







# Introduction to Big Data Optimization

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EPSRC Fellow in Mathematical Sciences (Mathematical Underpinnings of OR)

OR58 - Portsmouth - September 6-8, 2016

My science is better than your science!



OPERATIONAL RESEARCH
THE SCIENCE OF BETTER

BEST

### Outline

- 1. Data Science, Big Data & Optimization
- 2. Applications
- 3. Methods

# Part 1 Data Science, Big Data & Optimization

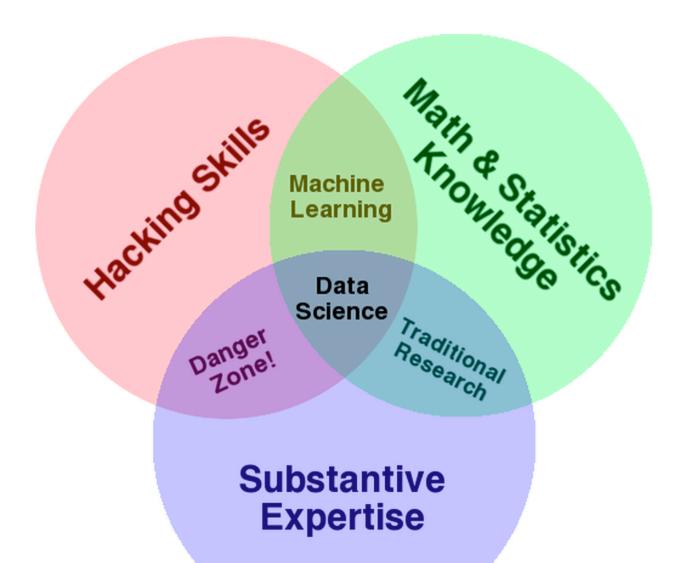
### Data Science and Machine Learning

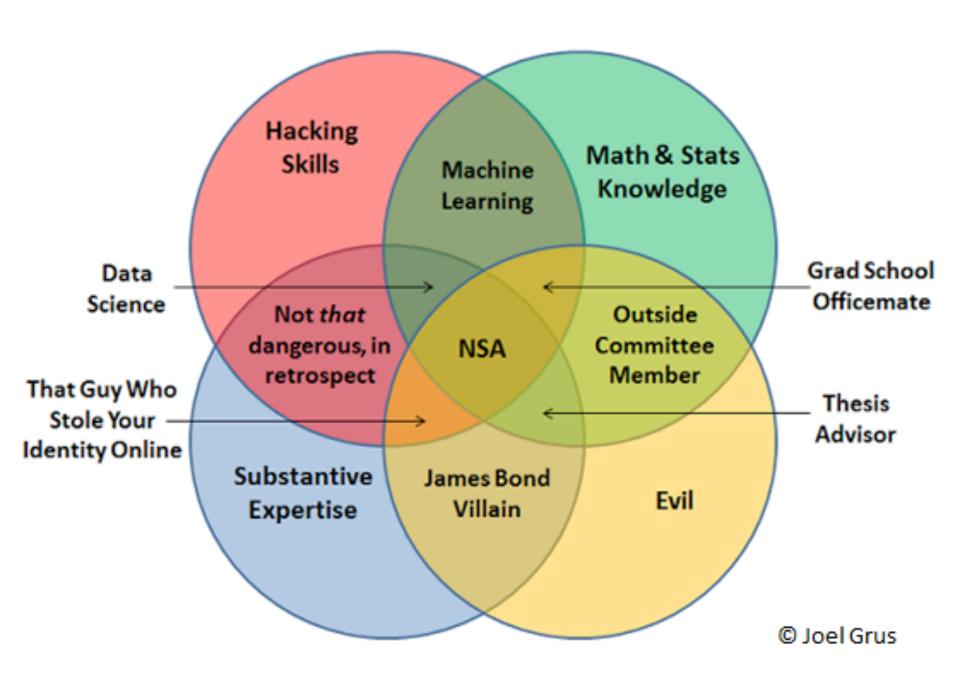
Data: Anything collected/recorded in digital form of potential value

- Text, music, video, images, scans, databases, health records, tax data, email, online clicks, tweets, blogs, ...
- Usually modelled statistically, or as a signal

Data Science: Extraction of knowledge from data

Machine Learning: Automated learning from available data to make predictions & decisions about unseen data







**Matrix Theory** 

**Machine Learning** 

## Translational Research



## Foundational Research











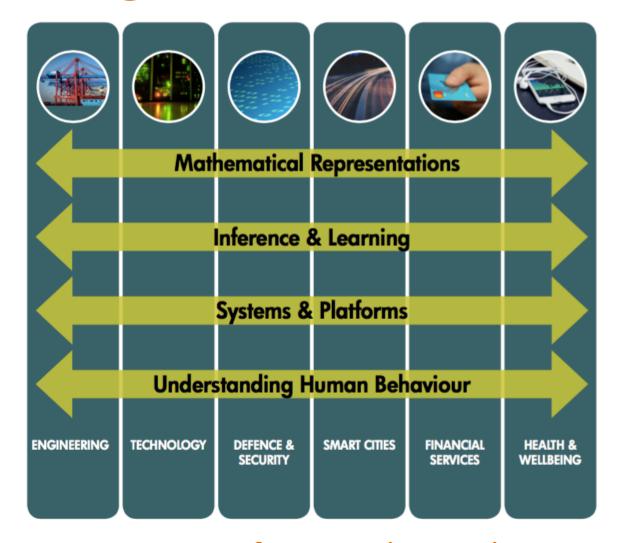
UK's national institute for data science

Leading Public Conversation



Training the Next Generation

### Strategic Priorities of the ATI



6 Priority Sectors for Translational Research

### **Big Data**

Too much hype?

"Big data opens the door to a new approach to understanding the world and making decisions" (New York Times, 2013)

"Don't be colonized by the Americans with their big data, colonize them" (Cathal MacSwiney Brugha, 8.9.2016)

Data that can't be stored on a "typical system" or analyzed via "normal procedures"

What to do with huge quantities of data?

- New models
- New algorithms

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### **Optimization & Big Data**

#### **Conference Series**

 Established & run in Edinburgh in 2012, 2013, 2015, 2017

### Optimization plays a key role in big data analysis

- Machine Learning = Stochastic Optimization (Srebro)
- Optimization is used to train ML models
- Optimization used in discovering new data representations
- Optimization used in turning extracted knowledge into action



# Optimization Objective in Big Data Problems

Objective is formed from collected data, and hence is not a "precise object"

- Low to medium accuracy solutions are fine!
- What methods can find rough solutions quickly?

### Objective often simple

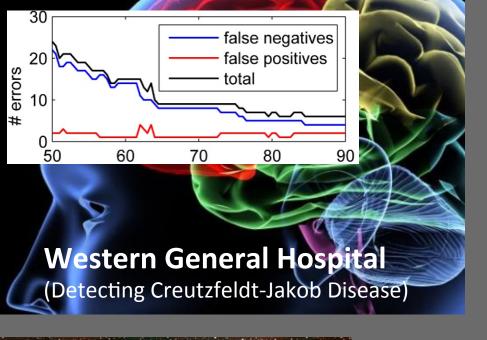
- The more data we have, the less modeling we should do: "the model is in the data"
- Typically: Data-fitting term + Prior knowledge term

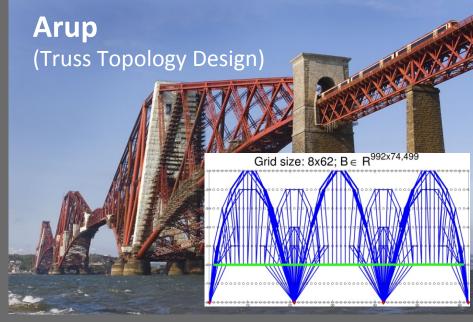
$$\min_{x} \frac{1}{2} ||Ax - b||_{2}^{2} + \lambda ||x||_{2}^{2}$$

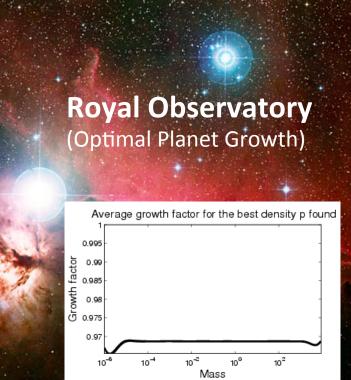
# Part 2 Applications

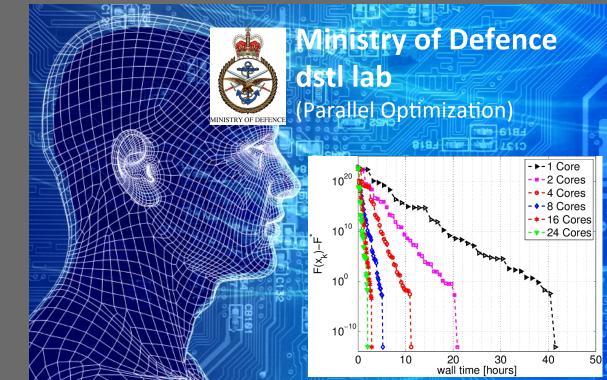
### **Application Areas**

- Natural language processing
  - speech recognition
- Text processing
  - text prediction, recognition, machine translation, spam filtering
- Image & video processing
  - deblurring, denoising, inpainting, face detection and recognition
- Social networks
  - community detection, geo-tagging of tweets
- Public records analysis
  - tax data, financial records, health records
- Online advertising
  - ad allocation, ad pricing
- Scientific measurements
  - truss topology design, inverse problems, data assimilation, gene expression analysis,

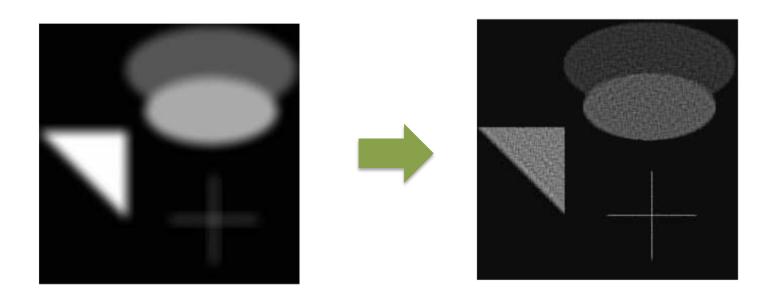








### Image Deblurring



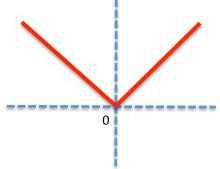


Amir Beck and Marc Teboulle. **A Fast Iterative Shrinking-Thresholding Algorithm for Linear Inverse Problems.** *SIAM J. Imaging Sciences* 2(1), 183-202, 2009



Jakub Konečný, Jie Liu, P.R., Martin Takáč. **Mini-Batch Semi-Stochastic Gradient Descent in the Proximal Setting.** *IEEE Journal of Selected Topics in Signal Processing* 10(2), 242-255, 2016

