where $D \in \mathbb{R}^{d \times d}$ and $H \in \mathbb{R}^{m \times d}$

- $m = \Omega(k^2/\epsilon^2)$ suffice for a subspace embedding with a probability $2/3$
- Computational Cost AX : $O(nnz(X))$

Randomized Dimensionality Reduction

- Johnson-Lindenstauss (JL) transforms
- Subspace embeddings
- Column (Row) sampling

Column sampling

- Column subset selection (feature selection)
- More interpretable
- Uniform sampling usually does not work (not a JL transform)
- Non-oblivious sampling (data-dependent sampling)
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Leverage-score sampling (Drineas et al., 2006)

Let $X \in \mathbb{R}^{d \times n}$ be a rank- k matrix

- $X = U\Sigma V^T$: $U \in \mathbb{R}^{d \times k}$, $\Sigma \in \mathbb{R}^{k \times k}$
- Leverage scores $\|U_{i*}\|_2^2$, $i = 1, \dots, d$
- Let $p_i = \frac{\|U_{i*}\|_2^2}{\sum_{i=1}^d \|U_{i*}\|_2^2}$, $i = 1, \dots, d$
- Let $i_1, \dots, i_m \in \{1, \dots, d\}$ denote m indices selected by following p_i
- Let $A \in \mathbb{R}^{m \times d}$ be sampling-and-rescaling matrix:

$$A_{ij} = \begin{cases} \frac{1}{\sqrt{mp_j}} & \text{if } j = i_j \\ 0 & \text{otherwise} \end{cases}$$

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- Let $i_1, \dots, i_m \in \{1, \dots, d\}$ denote m indices selected by following p_i
- Let $A \in \mathbb{R}^{m \times d}$ be sampling-and-rescaling matrix:

$$A_{ij} = \begin{cases} \frac{1}{\sqrt{mp_j}} & \text{if } j = i_j \\ 0 & \text{otherwise} \end{cases}$$

- $AX \in \mathbb{R}^{m \times n}$ is a small sketch of X

Leverage-score sampling (Drineas et al., 2006)

Let $X \in \mathbb{R}^{d \times n}$ be a rank- k matrix

- $X = U\Sigma V^T$: $U \in \mathbb{R}^{d \times k}$, $\Sigma \in \mathbb{R}^{k \times k}$
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Properties of Leverage-score sampling

When $m = \Theta\left(\frac{k}{\epsilon^2} \log\left[\frac{2k}{\delta}\right]\right)$, w.h.p $1 - \delta$,

- $AU \in \mathbb{R}^{m \times k}$ is full column rank
- $\sigma_i^2(AU) \geq (1 - \epsilon) \geq (1 - \epsilon)^2$
- $\sigma_i^2(AU) \leq 1 + \epsilon \leq (1 + \epsilon)^2$
- Leverage-score sampling performs like a subspace embedding (only for U , the top singular vector matrix of X)
- Computational cost: compute top- k SVD of X , expensive
- Randomized algorithms to compute approximate leverage scores

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When uniform sampling makes sense?

Coherence measure

$$\mu_k = \frac{d}{k} \max_{1 \leq i \leq d} \|U_{i*}\|_2^2$$

- Valid when the coherence measure is small (some real data mining datasets have small coherence measures)
- The Nyström method usually uses uniform sampling (Gittens, 2011)

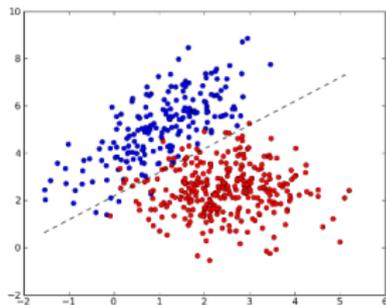
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- 4 Randomized Algorithms
 - Randomized Classification (Regression)
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Classification

Classification problems:

$$\min_{\mathbf{w} \in \mathbb{R}^d} \frac{1}{n} \sum_{i=1}^n \ell(y_i \mathbf{w}^\top \mathbf{x}_i) + \frac{\lambda}{2} \|\mathbf{w}\|_2^2$$



- $y_i \in \{+1, -1\}$: label
- Loss function $\ell(z)$: $z = \mathbf{y}\mathbf{w}^\top \mathbf{x}$
 1. **SVMs**: (squared) hinge loss $\ell(z) = \max(0, 1 - z)^p$, where $p = 1, 2$
 2. **Logistic Regression**: $\ell(z) = \log(1 + \exp(-z))$

Randomized Classification

For large-scale high-dimensional problems, the computational cost of optimization is $O((nd + d\kappa) \log(1/\epsilon))$.

Use random reduction $A \in \mathbb{R}^{d \times m}$ ($m \ll d$), we reduce $X \in \mathbb{R}^{n \times d}$ to $\hat{X} = XA \in \mathbb{R}^{n \times m}$. Then solve

$$\min_{\mathbf{u} \in \mathbb{R}^m} \frac{1}{n} \sum_{i=1}^n \ell(y_i \mathbf{u}^\top \hat{\mathbf{x}}_i) + \frac{\lambda}{2} \|\mathbf{u}\|_2^2$$

- JL transforms
- Sparse subspace embeddings

Randomized Classification

Two questions:

- Is there any performance guarantee?
 - margin is preserved: if data is linearly separable (Balcan et al., 2006) as long as $m \geq \frac{12}{\epsilon^2} \log(\frac{6m}{\delta})$
 - generalization performance is preserved: if the data matrix is of low rank and $m = \Omega(\frac{k \text{poly}(\log(k/\delta\epsilon))}{\epsilon^2})$ (Paul et al., 2013)
- How to recover an accurate model in the original high-dimensional space?

