

EE270

Large scale matrix computation, optimization and learning

Instructor : Mert Pilanci

Stanford University

Tuesday, Jan 12 2021

Outline

- Introduction
- Administrative
- Overview of topics and applications

Administrative

Teaching staff

- ▶ Instructor: Mert Pilanci
 - ▶ Email: pilanci@stanford.edu
 - ▶ Office hours: Wednesdays 11am-12pm via Zoom (see Canvas homepage for the Zoom link)
- TA: Tolga Ergen, ergen@stanford.edu
 - ▶ TA office hours: TBA
- ▶ Public web page :
<http://web.stanford.edu/class/ee270/>

Please check Canvas for up-to-date info
For all questions please use Piazza

About EE-270

This course will explore the theory and practice of randomized matrix computation and optimization for large-scale problems to address challenges in modern massive data sets.

- ▶ Our goal in this course is to help you to learn:
 - ▶ **randomized methods** for linear algebra, optimization and machine learning

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 - ▶ **randomized methods** for linear algebra, optimization and machine learning
 - ▶ **probabilistic tools** for analyzing randomized approximations
 - ▶ how to implement **optimization algorithms** for large scale problems
 - ▶ applications in **machine learning, statistics, signal processing and data mining**.

Resources

- ▶ EE 270 Lecture notes, M. Pilanci
(<https://web.stanford.edu/class/ee270/>)
- ▶ Lecture notes on randomized linear algebra. M. Mahoney
- ▶ Sketching as a tool for numerical linear algebra. D. Woodruff
- ▶ Randomized algorithms in numerical linear algebra. R. Kannan and S. Vempala
- ▶ A Practical Guide to Randomized Matrix Computations with MATLAB Implementations. S. Wang
- ▶ Information-theoretic bounds on sketching. M. Pilanci

Prerequisites

- ▶ Familiarity with linear algebra (EE 103 or equivalent).
- ▶ Probability theory and statistics (EE 178 or equivalent)
- ▶ Basic programming skills

Grading policy

- ▶ Homework: 60%, submission via Gradescope.
- ▶ Project: 40% (proposal 10%, poster presentation 15%, report 15%)
- ▶ Extra credit: 5% for Piazza contributions, 5% for scribing/revising lecture notes.

Homework

- ▶ Assigned homeworks will be bi-weekly.
- ▶ The problem sets will include programming assignments to implement algorithms covered in the class.
- ▶ We will also analyze randomized algorithms using probabilistic tools.
- ▶ We support Python and Matlab.

Group Study

- ▶ **Homework:**
 - ▶ Working in groups is allowed, but each member must submit their own writeup.
 - ▶ Write the members of your group on your solutions (Up to four people are allowed).
 - ▶ **Project:**
 - ▶ You will be asked to form groups of about 1-2 people and choose a topic
 - ▶ We'll suggest a list of research problems on the course website
 - ▶ Proposal (1 page)
 - ▶ Poster presentation (last week of classes via Gather.town)
 - ▶ Project report (6 pages max)

Topics

- ▶ randomized linear algebra
 - ▶ approximate matrix and tensor multiplication
 - ▶ approximate verification
 - ▶ sampling and projection methods
 - ▶ bootstrap
- ▶ randomized linear system solvers and regression
 - ▶ Johnson Lindenstrauss embeddings
 - ▶ leverage scores
 - ▶ iterative sketching and preconditioning
 - ▶ high dimensional problems
 - ▶ robust regression
- ▶ matrix decompositions
 - ▶ subspace embeddings
 - ▶ randomized QR decomposition
 - ▶ randomized Singular Value Decomposition
 - ▶ column subset selection