# Image Deblurring: "LASSO" Problem



blurred image

$$\min_{x \in \mathbb{R}^n} \frac{1}{2} ||Ax - b||_2^2 + \lambda ||x||_1$$

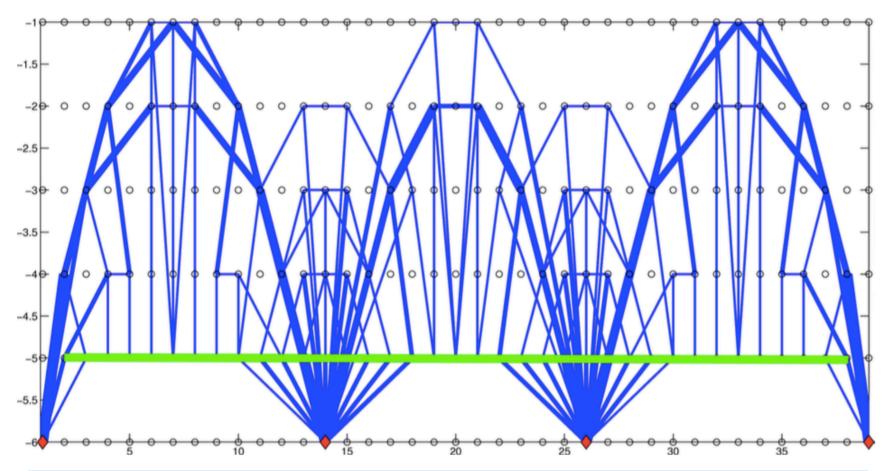
image

# pixels in the image

Blurring matrix multiplied by a wavelet basis matrix

Encourages sparsity in the wavelet basis

### Truss Topology Design

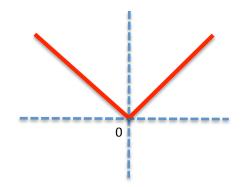




P.R. and Martin Takáč. Efficient Serial and Parallel Coordinate Descent Methods for Huge-Scale Truss Topology Design. Operations Research Proceedings, pp 27-32, 2012

### Truss Topology Design: "LASSO" Problem

**Encodes all** potential bars



$$\min_{x \in \mathbb{R}^n}$$

$$\min_{x \in \mathbb{R}^n} \frac{1}{2} ||Ax - b||_2^2 + \lambda ||x||_1$$

- 
$$\lambda \|x\|_1$$



# potential bars (quadratic in mesh size)

Least-squares (convex, smooth, quadratic)

L1 norm (convex, nonsmooth, but "simple")

### **Image Segmentation**









Olivier Fercoq and P.R. **Accelerated, Parallel and Proximal Coordinate Descent.** *SIAM Journal on Optimization* 25(4), 1997-2023, 2015



Alina Ene and Huy L. Nguyen. Random Coordinate Descent Methods for Minimizing Decomposable Submodular Functions. *ICML* 2015

# Image Segmentation: Reformulated Submodular Optimization

minimize

$$\frac{1}{2} \left\| \sum_{i=1}^{n} x^{i} \right\|^{2}$$
Smooth, convex, quadratic

subject to

$$x^{i} \in P^{i}, i = 1, 2, \dots, n$$

# polytope

grows with the image size

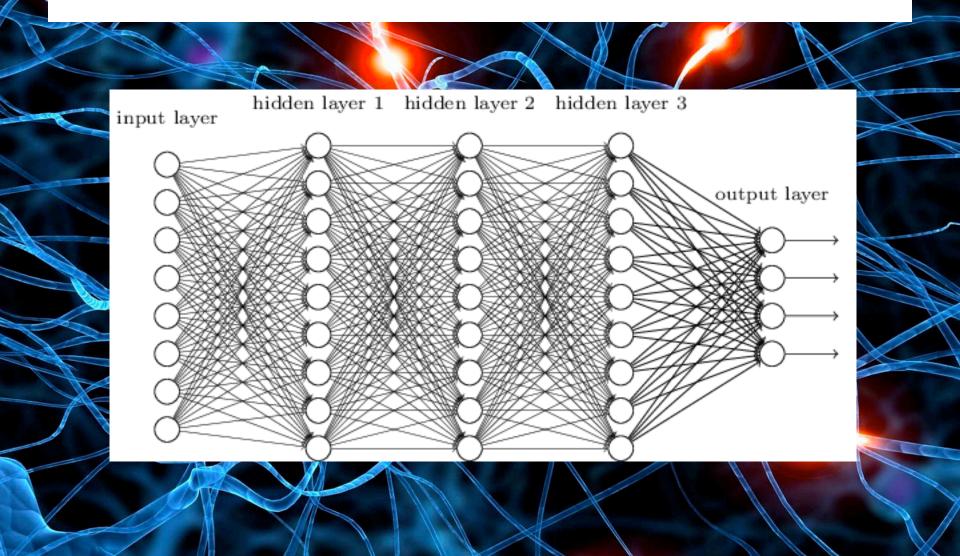
### Predicting Expert Moves in Go



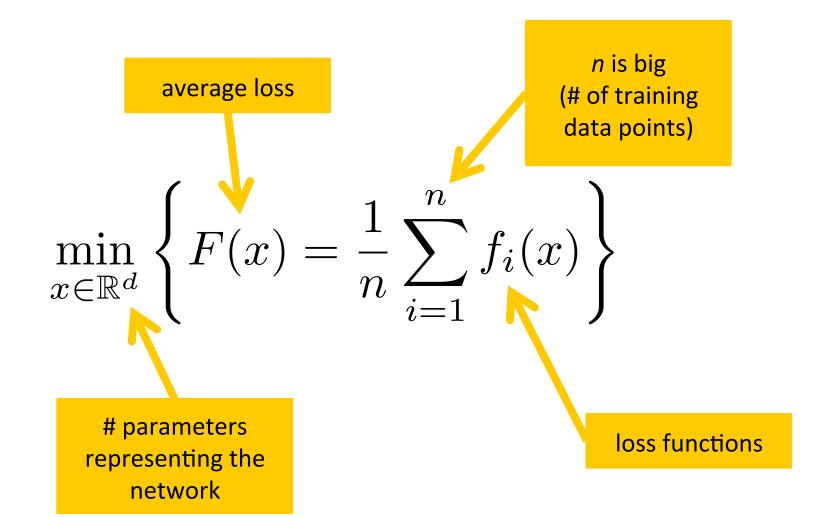


Silver et al. Mastering the Game of Go with Deep Neural Networks and Tree Search. *Nature* 529, pp 484–489, 2016

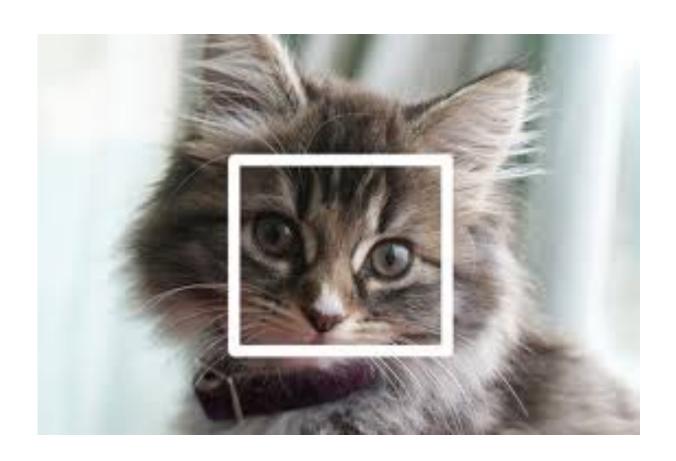
### Go: Training a Neural Network



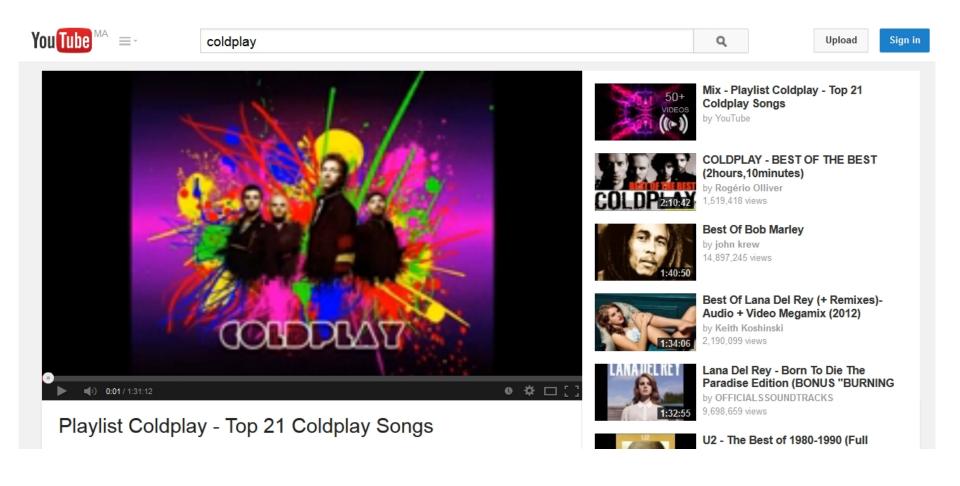
### Go: Training a Neural Network



### **Face Detection**



### Recommender Systems



### **Geotagging Tweets**





arXiv.org > cs > arXiv:1404.7152

Search or Ar

Computer Science > Social and Information Networks

### Geotagging One Hundred Million Twitter Accounts with Total Variation Minimization

Ryan Compton, David Jurgens, David Allen

(Submitted on 28 Apr 2014)

Geographically annotated social media is extremely valuable for modern information retrieval. However, when researchers can only access publicly-visible data, one quickly finds that social media users rarely publish location information. In this work, we provide a method which can geolocate the overwhelming majority of active Twitter users, independent of their location sharing preferences, using only publicly-visible Twitter data.

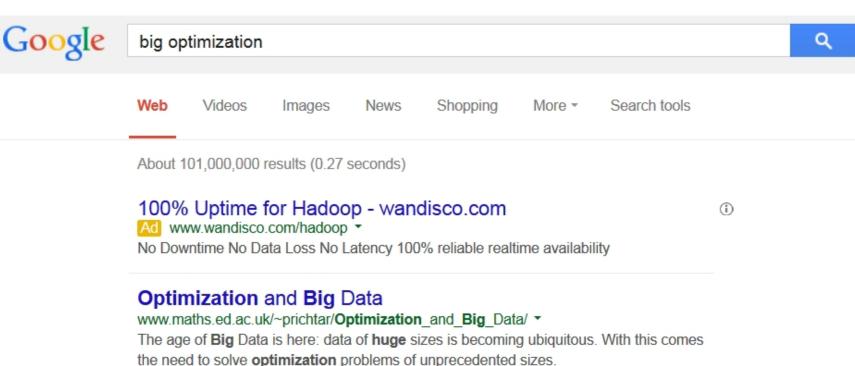
Our method infers an unknown user's location by examining their friend's locations. We frame the geotagging problem as an optimization over a social network with a total variation-based objective and provide a scalable and distributed algorithm for its solution. Furthermore, we show how a robust estimate of the geographic dispersion of each user's ego network can be used as a per-user accuracy measure, allowing us to discard poor location inferences and



## Spam Filtering



### Ranking



### Optimization and Big Data - School of Mathematics ...

www.maths.ed.ac.uk/~prichtar/**Optimization\_**and\_**Big...**/schedule.html ▼ Big data optimization at SAS. 14:30-15:10, Olivier Fercoq (Edinburgh, UK).