Dual Recovery (Zhang et al., 2014) and Dual Sparse Recovery (Yang et al., 2015)

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The Dual problem

Using Fenchel conjugate

$$\ell_i^*(\alpha_i) = \max_{\alpha_i} \alpha_i z - \ell(z, y_i)$$

Primal:

$$\mathbf{w}_* = \arg \min_{\mathbf{w} \in \mathbb{R}^d} \frac{1}{n} \sum_{i=1}^n \ell(\mathbf{w}^\top \mathbf{x}_i, y_i) + \frac{\lambda}{2} \|\mathbf{w}\|_2^2$$

Dual:

$$\alpha_* = \arg \max_{\alpha \in \mathbb{R}^n} -\frac{1}{n} \sum_{i=1}^n \ell_i^*(\alpha_i) - \frac{1}{2\lambda n^2} \alpha^\top \mathbf{X} \mathbf{X}^\top \alpha$$

From dual to primal:

$$\mathbf{w}_* = -\frac{1}{\lambda n} \mathbf{X}^\top \alpha_*$$

Dual Recovery for Randomized Reduction

From dual formulation: \mathbf{w}_* lies in the row space of the data matrix $X \in \mathbb{R}^{n \times d}$

- Dual Recovery: $\tilde{\mathbf{w}}_* = -\frac{1}{\lambda n} X^\top \hat{\alpha}_*$, where

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and $\hat{X} = XA \in \mathbb{R}^{n \times m}$

- Subspace Embedding A with $m = \Theta(r \log(r/\delta) \epsilon^{-2})$
- Guarantee: under low-rank assumption of the data matrix X (e.g., $\text{rank}(X) = r$), with a high probability $1 - \delta$,

$$\|\tilde{\mathbf{w}}_* - \mathbf{w}_*\|_2 \leq \frac{\epsilon}{1 - \epsilon} \|\mathbf{w}_*\|_2$$

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Assume the optimal dual solution α_* is sparse (i.e., the number of support vectors is small)

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where $\hat{X} = XA \in \mathbb{R}^{n \times m}$

- JL transform A with $m = \Theta(s \log(n/\delta) \epsilon^{-2})$
- Guarantee: if α_* is s -sparse, with a high probability $1 - \delta$,

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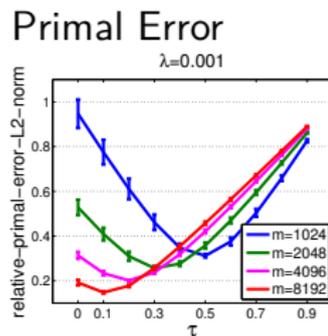
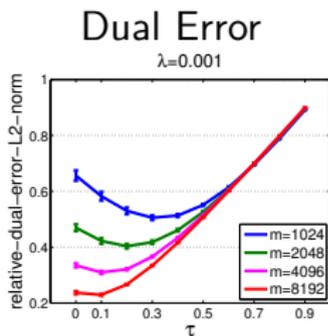
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Dual Sparse Recovery

RCV1 text data, $n = 677,399$, and $d = 47,236$



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4 Randomized Algorithms

- Randomized Classification (Regression)
- **Randomized Least-Squares Regression**
- Randomized K-means Clustering
- Randomized Kernel methods
- Randomized Low-rank Matrix Approximation

Least-squares regression

Let $X \in \mathbb{R}^{n \times d}$ with $d \ll n$ and $b \in \mathbb{R}^n$. The least-squares regression problem is to find \mathbf{w}_* such that

$$\mathbf{w}_* = \arg \min_{\mathbf{w} \in \mathbb{R}^d} \|X\mathbf{w} - b\|_2$$

- Computational Cost: $O(nd^2)$
- Goal of RA: $o(nd^2)$

Randomized Least-squares regression

Let $A \in \mathbb{R}^{m \times n}$ be a random reduction matrix. Solve

$$\hat{\mathbf{w}}_* = \arg \min_{\mathbf{w} \in \mathbb{R}^d} \|A(X\mathbf{w} - b)\|_2 = \|AX\mathbf{w} - Ab\|_2$$

- Computational Cost: $O(md^2)$ + reduction time

Randomized Least-squares regression

Theoretical Guarantees (Sarlós, 2006; Drineas et al., 2011; Nelson & Nguyen, 2012):

$$\|X\hat{\mathbf{w}}_* - \mathbf{b}\|_2 \leq (1 + \epsilon)\|X\mathbf{w}_* - \mathbf{b}\|_2$$

Total Time $O(\text{nnz}(X) + d^3 \log(d/\epsilon)\epsilon^{-2})$

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K-means Clustering

Let $\mathbf{x}_1, \dots, \mathbf{x}_n \in \mathbb{R}^d$ be a set of data points.

K-means clustering aims to solve

$$\min_{C_1, \dots, C_k} \sum_{j=1}^k \sum_{\mathbf{x}_i \in C_j} \|\mathbf{x}_i - \mu_j\|_2^2$$

Computational Cost: $O(ndkt)$, where t is number of iterations.

Randomized Algorithms for K-means Clustering

Let $X = (\mathbf{x}_1, \dots, \mathbf{x}_n)^\top \in \mathbb{R}^{n \times d}$ be the data matrix.

High-dimensional data: Random Sketch: $\hat{X} = XA \in \mathbb{R}^{n \times m}$, $\ell \ll d$

Approximate K-means:

$$\min_{C_1, \dots, C_k} \sum_{j=1}^k \sum_{\hat{\mathbf{x}}_i \in C_j} \|\hat{\mathbf{x}}_i - \hat{\mu}_j\|_2^2$$

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Randomized Algorithms for K-means Clustering

For random sketch: JL transforms, sparse subspace embedding all work

- JL transform: $m = O\left(\frac{k \log(k/(\epsilon\delta))}{\epsilon^2}\right)$
- Sparse subspace embedding: $m = O\left(\frac{k^2}{\epsilon^2\delta}\right)$
- ϵ relates to the approximation accuracy
- Analysis of approximation error for K-means can be formulated as Constrained Low-rank Approximation (Cohen et al., 2015)

$$\min_{Q^T Q = I} \|X - QQ^T X\|_F^2$$

where Q is orthonormal.