Topics

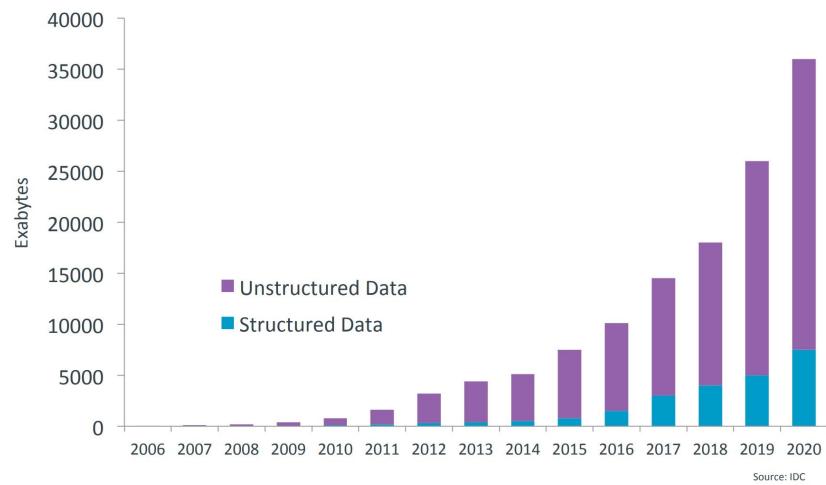
- ▶ large-scale optimization
 - ▶ empirical risk minimization
 - ▶ gradient descent and acceleration
 - ▶ stochastic gradient methods and variants
 - ▶ second order methods and Hessian approximations
- ▶ kernel methods
 - ▶ Reproducing kernel Hilbert spaces
 - ▶ Nystrom approximations
 - ▶ Randomized kernel approximations
- ▶ neural networks
 - ▶ large scale non-convex optimization
 - ▶ kernel approximations
 - ▶ convex optimization for neural networks

For details see Canvas!

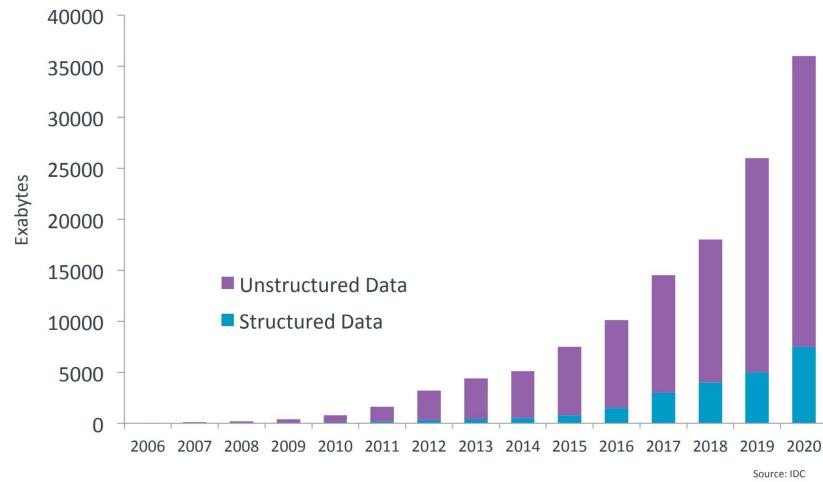
Any questions?