#### IBM - Business Analytics and Optimization - Big Data ...

www.ibm.com/services/us/gbs/business-analytics/ ▼ IBM ▼

Business analytics and **big** data consulting services from IBM help discover predictive insights and turn them into operational reality to close the gap between ...

### **Application in Focus**

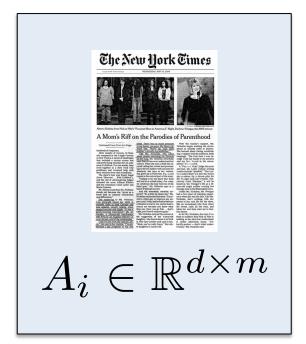
# **Training Linear Predictors**

"Predict based on past observations"

### Statistical Nature of Data

$$(A_i, y_i) \sim Distribution$$

#### **DATA**



#### **LABEL**

"politics"

$$y_i \in \mathbb{R}^m$$

### Prediction of Labels from Data

Find 
$$w \in \mathbb{R}^d$$
 Linear predictor

such that when a (data, label) pair is drawn from the distribution

$$(A_i, y_i) \sim Distribution$$

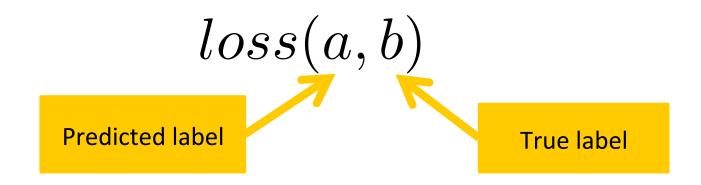
then

$$A_i^{\top} w \approx y_i$$

**Predicted label** 

True label

### Measure of Success



We want the expected loss (=risk) to be small:

$$\mathbf{E}\left[loss(A_i^\top w, y_i)\right]$$

$$(A_i, y_i) \sim Distribution$$

#### Replace Expectation by Average

Draw i.i.d. data samples from the distribution

$$(A_1, y_1), (A_2, y_2), \ldots, (A_n, y_n) \sim Distribution$$

Output predictor which minimizes the empirical risk:

$$\min_{w \in \mathbb{R}^d} \frac{1}{n} \sum_{i=1}^n loss(A_i^\top w, y_i)$$

## Minimize the Average of a Large Number of Functions

$$\min_{x \in \mathbb{R}^d} \left\{ F(x) = rac{1}{n} \sum_{i=1}^n f_i(x) 
ight\}$$

# Part 3 Methods

### Optimization with Big Data

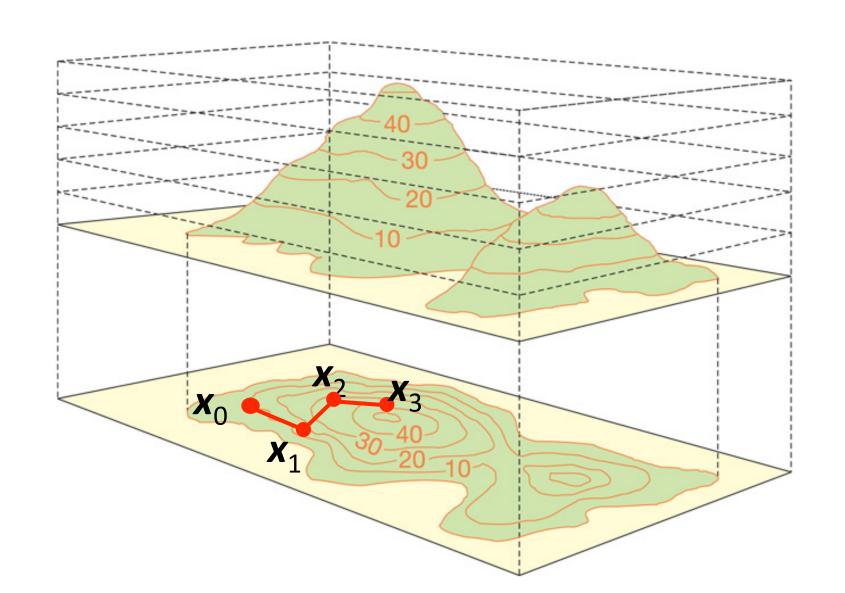
= Extreme\* Mountain Climbing

\* in a billion dimensional space on a foggy day

### God's Algorithm = Teleportation



#### Mortals Have to Walk...



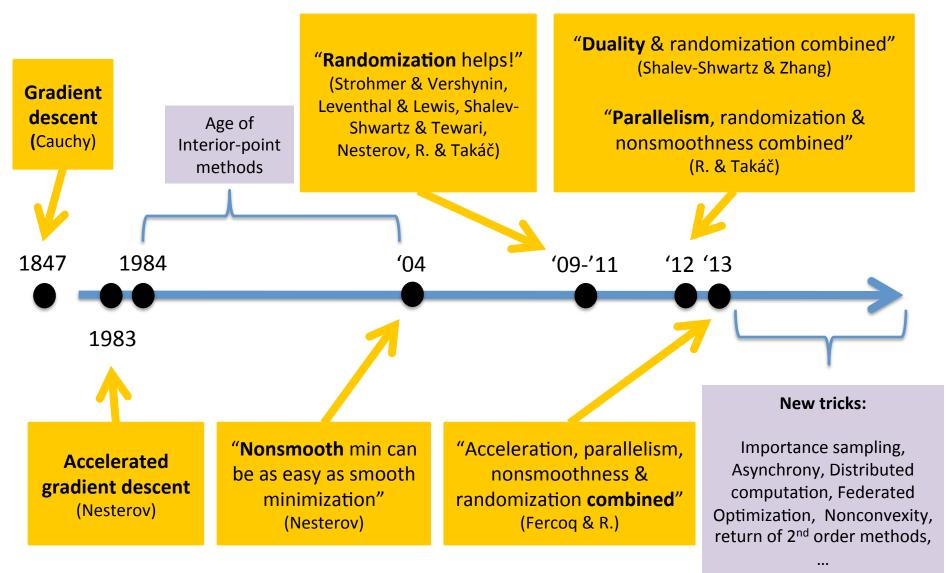
#### Algorithmic Tricks

- Gradient descent
- 2. Handling nonsmoothness via the proximal trick
- 3. Acceleration
- 4. Randomized decomposition
- 5. Parallelism/Minibatching & Sparsity
- 6. Distributed computation
- 7. Importance sampling

All these tricks can be combined!

There are more tricks: duality, variance reduction, asynchrony, curvature, ...

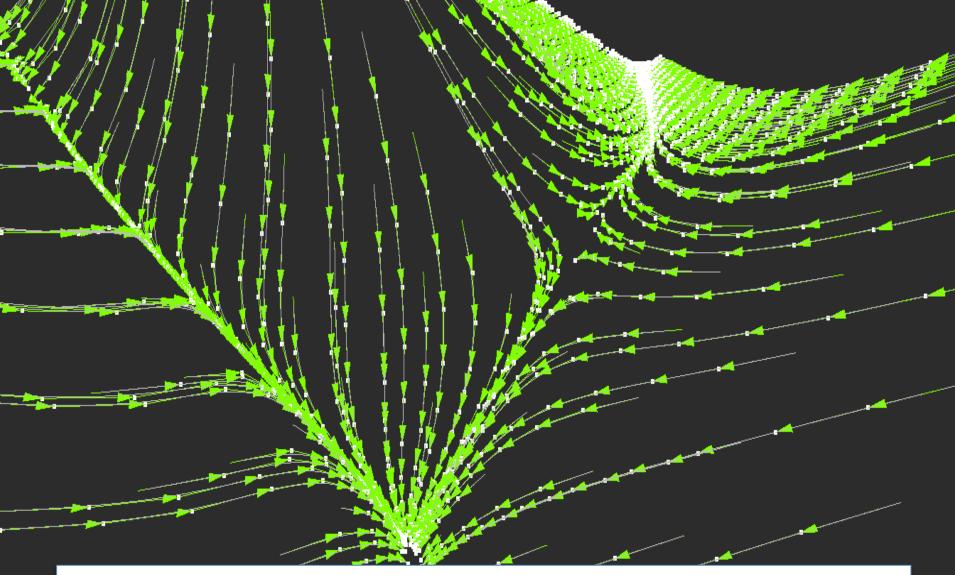
# Brief, Biased and Severely Incomplete History of Big Data Optimization



#### Tool 1

### **Gradient Descent (1847)**

"Just follow a ball rolling down the hill"





**Augustin Cauchy** 

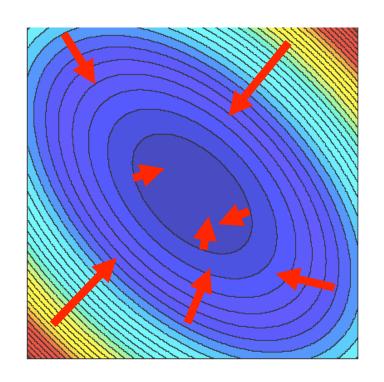
Méthode générale pour la résolution des systèmes d'équations simultanées, pp. 536-538, 1847

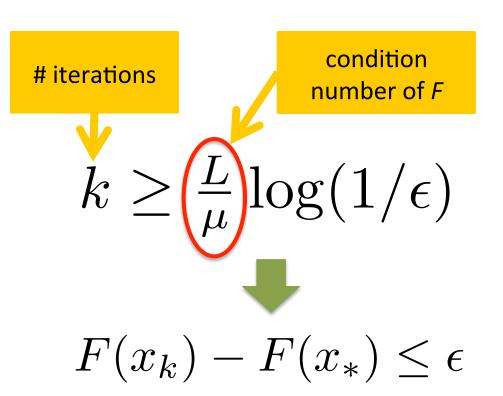
#### The Problem

$$\min_{x \in \mathbb{R}^d} F(x)$$

#### **Gradient Descent (GD)**

$$x_{k+1} = x_k - \frac{1}{L}\nabla F(x_k)$$



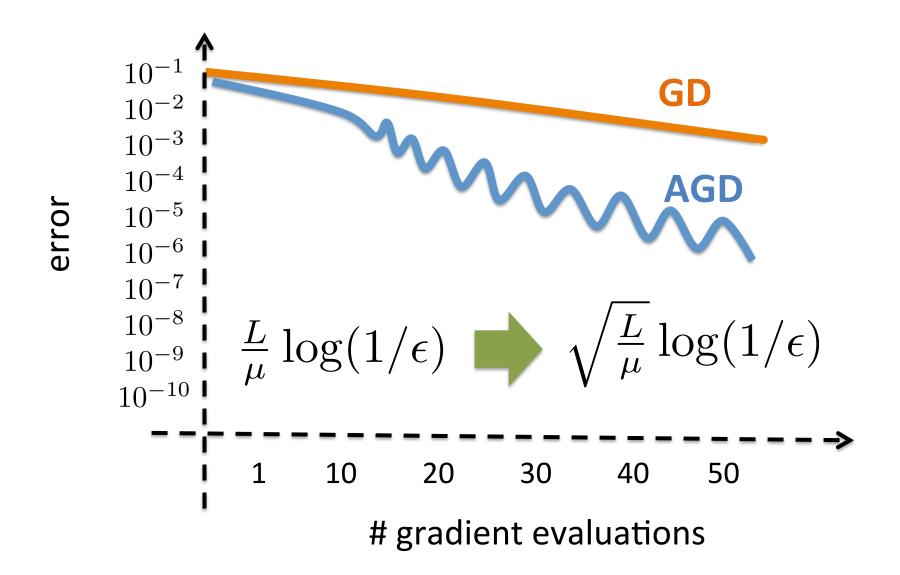


#### Tool 2

## Acceleration (1983/2003)

"Gradient descent can be made much faster!"