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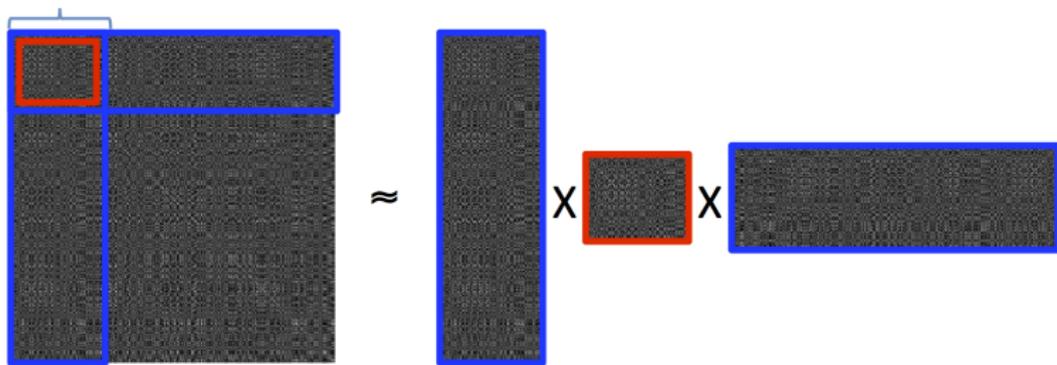
Kernel methods

- Kernel function: $\kappa(\cdot, \cdot)$
- a set of examples $\mathbf{x}_1, \dots, \mathbf{x}_n$
- Kernel matrix: $K \in \mathbb{R}^{n \times n}$ with $K_{ij} = \kappa(\mathbf{x}_i, \mathbf{x}_j)$
- K is a PSD matrix
- Computational and memory costs: $\Omega(n^2)$
- Approximation methods
 - The Nyström method
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The Nyström method



Let $A \in \mathbb{R}^{n \times \ell}$ be uniform sampling matrix.

$$B = KA \in \mathbb{R}^{n \times \ell}$$

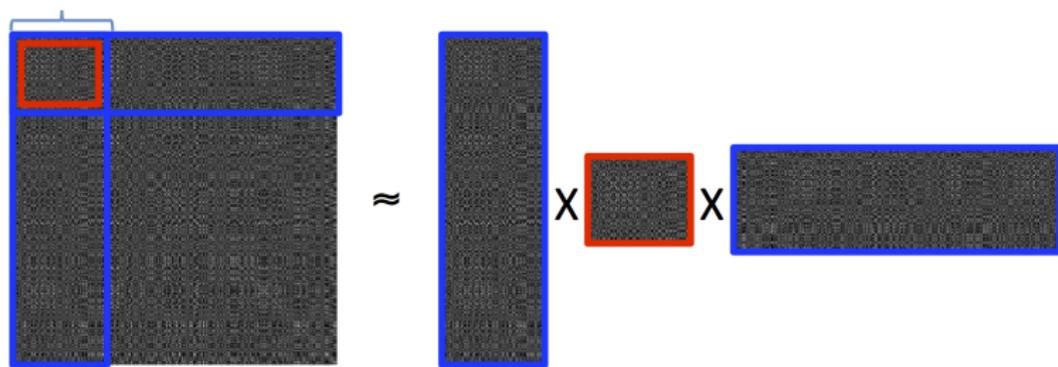
$$C = A^T B = A^T KA$$

The Nyström approximation (Drineas & Mahoney, 2005)

$$\hat{K} = BC^{\dagger}B^T$$

Computational Cost: $O(\ell^3 + n\ell^2)$

The Nyström method



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The Nyström based kernel machine

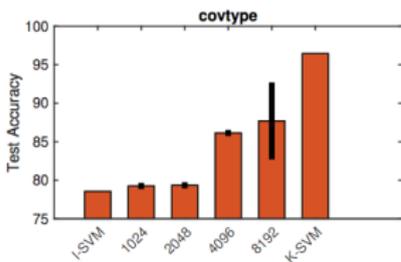
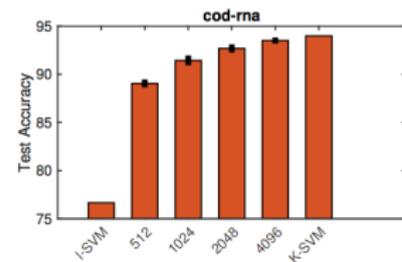
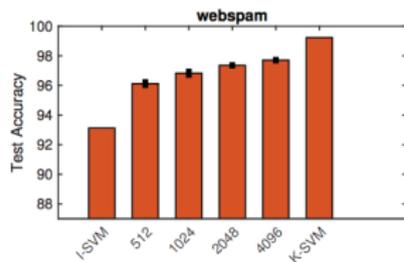
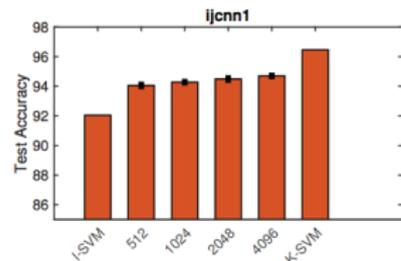
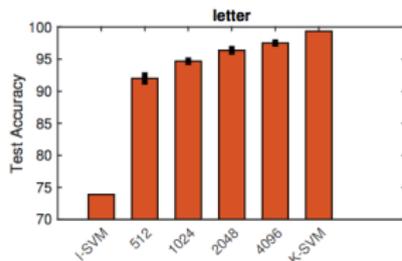
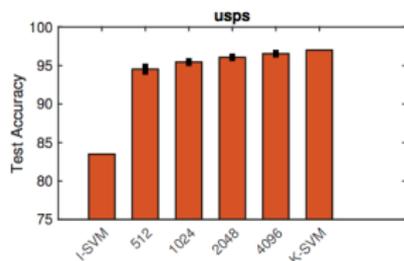
The dual problem:

$$\arg \max_{\alpha \in \mathbb{R}^n} -\frac{1}{n} \sum_{i=1}^n \ell_i^*(\alpha_i) - \frac{1}{2\lambda n^2} \alpha^\top BC^\dagger B^\top \alpha$$

Solve it like solving a linear method: $\hat{X} = BC^{-1/2} \in \mathbb{R}^{n \times \ell}$

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Random Fourier Features (RFF)

Bochner's theorem

A shift-invariant kernel $\kappa(\mathbf{x}, \mathbf{y}) = \kappa(\mathbf{x} - \mathbf{y})$ is a valid kernel if and only if $\kappa(\delta)$ is the Fourier transform of a non-negative measure, i.e.,

$$\kappa(\mathbf{x} - \mathbf{y}) = \int p(\omega) e^{-j\omega^\top(\mathbf{x}-\mathbf{y})} d\omega$$