Overview of topics and applications

Scale of data

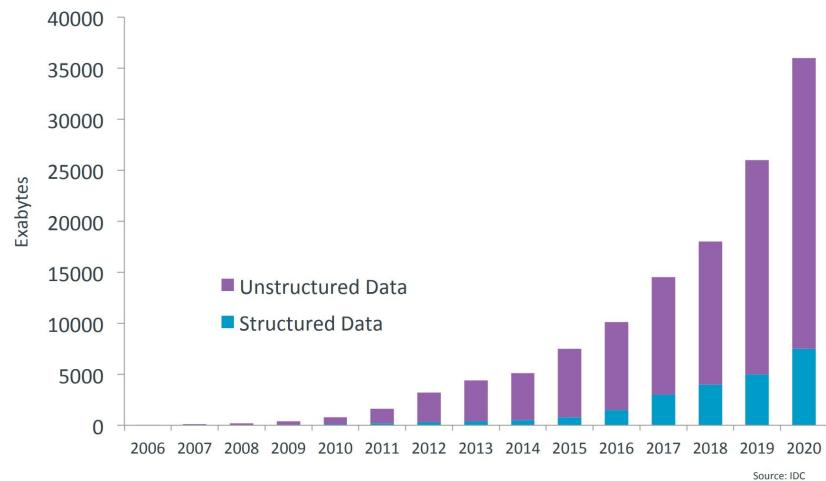


Scale of data



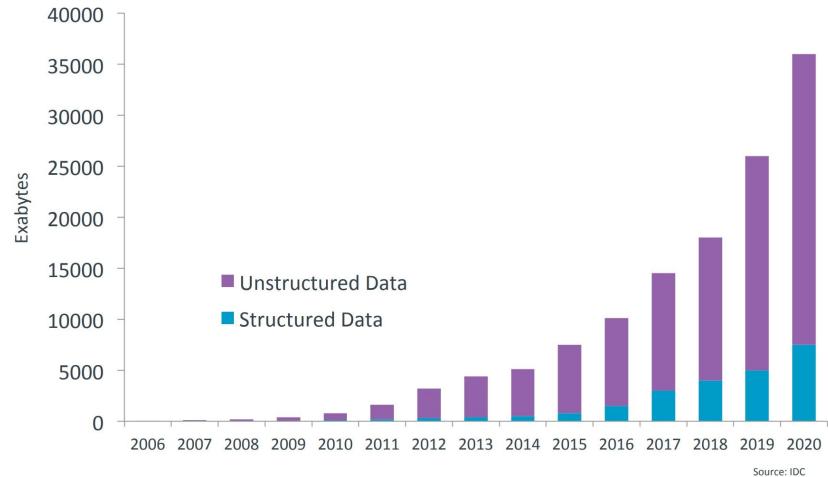
- ▶ Every day, we create 2.5 billion gigabytes of data

Scale of data

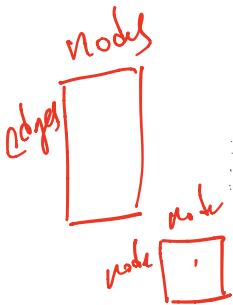


- ▶ Every day, we create 2.5 billion gigabytes of data
- ▶ Data stored grows 4x faster than world economy (Mayer-Schonberger)

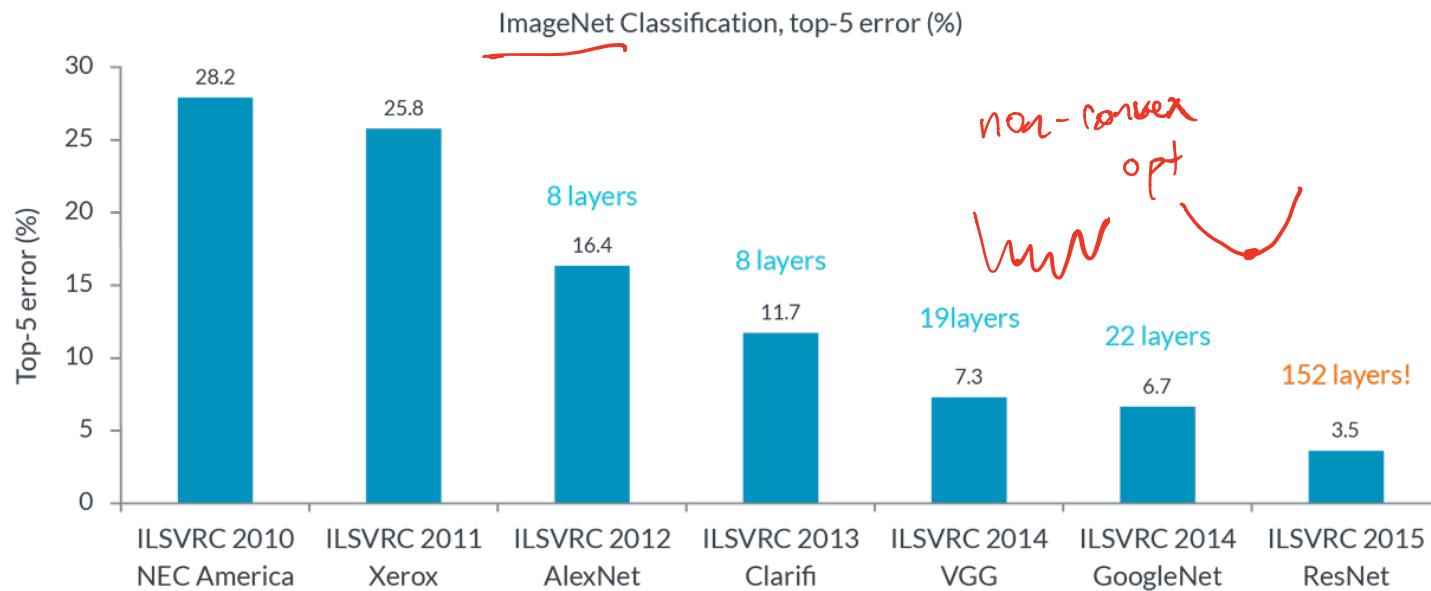
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Deep learning revolution