#### Acceleration Works (Mysteriously)



#### Acceleration

- Reignited interest in gradient methods
- Usage in all areas of data science (called momentum in deep neural networks literature)
- Oscilation can be tamed (e.g., by restarting)
- Can be combined with other tricks
  - Duality [Shai-Shalev Shwartz & Zhang 2013]
  - Randomized decomposition, Parallelism, Proximal trick [Fercog & R 2013]



Yurii Nesterov

Introductory lectures on convex optimization: a basic course Kluwer, Boston, 2003



Yurii Nesterov

A method for unconstrained convex minimization problem with the rate of convergence  $O(1 / k^2)$ 

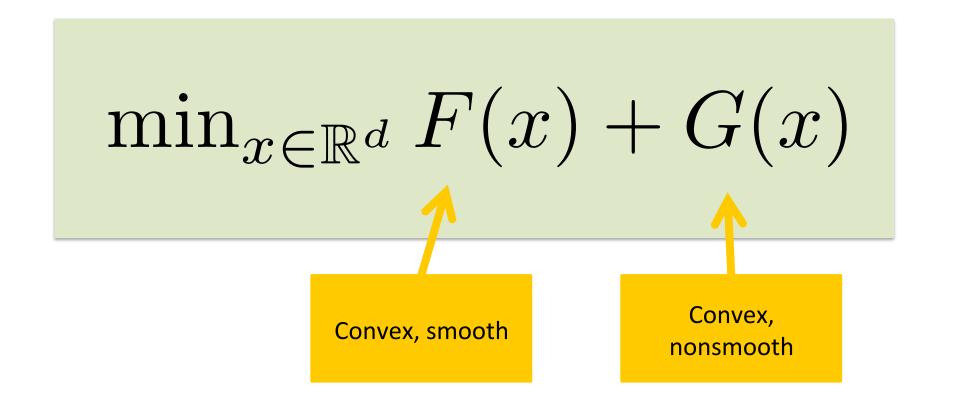
Soviet Math. Doclady 269, 543-547, 1983

#### Tool 3

## Proximal Trick (2004)

"Some nonsmooth problems are as easy as smooth problems"

#### The Problem



#### Proximal Gradient Descent (PGD)

#### **STEP 1:** Pretend there is no *G*

$$z_{k+1} = x_k - \frac{1}{L}\nabla F(x_k)$$

**STEP 2:** Take a "proximal" step with respect to *G* 

$$x_{k+1} = \arg\min_{x} \frac{1}{2} ||x - z_{k+1}||^2 + \frac{1}{L}G(x)$$

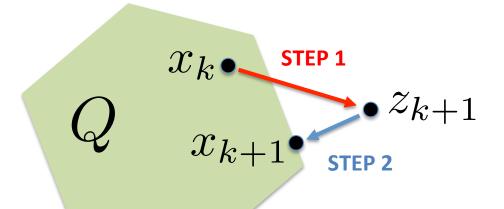
- 1. Gradient Descent is a special case for G = 0
- 2. Even though this is a nonsmooth problem, # steps is the same as for Gradient Descent!!!  $\frac{L}{\mu} \log(1/\epsilon)$
- 3. Efficient if Step 2 is easy to do

#### Example: Projected Gradient Descent

$$\min_{x \in Q} F(x) \quad \Leftrightarrow \quad \min_{x} F(x) + G(x)$$

Convex set

$$G(x) = \begin{cases} 0 & x \in Q \\ +\infty & x \notin Q \end{cases}$$



$$z_{k+1} = x_k - \frac{1}{L}\nabla F(x_k)$$

$$x_{k+1} = \arg\min_{x} \frac{1}{2} ||x - z_{k+1}||^2 + \frac{1}{L}G(x)$$

#### Tool 4

# Randomized Decomposition

"Doing many simple decisions is better than doing a few smart ones"

#### Why Randomize?



# Stochastic Gradient Descent



H. Robbins and S. Monro

**A Stochastic Approximation Method** 

Annals of Mathematical Statistics 22, pp. 400–407, 1951

#### The Problem

$$\min_{x \in \mathbb{R}^d} \left\{ F(x) = \frac{1}{n} \sum_{i=1}^n f_i(x) \right\}$$

#### Stochastic Gradient Descent (SGD)

stepsize

Update rule:

$$x_{k+1} = x_k - h_k \nabla f_i(x_k)$$

$$\mathbb{E}[\nabla f_i(x)] = \nabla F(x)$$

Complexity:

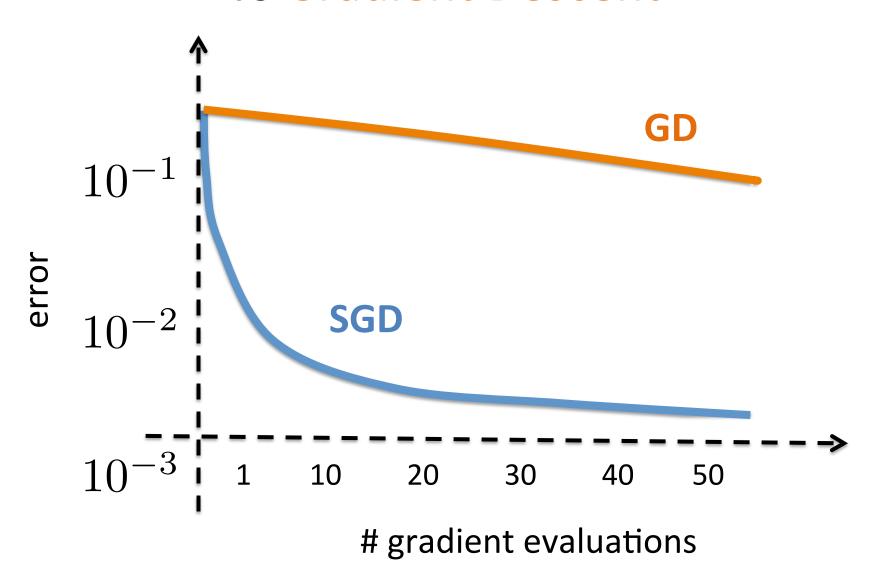
*i* = chosen uniformly at random

$$\mathcal{O}\left(\frac{L}{\mu}\frac{1}{\epsilon}\right)$$

Cost of a single iteration: 1

# stochastic gradient evaluations

## Stochastic Gradient Descent vs Gradient Descent



# Randomized Coordinate Descent



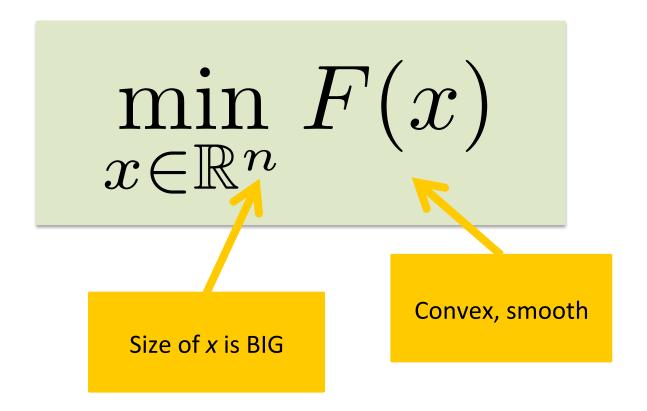
P.R. and Martin Takáč

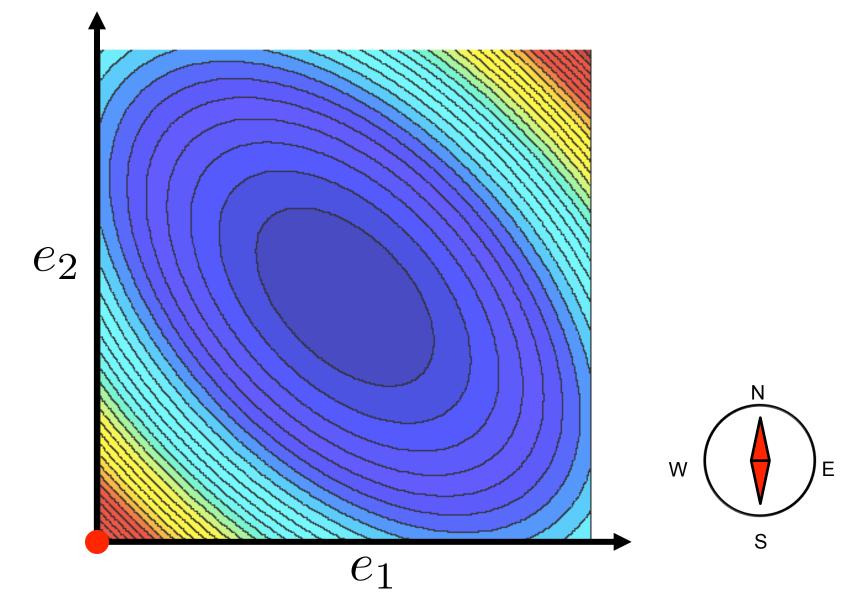
**Iteration Complexity of Randomized Block Coordinate Descent Methods for Minimizing a Composite Function** *Mathematical Programming* 144(2), 1-38, 2014

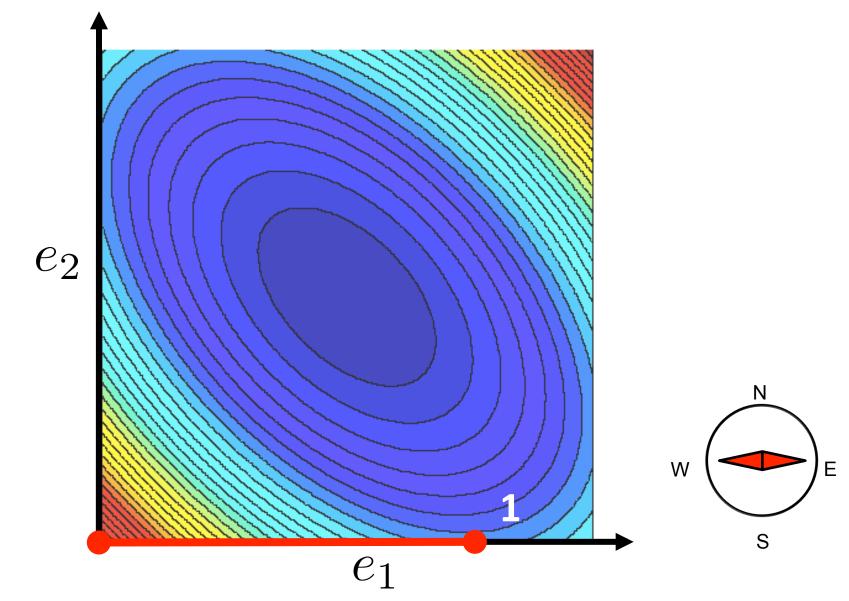
INFORMS Computing Society Best Student Paper Prize (runner up), 2012