RFF (Rahimi & Recht, 2008): generate a set of $\omega_1, \dots, \omega_m \in \mathbb{R}^d$ following $p(\omega)$. For an example $\mathbf{x} \in \mathbb{R}^d$, construct

$$\hat{\mathbf{x}} = (\cos(\omega_1^\top \mathbf{x}), \sin(\omega_1^\top \mathbf{x}), \dots, \cos(\omega_m^\top \mathbf{x}), \sin(\omega_m^\top \mathbf{x}))^\top \in \mathbb{R}^{2m}$$

RBF kernel $\exp(-\frac{\|\mathbf{x}-\mathbf{y}\|_2^2}{2\gamma^2})$: $p(\omega) = \mathcal{N}(0, \gamma^2)$

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$$\kappa(\mathbf{x} - \mathbf{y}) = \int p(\omega) e^{-j\omega^\top(\mathbf{x}-\mathbf{y})} d\omega$$

RFF (Rahimi & Recht, 2008): generate a set of $\omega_1, \dots, \omega_m \in \mathbb{R}^d$ following $p(\omega)$. For an example $\mathbf{x} \in \mathbb{R}^d$, construct

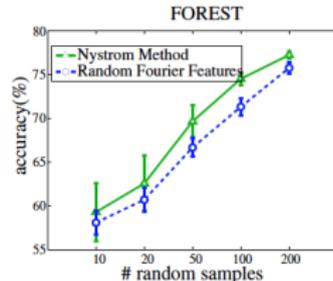
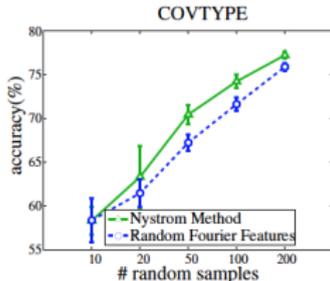
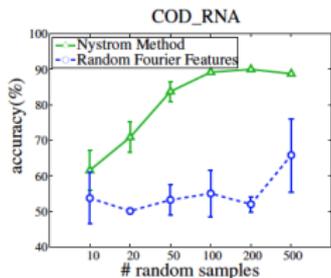
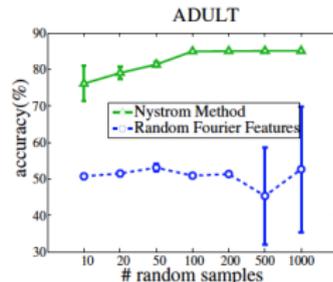
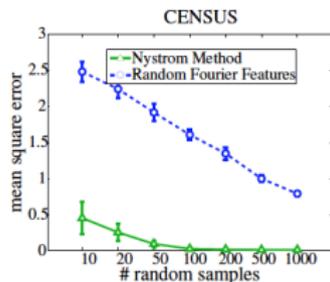
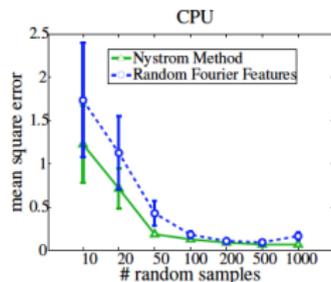
$$\hat{\mathbf{x}} = (\cos(\omega_1^\top \mathbf{x}), \sin(\omega_1^\top \mathbf{x}), \dots, \cos(\omega_m^\top \mathbf{x}), \sin(\omega_m^\top \mathbf{x}))^\top \in \mathbb{R}^{2m}$$

RBF kernel $\exp(-\frac{\|\mathbf{x}-\mathbf{y}\|_2^2}{2\gamma^2})$: $p(\omega) = \mathcal{N}(0, \gamma^2)$

The Nyström method vs RFF (Yang et al., 2012)

- functional approximation framework
- The Nyström method: data-dependent bases
- RFF: data independent bases
- In certain cases (e.g., large eigen-gap, skewed eigen-value distribution): the generalization performance of the Nyström method is better than RFF

The Nyström method vs RFF



Outline

- 4 Randomized Algorithms
 - Randomized Classification (Regression)
 - Randomized Least-Squares Regression
 - Randomized K-means Clustering
 - Randomized Kernel methods
 - Randomized Low-rank Matrix Approximation

Randomized low-rank matrix approximation

Let $X \in \mathbb{R}^{n \times d}$. The goal is to obtain

$$\hat{U}\hat{\Sigma}\hat{V}^T \approx X$$

where $\hat{U} \in \mathbb{R}^{n \times k}$, $\hat{V} \in \mathbb{R}^{d \times k}$ have orthonormal columns, $\hat{\Sigma} \in \mathbb{R}^{k \times k}$ is a diagonal matrix with nonnegative entries

- k is target rank
- The best rank- k approximation $X_k = U_k \Sigma_k V_k^T$
- Approximation error

$$\|\hat{U}\hat{\Sigma}\hat{V}^T - X\|_{\xi} \leq (1 + \epsilon) \|U_k \Sigma_k V_k^T - X\|_{\xi}$$

where $\xi = F$ or $\xi = 2$

Why low-rank approximation?

Applications in Data mining and Machine learning

- PCA
- Spectral clustering
- ...

Why randomized algorithms?

Deterministic Algorithms

- Truncated SVD $O(nd \min(n, d))$
- Rank-Revealing QR factorization $O(ndk)$
- Krylov subspace method (e.g. Lanczos algorithm):
 $O(kT_{mult} + (n + d)k^2)$, where T_{mult} denotes the cost of matrix-vector product.

Randomized Algorithms

- Speed can be faster (e.g., $O(nd \log(k))$)
- Output more robust (e.g. Lanczos requires sophisticated modifications)
- Can be pass efficient
- Can exploit parallel algorithms

Why randomized algorithms?