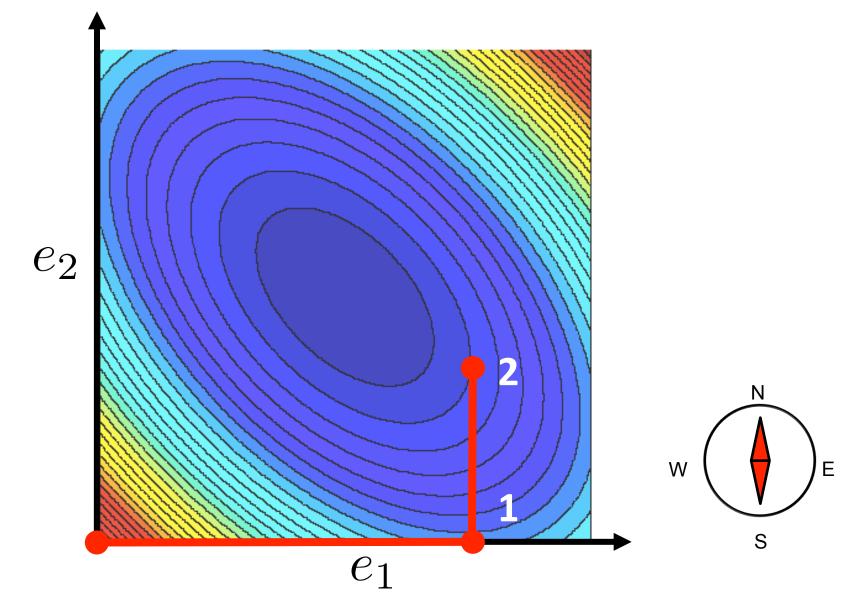
2014 OR Society Doctoral Prize

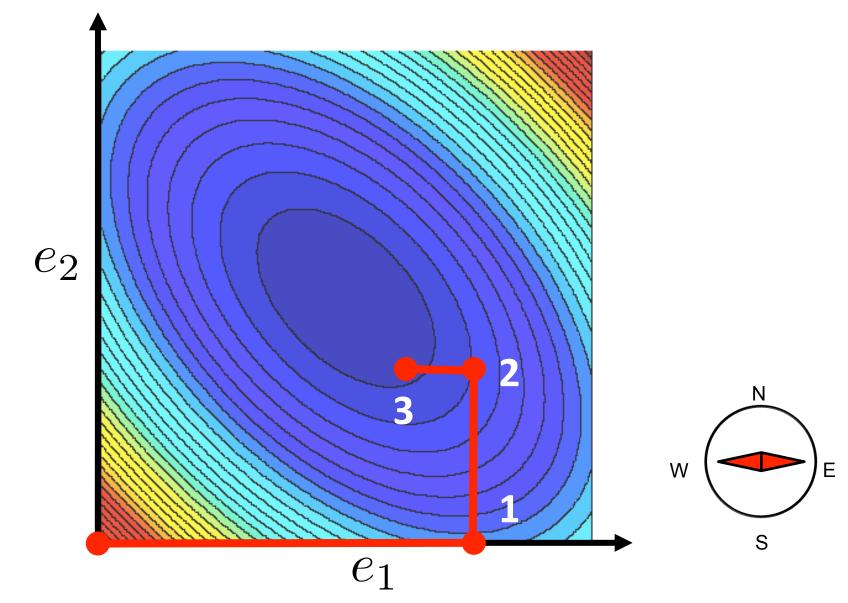
#### The Problem

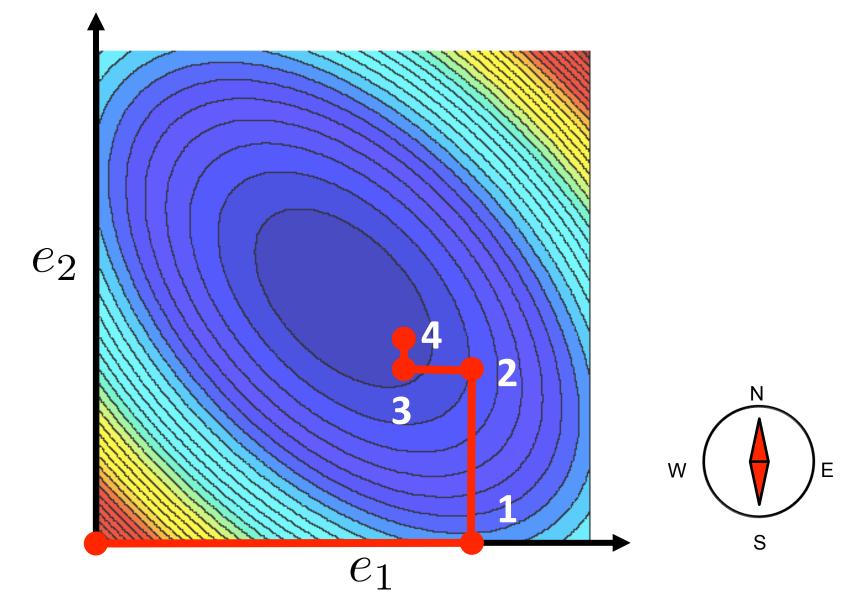


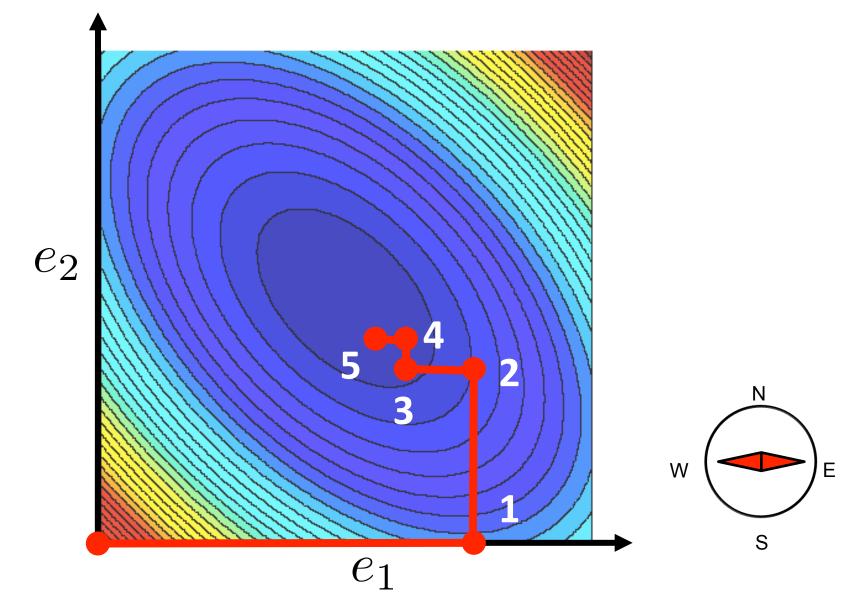


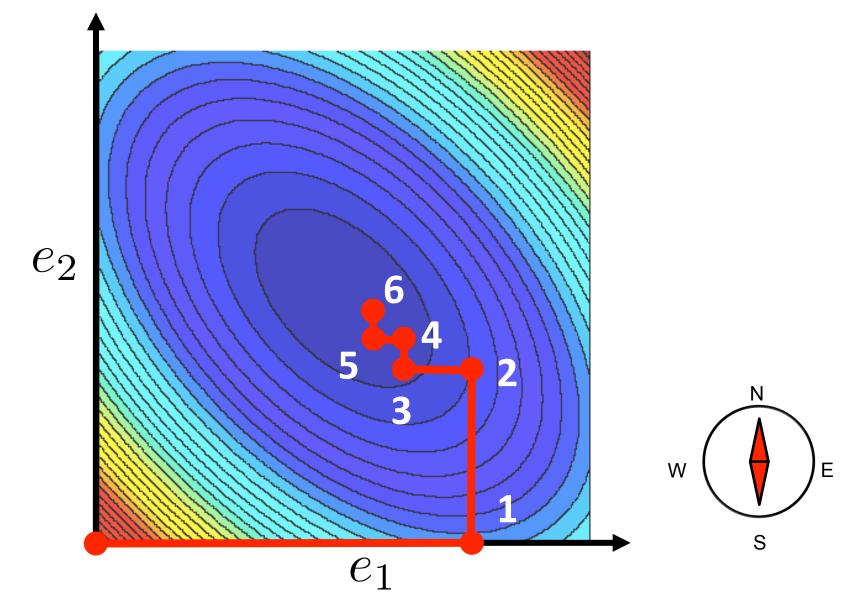


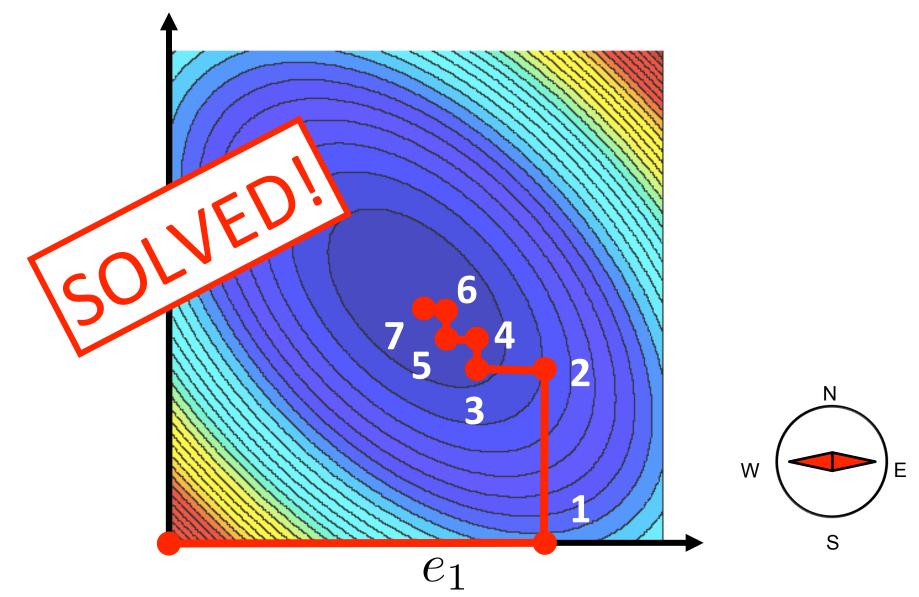


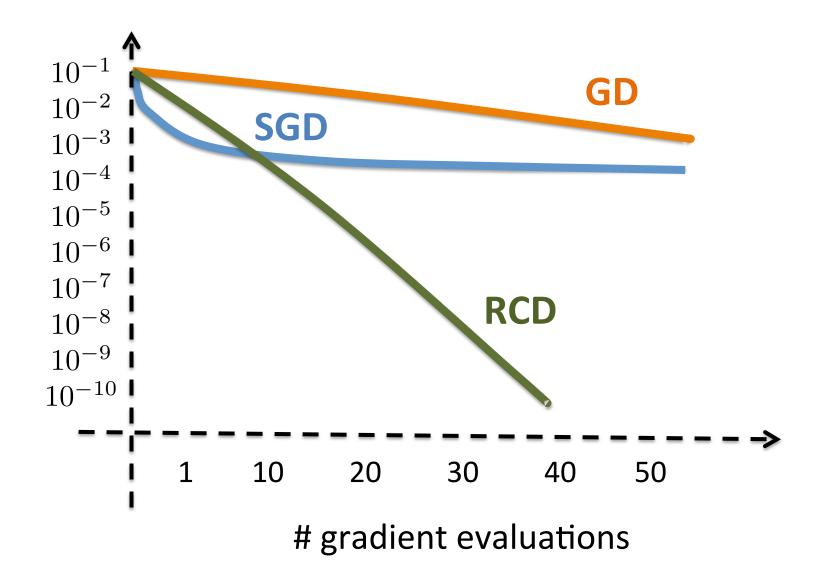












#### 1 Billion Rows & 100 Million Variables

$$A \in \mathbf{R}^{10^9 \times 10^8}$$

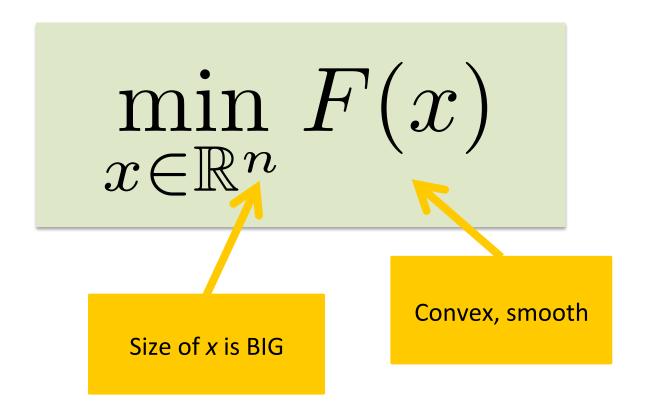
k/n	$F(x_k) - F^*$	$\#$ nonzeros in $x_k$	time [s]
0.01	$< 10^{18}$	18,486	1.32
9.35	$< 10^{14}$	$99,\!837,\!255$	1294.72
11.97	$< 10^{13}$	99,567,891	1657.32
14.78	$< 10^{12}$	98,630,735	2045.53
17.12	$< 10^{11}$	96,305,090	2370.07
20.09	$< 10^{10}$	86,242,708	2781.11
22.60	$< 10^9$	58,157,883	3128.49
24.97	$< 10^8$	19,926,459	3455.80
28.62	$< 10^7$	$747{,}104$	3960.96