Deterministic Algorithms

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Randomized algorithms for low-rank matrix approximation

The Basic Randomized Algorithms for Approximating $X \in \mathbb{R}^{n \times d}$ (Halko et al., 2011)

- ① Obtain a small sketch by $Y = XA \in \mathbb{R}^{n \times m}$
- ② Compute $Q \in \mathbb{R}^{n \times m}$ that contains the orthonormal basis of $\text{col}(Y)$
- ③ Compute SVD of $Q^T X = U \Sigma V^T$
- ④ Approximation $X \approx \tilde{U} \Sigma V^T$, where $\tilde{U} = QU$

Explanation: If $\text{col}(XA)$ captures the top- k column space of X well, i.e.,

$$\|X - QQ^T X\| \leq \varepsilon$$

then

$$\|X - \tilde{U} \Sigma V^T\| \leq \varepsilon$$

Randomized algorithms for low-rank matrix approximation

Three questions:

- 1 What is the value of m ?
 - $m = k + p$, p is the oversampling parameter. In practice $p = 5$ or 10 gives superb results
- 2 What is the computational cost?
 - Subsampled Randomized Hadmard Transform: can be as fast as $O(nd \log(k) + k^2(n + d))$
- 3 What is the quality?
 - Theoretical Guarantee:
 - Practically, very accurate

Randomized algorithms for low-rank matrix approximation

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Randomized algorithms for low-rank matrix approximation

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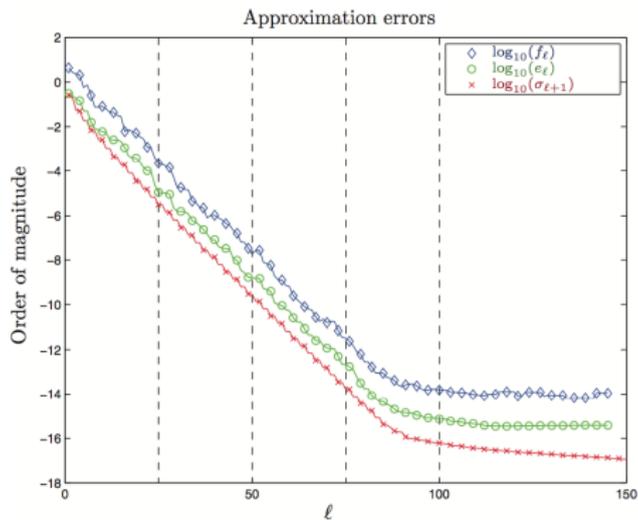
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Randomized algorithms for low-rank matrix approximation

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Randomized algorithms for low-rank matrix approximation



Randomized algorithms for low-rank matrix approximation

Other things

- Use power iteration to reduce the error: use $(XX^T)^q X$
- Can use sparse JL transform/subspace embedding matrices (Frobenius norm guarantee only)

Outline

- 1 Basics
- 2 Optimization
- 3 Randomized Dimension Reduction
- 4 Randomized Algorithms
- 5 Concluding Remarks**

How to address big data challenge?

- Optimization perspective: improve convergence rates, exploring properties of functions
 - stochastic optimization (e.g., SDCA, SVRG, SAGA)
 - distributed optimization (e.g., DisDCA)
- Randomization perspective: reduce data size, exploring properties of data
 - randomized feature reduction (e.g., reduce the number of features)
 - randomized instance reduction (e.g., reduce the number of instances)

How can we address big data challenge?

- Optimization perspective: improve convergence rates, exploring properties of functions
 - Pro: can obtain the optimal solution
 - Con: high computational/communication costs
- Randomization perspective: reduce data size, exploring properties of data
 - Pro: fast
 - Con: still exists recovery error

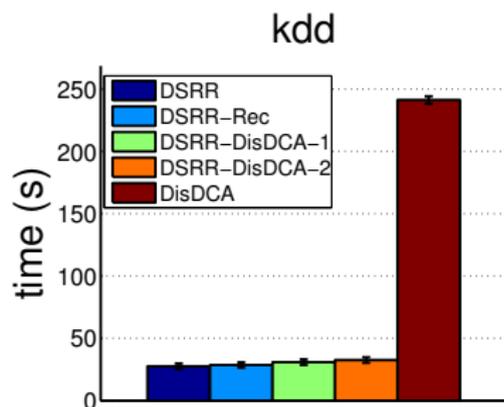
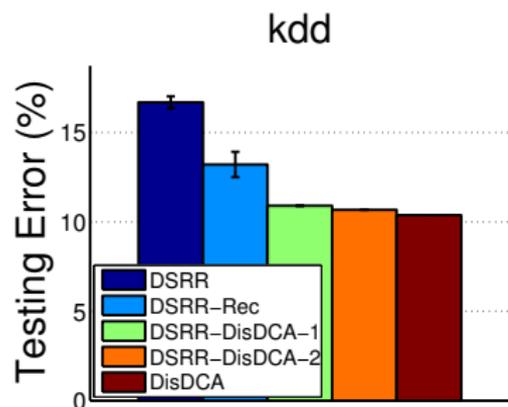
Can we combine the benefits of two techniques?

Combine Randomization and Optimization (Yang et al., 2015)

- Use randomization (Dual Spare Recovery) to obtain a good initial solution
- Initialize distributed optimization (DisDCA) to reduce cost of computation/communication
- Observe 1 or 2 epochs of computations (1 or 2 communications) suffice to obtain the same performance of pure optimization

Big Data Experiments

KDDcup Data: $n = 8,407,752$, $d = 29,890,095$, 10 machines, $m = 1024$



THANK YOU! QUESTIONS?

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Examples of Convex functions

- $ax + b$, $A\mathbf{x} + b$
- x^2 , $\|\mathbf{x}\|_2^2$
- $\exp(ax)$, $\exp(\mathbf{w}^\top \mathbf{x})$
- $\log(1 + \exp(ax))$, $\log(1 + \exp(\mathbf{w}^\top \mathbf{x}))$
- $x \log(x)$, $\sum_i x_i \log(x_i)$
- $\|\mathbf{x}\|_p$, $p \geq 1$, $\|\mathbf{x}\|_p^2$
- $\max_i(x_i)$

Operations that preserve convexity

- Nonnegative scale: $a \cdot f(\mathbf{x})$ where $a \geq 0$
- Sum: $f(\mathbf{x}) + g(\mathbf{x})$
- Composition with affine function $f(A\mathbf{x} + b)$
- Point-wise maximum: $\max_j f_j(\mathbf{x})$

Examples:

- Least-squares regression: $\|A\mathbf{x} - b\|_2$
- SVM: $\frac{1}{n} \sum_{i=1}^n \max(0, 1 - y_i \mathbf{w}^\top \mathbf{x}_i) + \frac{\lambda}{2} \|\mathbf{w}\|_2^2$

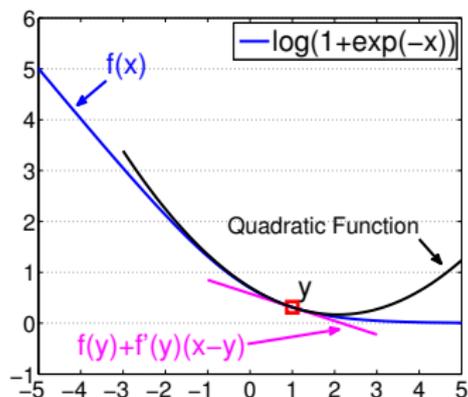
Smooth Convex function

- smooth: e.g. **logistic loss** $f(x) = \log(1 + \exp(-x))$

$$\|\nabla f(x) - \nabla f(y)\|_2 \leq L\|x - y\|_2$$

where $L > 0$

Second Order Derivative is upper bounded $\|\nabla^2 f(x)\|_2 \leq L$



Smooth Convex function

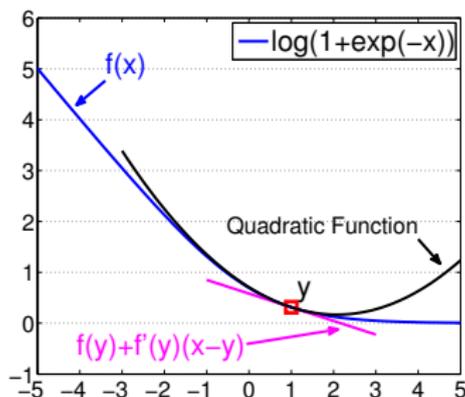
- smooth: e.g. $\log(1 + \exp(-x))$

smoothness
constant

$$\|\nabla f(x) - \nabla f(y)\|_2 \leq L\|x - y\|_2$$

where $L > 0$

Second Order Derivative is upper bounded $\|\nabla^2 f(x)\|_2 \leq L$



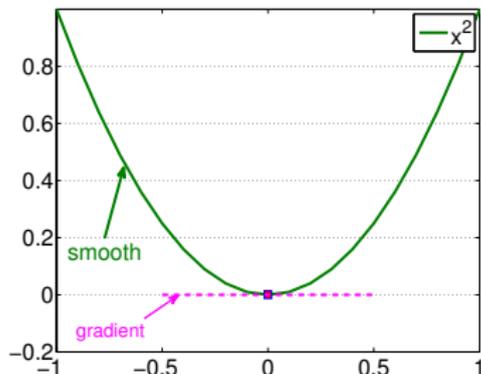
Strongly Convex function

- strongly convex: e.g. Euclidean norm $f(x) = \frac{1}{2}\|x\|_2^2$

$$\|\nabla f(x) - \nabla f(y)\|_2 \geq \lambda \|x - y\|_2$$

where $\lambda > 0$

Second Order Derivative is lower bounded $\|\nabla^2 f(x)\|_2 \geq \lambda$



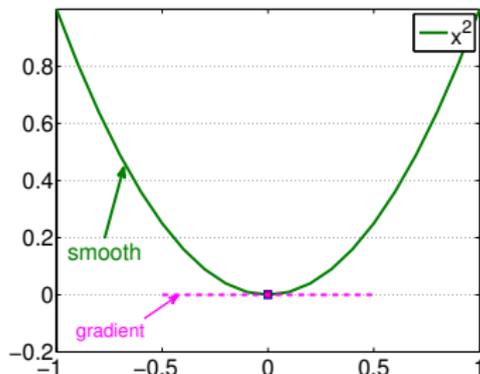
Strongly Convex function

- strongly convex: strong convexity
constant e.g. $f(x) = \frac{1}{2}\|x\|_2^2$

$$\|\nabla f(x) - \nabla f(y)\|_2 \geq \lambda \|x - y\|_2$$

where $\lambda > 0$

Second Order Derivative is lower bounded $\|\nabla^2 f(x)\|_2 \geq \lambda$



Smooth and Strongly Convex function

- smooth and strongly convex: e.g. **quadratic function**:

$$f(z) = \frac{1}{2}(z - 1)^2$$

$$\lambda \|x - y\|_2 \leq \|\nabla f(x) - \nabla f(y)\|_2 \leq L \|x - y\|_2, \quad L \geq \lambda > 0$$

Chernoff bound

Let X_1, \dots, X_n be independent random variables. Assume $0 \leq X_i \leq 1$.
 Let $X = X_1 + \dots + X_n$. $\mu = \mathbb{E}[X]$. Then

$$\Pr(X \geq (1 + \epsilon)\mu) \leq \exp\left(-\frac{\epsilon^2}{2 + \epsilon}\mu\right)$$

$$\Pr(X \leq (1 - \epsilon)\mu) \leq \exp\left(-\frac{\epsilon^2}{2}\mu\right)$$

or

$$\Pr(|X - \mu| \geq \epsilon\mu) \leq 2 \exp\left(-\frac{\epsilon^2}{2 + \epsilon}\mu\right) \leq 2 \exp\left(-\frac{\epsilon^2}{3}\mu\right)$$

the last inequality holds when $0 < \epsilon \leq 1$

Theoretical Guarantee of RA for low-rank approximation

$$X = U \begin{bmatrix} \Sigma_1 & \\ & \Sigma_2 \end{bmatrix} \begin{bmatrix} V_1^T \\ V_2^T \end{bmatrix}$$

- $X \in \mathbb{R}^{m \times n}$: the target matrix
- $\Sigma_1 \in \mathbb{R}^{k \times k}$, $V_1 \in \mathbb{R}^{n \times k}$
- $A \in \mathbb{R}^{n \times \ell}$: random reduction matrix
- $Y = XA \in \mathbb{R}^{m \times \ell}$: the small sketch