31.47	$< 10^{6}$	$266,\!180$	4325.60
34.47	$< 10^5$	175,981	4693.44
36.84	$< 10^4$	$163,\!297$	5004.24
39.39	$< 10^3$	$160,\!516$	5347.71
41.08	$< 10^2$	$160,\!138$	5577.22
43.88	$< 10^{1}$	160,011	5941.72
45.94	$< 10^{0}$	$160,\!002$	6218.82
46.19	$< 10^{-1}$	160,001	6252.20
46.25	$< 10^{-2}$	160,000	6260.20
46.89	$< 10^{-3}$	160,000	6344.31
46.91	$< 10^{-4}$	160,000	6346.99
46.93	$< 10^{-5}$	160,000	6349.69

#### Tool 5

# **Parallelism**

"Work on random subsets"

#### The Problem



# Parallel Randomized Coordinate Descent

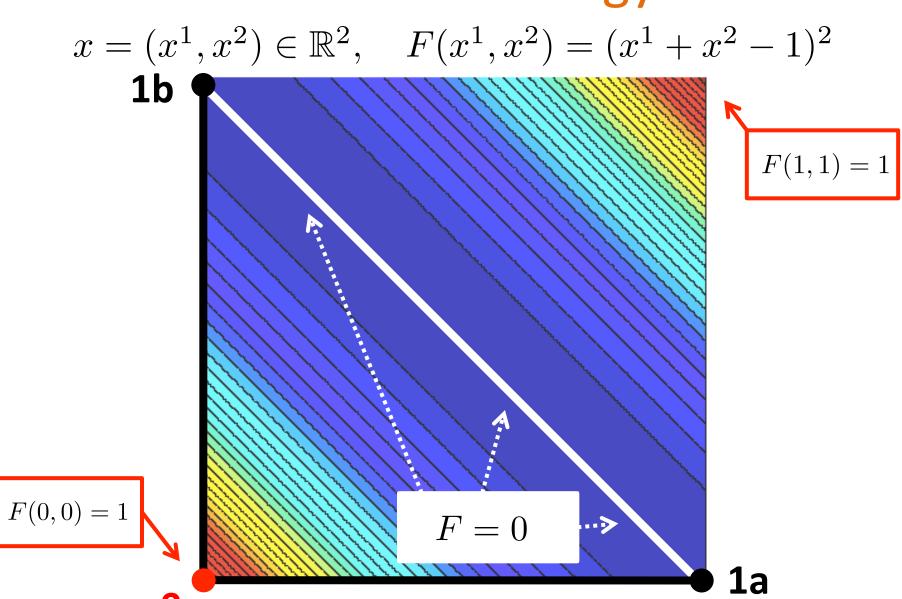


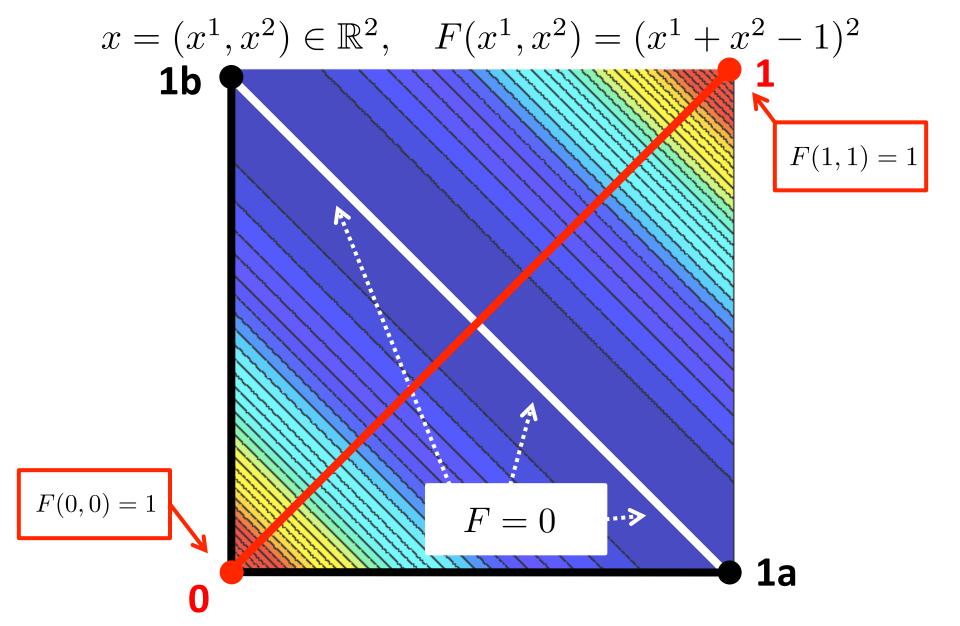
P.R. and Martin Takáč

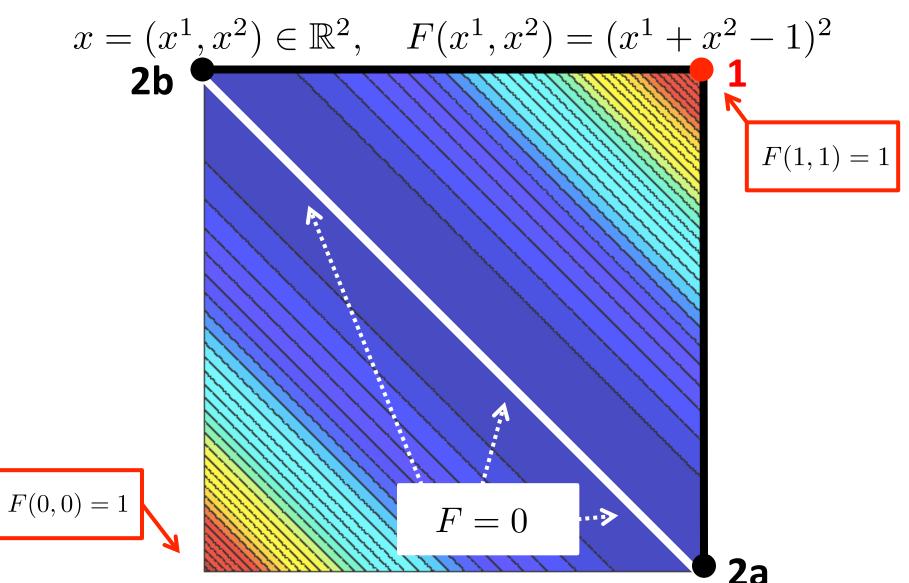
Parallel Coordinate Descent Methods for Big Data Optimization Mathematical Programming 156(1), 433-484, 2016

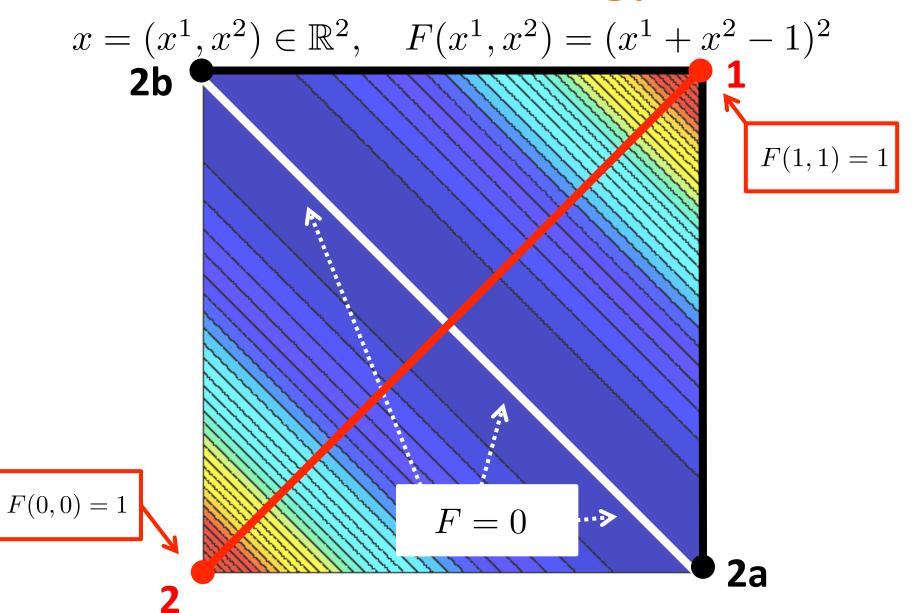
16<sup>th</sup> IMA Leslie Fox Prize (2<sup>nd</sup>), 2013