Key inequality:

$$\|(I - P_Y)X\|^2 \leq \|\Sigma_2\|^2 + \|\Sigma_2 \Omega_2 \Omega_1^\dagger\|^2$$

Gaussian Matrices

- G is a standard Gaussian matrix
- U and V are orthonormal matrices
- $U^T G V$ follows the standard Gaussian distribution
- $\mathbb{E}[\|SGT\|_F^2] = \|S\|_F^2 \|T\|_F^2$
- $\mathbb{E}[\|SGT\|] \leq \|S\| \|T\|_F + \|S\|_F \|T\|$
- Concentration for function of a Gaussian matrix. Suppose h is a Lipschitz function on matrices

$$h(X) - h(Y) \leq L\|X - Y\|_F$$

Then

$$\Pr(h(G) \geq \mathbb{E}[h(G)] + Lt) \leq e^{-t^2/2}$$

Analysis for Randomized Least-square regression

Let $X = U\Sigma V^\top$

$$\mathbf{w}_* = \arg \min_{\mathbf{w} \in \mathbb{R}^d} \|X\mathbf{w} - b\|_2$$

Let $Z = \|X\mathbf{w}_* - b\|_2$, $\omega = b - X\mathbf{w}_*$, and $X\mathbf{w}_* = U\alpha$

$$\hat{\mathbf{w}}_* = \arg \min_{\mathbf{w} \in \mathbb{R}^d} \|A(X\mathbf{w} - b)\|_2$$

Since $b - X\mathbf{w}_* = b - X(X^\top X)^\dagger X^\top b = (I - UU^\top)b$, $X\hat{\mathbf{w}}_* - X\mathbf{w}_* = U\beta$.
Then

$$\|X\hat{\mathbf{w}}_* - b\|_2 = \|X\mathbf{w}_* - b\|_2 + \|X\hat{\mathbf{w}}_* - X\mathbf{w}_*\|_2 = Z + \|\beta\|_2$$

Analysis for Randomized Least-square regression

$$AU(\alpha + \beta) = AX\hat{\mathbf{w}}_* = AX(AX)^\dagger Ab = P_{AX}(Ab) = P_{AU}(Ab)$$

$$P_{AU}(Ab) = P_{AU}(A(\omega + U\alpha)) = AU\alpha + P_{AU}(A\omega)$$

Hence

$$U^\top A^\top AU\beta = (AU)^\top (AU)(AU)^\dagger A\omega = (AU)^\top (AU)((AU)^\top AU)^{-1}(AU)^\top A\omega$$

where we use AU is full column matrix. Then

$$U^\top A^\top AU\beta = U^\top A^\top A\omega$$

$$\|\beta\|_2^2/2 \leq \|U^\top A^\top AU\beta\|_2^2 = \|U^\top A^\top A\omega\|_2^2 \leq \epsilon'^2 \|U\|_F^2 \|\omega\|_2^2$$

where the last inequality uses the matrix products approximation shown in next slide. Since $\|U\|_F^2 \leq d$, setting $\epsilon' = \sqrt{\frac{\epsilon}{d}}$ suffices.

Approximate Matrix Products

Given $X \in \mathbb{R}^{n \times d}$ and $Y \in \mathbb{R}^{d \times p}$, let $A \in \mathbb{R}^{m \times d}$ one of the following matrices

- a JL transform matrix with $m = \Theta(\epsilon^{-2} \log((n + p)/\delta))$
- the sparse subspace embedding with $m = \Theta(\epsilon^{-2})$
- leverage-score sampling matrix based on $p_i \geq \frac{\|X_{i*}\|_2^2}{2\|X\|_F^2}$ and $m = \Theta(\epsilon^{-2})$

Then w.h.p $1 - \delta$

$$\|XA^T AY - XY\|_F \leq \epsilon \|X\|_F \|Y\|_F$$

Analysis for Randomized Least-square regression

$$A \in \mathbb{R}^{m \times n}$$

1. Subspace embedding: AU full column rank
2. Matrix product approximation: $\sqrt{\epsilon/d}$

Order of m

- JL transforms: 1. $O(d \log(d))$, 2. $O(d \log(d)\epsilon^{-1}) \Rightarrow O(d \log(d)\epsilon^{-1})$
- Sparse subspace embedding: 1. $O(d^2)$, 2. $O(d\epsilon^{-1}) \Rightarrow O(d^2\epsilon^{-1})$

If we use SSE ($A_1 \in \mathbb{R}^{m_1 \times n}$) and JL transform $A_2 \in \mathbb{R}^{m_2 \times m_1}$

$$\begin{aligned} \|A_2 A_1 (X \mathbf{w}_*^2 - b)\|_2 &\leq (1 + \epsilon) \|A_1 (X \mathbf{w}_*^1 - b)\|_2 \\ &\leq (1 + \epsilon) \|A_1 (X \mathbf{w}_* - b)\|_2 \leq (1 + \epsilon)^2 \|X \mathbf{w}_* - b\| \end{aligned}$$

with $m_1 = O(d^2 \epsilon^{-2})$ and $m_2 = d \log(d) \epsilon^{-1}$, \mathbf{w}_*^2 is the optimal solution using $A_2 A_1$ and \mathbf{w}_*^1 is the optimal using A_1 and \mathbf{w}_* is the original optimal solution.

Randomized Least-squares regression

Theoretical Guarantees (Sarlós, 2006; Drineas et al., 2011; Nelson & Nguyen, 2012):

$$\|X\widehat{\mathbf{w}}_* - b\|_2 \leq (1 + \epsilon)\|X\mathbf{w}_* - b\|_2$$

- If A is a fast JL transform with $m = \Theta(\epsilon^{-1}d \log(d))$: Total Time $O(nd \log(m) + d^3 \log(d)\epsilon^{-1})$
- If A is a Sparse Subspace Embedding with $m = \Theta(d^2\epsilon^{-1})$: Total Time $O(nnz(X) + d^4\epsilon^{-1})$
- If $A = A_1A_2$ combine fast JL ($m_1 = \Theta(\epsilon^{-1}d \log(d))$) and SSE ($m_2 = \Theta(d^2\epsilon^{-2})$): **Total Time $O(nnz(X) + d^3 \log(d/\epsilon)\epsilon^{-2})$**

Matrix Chernoff bound

Lemma (Matrix Chernoff (Tropp, 2012))

Let \mathcal{X} be a finite set of PSD matrices with dimension k , and suppose that $\max_{X \in \mathcal{X}} \lambda_{\max}(X) \leq B$. Sample $\{X_1, \dots, X_\ell\}$ independently from \mathcal{X} .