2014 OR Society Doctoral Prize





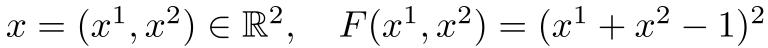


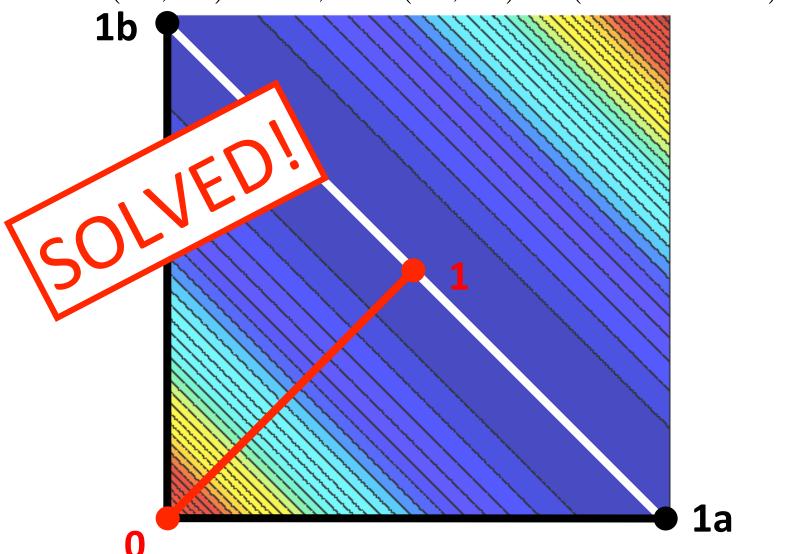


$$x = (x^1, x^2) \in \mathbb{R}^2, \quad F(x^1, x^2) = (x^1 + x^2 - 1)^2$$



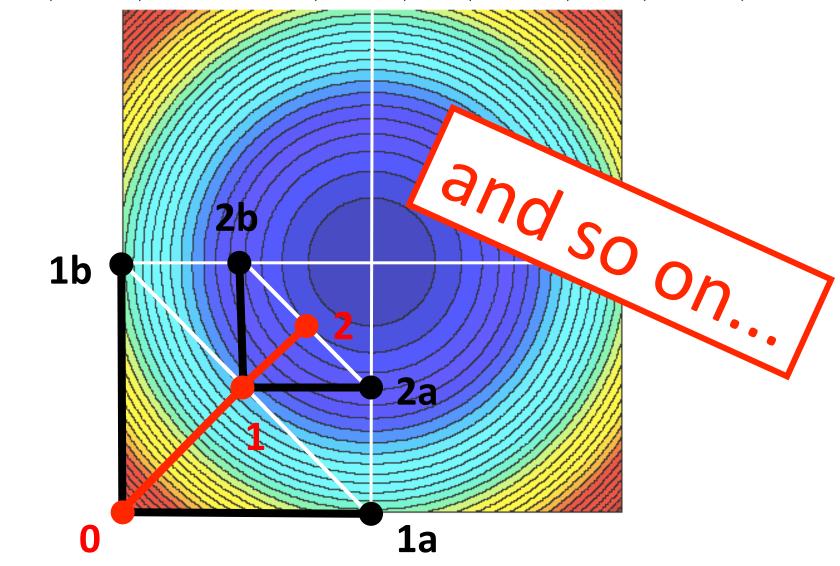
# **Averaging Strategy**





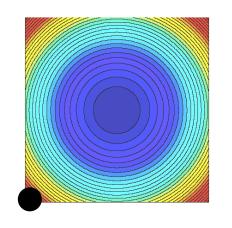
#### Averaging Can Be Bad, Too!

$$x = (x^1, x^2) \in \mathbb{R}^2, \quad F(x^1, x^2) = (x^1 - 1)^2 + (x^2 - 1)^2$$

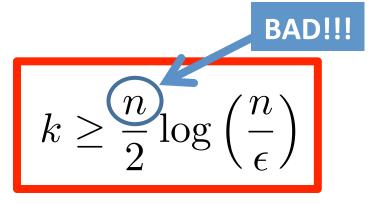


# Actually, Averaging Can Be Very Bad!

$$F(x) = (x^{1} - 1)^{2} + (x^{2} - 1)^{2} + \dots + (x^{n} - 1)^{2}$$



$$x_0 = 0 \in \mathbb{R}^n \implies F(x_0) = n$$

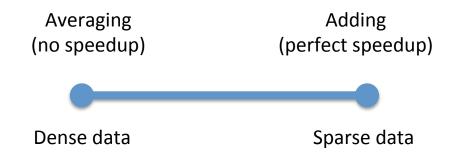




$$F(x_k) = n\left(1 - \frac{1}{n}\right)^{2k} \le \epsilon$$

#### How to Combine the Updates?

- We should do datadependent combination of the results obtained in parallel
- There is rich theory for this now



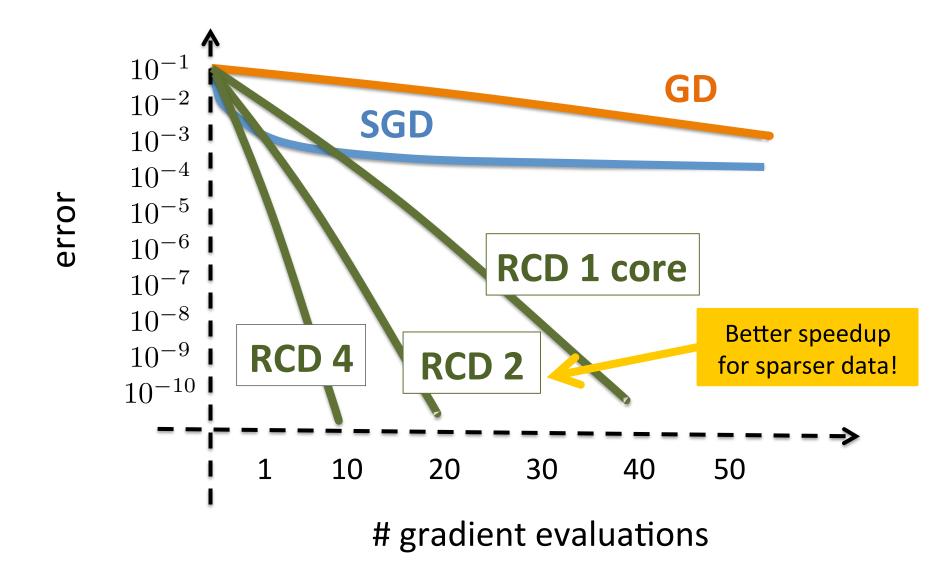


Zheng Qu and P.R.

**Coordinate Descent with Arbitrary Sampling II: Expected Separable Overapproximation** 

Optimization Methods and Software 31(5), 858-884, 2016

#### Performance



#### Problem with 1 Billion Variables

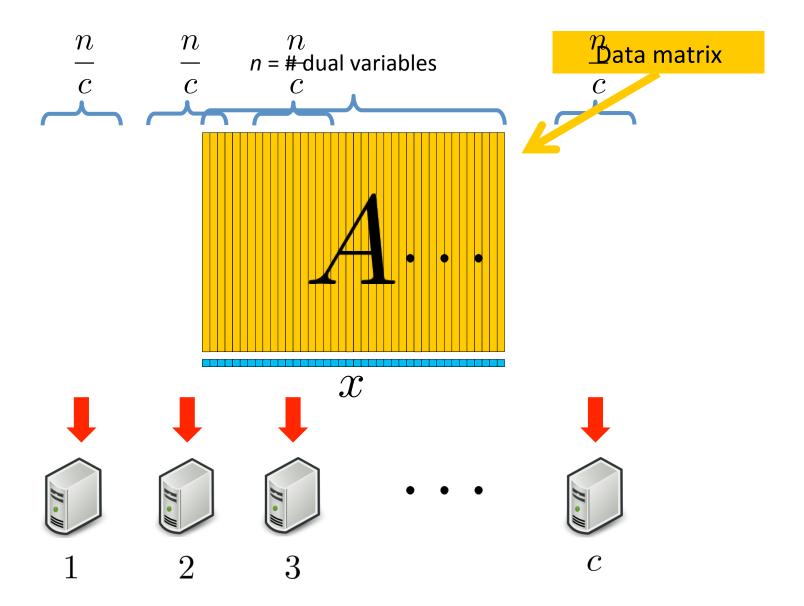
	$F(x_k) - F^*$		Elapsed Time			
$(k \cdot \tau)/n$	1 core	8 cores	16 cores	1 core	8 cores	16 cores
0	6.27e+22	6.27e+22	6.27e+22	0.00	0.00	0.00
1	2.24e+22	2.24e+22	2.24e+22	0.89	0.11	0.06
2	2.25e+22	3.64e+19	2.24e+22	1.97	0.27	0.14
3	1.15e+20	1.94e+19	1.37e+20	3.20	0.43	0.21
4	5.25e+19	1.42e+18	8.19e+19	4.28	0.58	0.29
5	1.59e+19	1.05e+17	3.37e+19	5.37	0.73	0.37
6	1.97e+18	1.17e+16	1.33e+19	6.64	0.89	0.45
7	2.40e+16	3.18e+15	8.39e+17	7.87	1.04	0.53
:	:	:	:	:	:	:
26	3.49e+02	4.11e+01	3.68e+03	31.71	3.99	2.02
27	1.92e+02	5.70e+00	7.77e+02	33.00	4.14	2.10
28	1.07e+02	2.14e+00	6.69e+02	34.23	4.30	2.17
29	6.18e+00	2.35e-01	3.64e+01	35.31	4.45	2.25
30	4.31e+00	4.03e-02	2.74e+00	36.60	4.60	2.33
31	6.17e-01	3.50e-02	6.20e-01	37.90	4.75	2.41
32	1.83e-02	2.41e-03	2.34e-01	39.17	4.91	2.48
33	3.80e-03	1.63e-03	1.57e-02	40.39	5.06	2.56
34	7.28e-14	7.46e-14	1.20e-02	41.47	5.21	2.64
35	-	-	1.23e-03	-	-	2.72
36	-	-	3.99e-04	-	-	2.80
37	-	-	7.46e-14	-	-	2.87

#### Tool 6

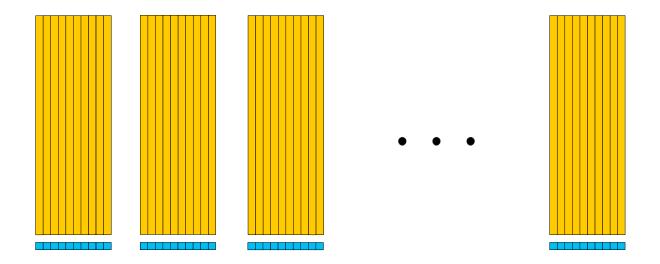
# **Distributed Computation**

"Communication hurts"

#### Distribution of Data

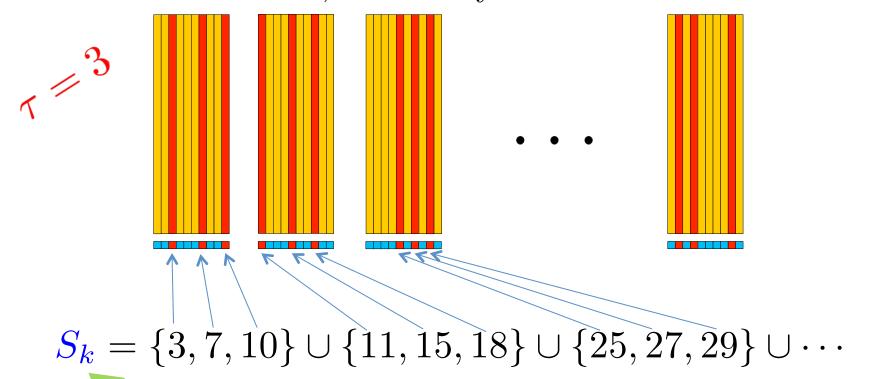


# Distributed sampling



# Distributed sampling

Each computer (node) independently pick  $\tau$  variables from those it owns, uniformly at random



Random set of variables

Also see: CoCoA+ [Ma, Smith, Jaggi et al 15]

# There is Theory for this...

**Key:** Get the right stepsize parameters *v* 

The leading term in the complexity bound then is:

$$\max_{i} \left( \frac{1}{p_i} + \frac{v_i}{p_i \lambda \gamma n} \right)$$

$$\frac{n}{c\tau} + \frac{\text{Something that looks complicated}}{\lambda \gamma c \tau}$$

$$\frac{n}{c\tau} + \max_{i} \frac{\lambda_{\max}\left(\sum_{j=1}^{d} \left(1 + \frac{(\tau-1)(\omega_{j}-1)}{\max\{n/c-1,1\}} + \left(\frac{\tau c}{n} - \frac{\tau-1}{\max\{n/c-1,1\}}\right) \frac{\omega_{j}'-1}{\omega_{j}'} \omega_{j}\right) A_{ji}^{\top} A_{ji}\right)}{\lambda \gamma c \tau}$$

#### Experiment

Machine: 128 nodes of Hector Supercomputer (4096 cores)

**Problem:** LASSO, n = 1 billion, d = 0.5 billion, 3 TB



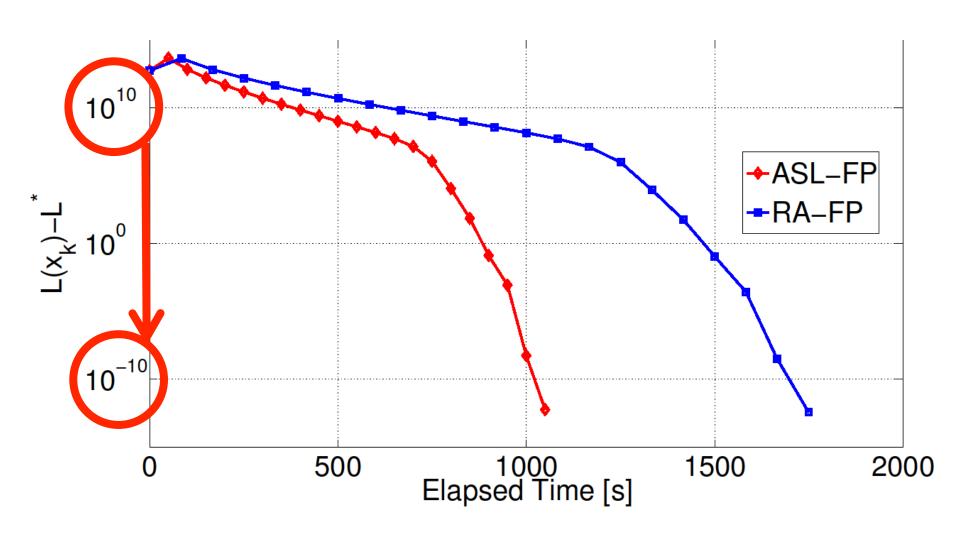
2014 OR Society Doctoral Prize



P.R. and Martin Takáč

**Distributed Coordinate Descent for Learning with Big Data** *Journal of Machine Learning Research* 17:1-25, 2016

#### LASSO: 3TB data + 128 nodes



#### Experiment

Machine: 128 nodes of Archer Supercomputer

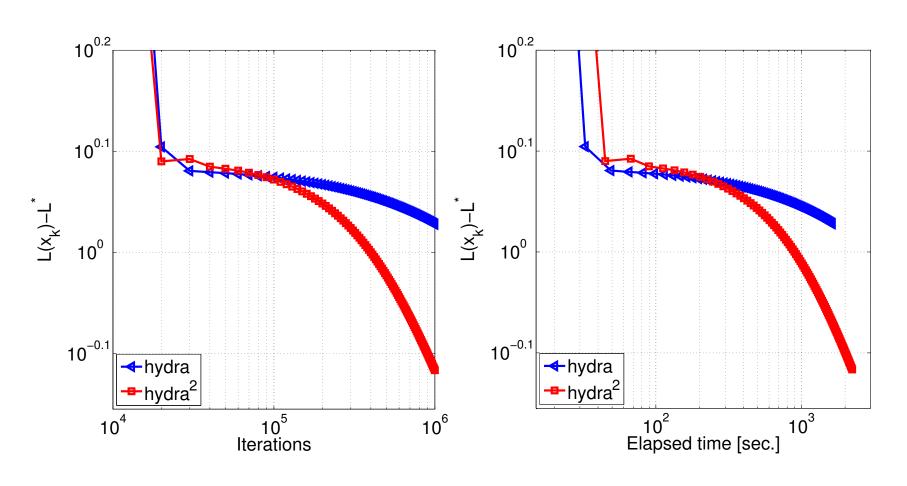
**Problem:** LASSO, n = 5 million, d = 50 billion, 5 TB (60,000 nnz per row of A)



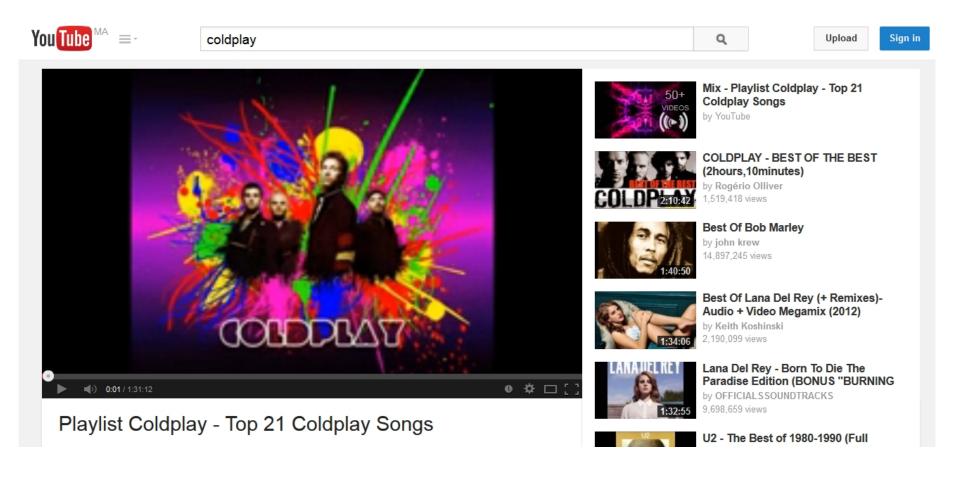


Olivier Fercoq, Zheng Qu, P.R. and Martin Takáč. Fast Distributed Coordinate Descent for Minimizing Non-strongly Convex Losses *IEEE Int. Workshop on Machine Learning for Signal Processing*, 2014

# LASSO: 5TB data (d = 50 billion) 128 nodes



#### Used in YouTube



#### Tool 7

# Importance Sampling

"Sample more important data more often"





P.R. and Martin Takáč

On Optimal Probabilities in Stochastic Coordinate Descent Methods Optimization Letters 10(6), 1233-1243, 2015

2014 OR Society Doctoral Prize

#### The Problem

$$\min_{x \in \mathbb{R}^n} F(x)$$

Smooth and strongly convex



#### **Arbitrary Sampling:**

$$S_k \subseteq \{1, 2, \dots, n\}$$

Choose a random set  $S_k$  of coordinates

For  $i \in S_k$  do

$$x_{k+1}^i \leftarrow x_k^i - \frac{1}{v_i} \nabla_i F(x_k)$$

For  $i \notin S_k$  do

$$x_{k+1}^i \leftarrow x_k^i$$

Partial derivative

Stepsize parameter

# **Complexity Theorem**

$$k \geq \left(\max_{i} \frac{v_{i}}{p_{i}\mu}\right) \log \left(\frac{F(x_{0}) - F(x_{*})}{\epsilon \rho}\right)$$

$$p_i = \mathbb{P}(i \in S_k)$$

strong convexity constant of *F* 

$$\mathbb{P}\left(F(x_k) - F(x_*) \le \epsilon\right) \ge 1 - \rho$$

# Uniform vs Optimal Sampling

$$p_i = \frac{1}{n}$$



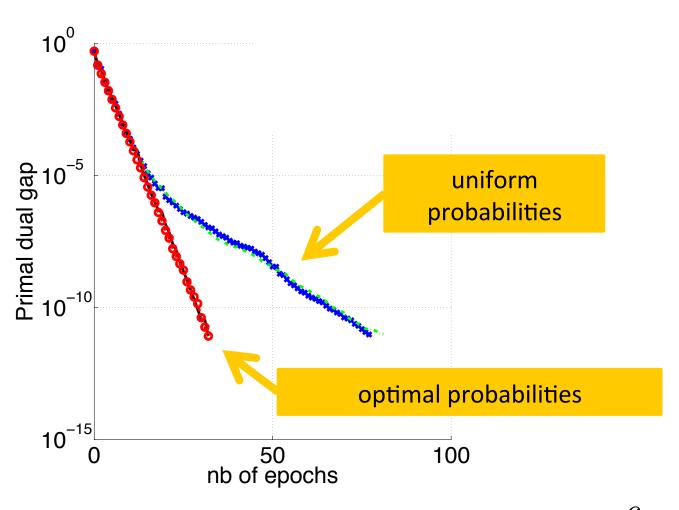
$$\max_{i} \frac{v_i}{p_i \mu} = \frac{n \max_{i} v_i}{\mu}$$

$$p_i = \frac{v_i}{\sum_i v_i}$$



$$\max_{i} \frac{v_i}{p_i \mu} = \frac{\sum_{i} v_i}{\mu}$$

#### Uniform vs Optimal Sampling



Data = cov1,  $n = 522,911, \mu = 10^{-6}$ 

# Part 4 Conclusion

#### Conclusion

- Data, data science, machine learning, ATI
- Data science applications
  - structure of the objective (simple, data-defined)
  - imaging, empirical risk minimization, truss topology design, spam filtering, ...
- Outlined a few key tools/tricks developed for big data optimization



Martin Takáč (Lehigh)



Jakub Mareček (IBM)



Zheng Qu (Hong Kong)



Olivier Fercoq (Telecom ParisTech)



Rachael Tappenden (Johns Hopkins)



Robert M Gower (Edinburgh)



Virginia Smith (Berkeley)



Jakub Konečný (Edinburgh)



**Jie Liu** (Lehigh)



Michael Jordan (Berkeley)



Dominik Csba (Edinburgh)



Tong Zhang (Rutgers & Baidu)



Zeyuan Allen-Zhu (Princeton)



Nati Srebro (TTI Chicago)



Donald Goldfarb (Columbia)



Chenxin Ma (Lehigh)



Martin Jaggi (ETH Zurich)