Compute

$$\mu_{\max} = \ell \lambda_{\max}(\mathbb{E}[X_1]), \quad \mu_{\min} = \ell \lambda_{\min}(\mathbb{E}[X_1])$$

Then

$$\Pr \left\{ \lambda_{\max} \left(\sum_{i=1}^{\ell} X_i \right) \geq (1 + \delta) \mu_{\max} \right\} \leq k \left[\frac{e^{\delta}}{(1 + \delta)^{1 + \delta}} \right]^{\frac{\mu_{\max}}{B}}$$

$$\Pr \left\{ \lambda_{\min} \left(\sum_{i=1}^{\ell} X_i \right) \leq (1 - \delta) \mu_{\min} \right\} \leq k \left[\frac{e^{-\delta}}{(1 - \delta)^{1 - \delta}} \right]^{\frac{\mu_{\min}}{B}}$$

To simplify the usage of Matrix Chernoff bound, we note that

$$\left[\frac{e^{-\delta}}{[1-\delta]^{1-\delta}} \right]^\mu \leq \exp\left(-\frac{\delta^2}{2}\right)$$

$$\left[\frac{e^\delta}{(1+\delta)^{1+\delta}} \right]^\mu \leq \exp\left(-\mu\delta^2/3\right), \delta \leq 1$$

$$\left[\frac{e^\delta}{(1+\delta)^{1+\delta}} \right]^\mu \leq \exp\left(-\mu\delta \log(\delta)/2\right), \delta > 1$$

Noncommutative Bernstein Inequality

Lemma (Noncommutative Bernstein Inequality (Recht, 2011))

Let Z_1, \dots, Z_L be independent zero-mean random matrices of dimension $d_1 \times d_2$. Suppose $\tau_j^2 = \max \{ \|\mathbb{E}[Z_j Z_j^\top]\|_2, \|\mathbb{E}[Z_j^\top Z_j]\|_2 \}$ and $\|Z_j\|_2 \leq M$ almost surely for all k . Then, for any $\epsilon > 0$,

$$\Pr \left[\left\| \sum_{j=1}^L Z_j \right\|_2 > \epsilon \right] \leq (d_1 + d_2) \exp \left[\frac{-\epsilon^2/2}{\sum_{j=1}^L \tau_j^2 + M\epsilon/3} \right]$$

Randomized Algorithms for K-means Clustering

K-means:

$$\sum_{j=1}^k \sum_{\mathbf{x}_i \in C_j} \|\mathbf{x}_i - \mu_j\|_2^2 = \|X - CC^T X\|_F^2$$

where $C \in \mathbb{R}^{n \times k}$ is the scaled cluster indicator matrix such that $C^T C = I$.

Constrained Low-rank Approximation (Cohen et al., 2015)

$$\min_{P \in \mathcal{S}} \|X - PX\|_F^2$$

where $\mathcal{S} = QQ^T$ is any set of rank k orthogonal projection matrix with orthonormal $Q \in \mathbb{R}^{n \times k}$

Low-rank Approximation: \mathcal{S} is the set of all rank k orthogonal projection matrix. $P^* = U_k U_k^T$

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Randomized Algorithms for K-means Clustering

Define

$$\hat{P}^* = \min_{P \in \mathcal{S}} \|\hat{X} - P\hat{X}\|_F^2$$

$$P^* = \min_{P \in \mathcal{S}} \|X - PX\|_F^2$$

Guarantees on Approximation

$$\|X - \hat{P}^*X\|_F^2 \leq \frac{1 + \epsilon}{1 - \epsilon} \|X - P^*X\|_F^2$$

Properties of Leverage-score sampling

We prove the properties using Matrix Chernoff bound. Let $\Omega = AU$.

$$\Omega^\top \Omega = (AU)^\top (AU) = \sum_{j=1}^m \frac{1}{mp_{ij}} \mathbf{u}_{ij} \mathbf{u}_{ij}^\top$$

Let $X_j = \frac{1}{mp_{ij}} \mathbf{u}_{ij} \mathbf{u}_{ij}^\top$. $E[X_j] = \frac{1}{m} I_k$. Therefore $\lambda_{\max}(X_j) = \lambda_{\min}(X_j) = \frac{1}{m}$.

And $\lambda_{\max}(X_j) \leq \max_i \frac{\|\mathbf{u}_{ij}\|_2^2}{mp_{ij}} = \frac{k}{m}$. Applying the Matrix Chernoff bound for the minimum and maximum eigen-value, we have

$$\Pr(\lambda_{\min}(\Omega^\top \Omega) \leq (1 - \epsilon)) \leq k \exp\left(-\frac{m\epsilon^2}{2k}\right) \leq k \exp\left(-\frac{m\epsilon^2}{3k}\right)$$

$$\Pr(\lambda_{\max}(\Omega^\top \Omega) \geq (1 + \epsilon)) \leq k \exp\left(-\frac{m\epsilon^2}{3k}\right)$$

When uniform sampling makes sense?

Coherence measure

$$\mu_k = \frac{d}{k} \max_{1 \leq i \leq d} \|U_{i*}\|_2^2$$

When $\mu_k \leq \tau$ and $m = \Theta\left(\frac{k\tau}{\epsilon^2} \log\left[\frac{2k}{\delta}\right]\right)$ w.h.p $1 - \delta$,

- A formed by uniform sampling (and scaling)
- $AU \in \mathbb{R}^{m \times k}$ is full column rank
- $\sigma_i^2(AU) \geq (1 - \epsilon) \geq (1 - \epsilon)^2$
- $\sigma_i^2(AU) \leq (1 + \epsilon) \leq (1 + \epsilon)^2$
- Valid when the coherence measure is small (some real data mining datasets have small coherence measures)
- The Nyström method usually uses uniform sampling (Gittens, 2011)