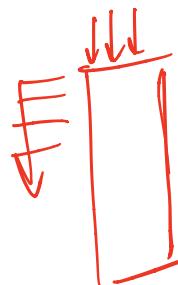
Big data matrices

- ▶ $n \times d$ datamatrix

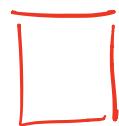
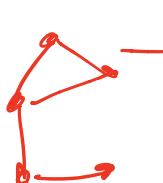
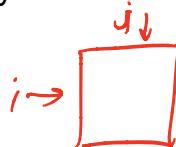


- ▶ **Small:** we can look at the data and find solutions easily
 - ▶ **Medium:** Fits into RAM and one can run computations in reasonable time
 - ▶ **Large:** Doesn't easily fit into RAM. One can't relatively easily run computations.
- cifar-10*
- imageNet*
- 1.2TB*

Typical data matrices



- ▶ Rectangular data (object-feature data): n objects, each of which are described by d features, e.g., document-term data, people-SNPs data.
- ▶ Correlation matrices
- ▶ Kernels and similarity matrices
- ▶ Laplacians or Adjacency matrices of graphs.
- ▶ Discretizations of dynamical systems, ODEs and PDEs
- ▶ Constraint matrices
- ▶ ...



$$A \cdot x \leq b$$

↑↑↑↑

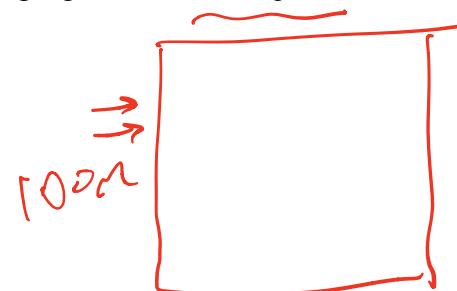
A hand-drawn red equation $A \cdot x \leq b$ with four arrows pointing up towards the inequality sign, representing linear constraints.

Typical data matrices

- ▶ Rectangular data:
essentially a two-dimensional matrix with rows indicating records (cases) and columns indicating features (variables)
- ▶ Example: Airline dataset

depart	arrive	origin	dest	dist	weather	delay	cancelled
00:00:01	13:35:01	RNO	LAS	345		0	1
07:20:01	08:40:01	SFO	SAN	447		40	0
07:25:01	10:15:01	OAK	PHX	646		0	0
07:30:01	08:30:01	OAK	BUR	325		0	0
:							

one-hot encoded
0 1 0 0 0 0 0



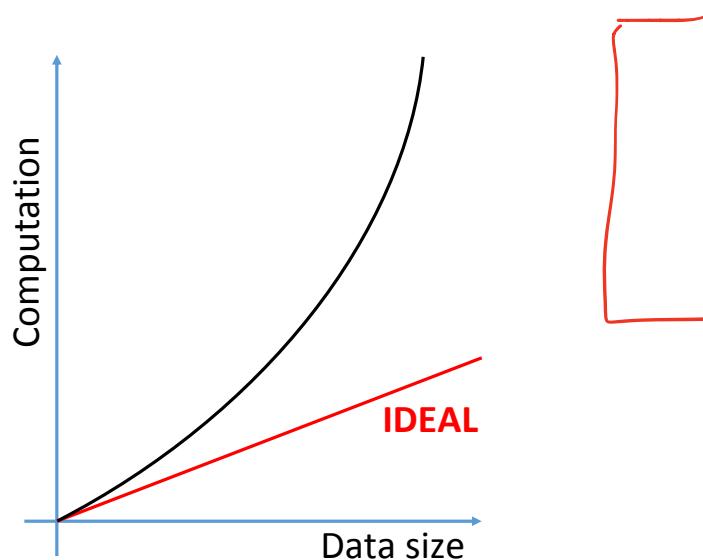
in machine learning, statistics and signal processing

- ▶ More data points typically increase the accuracy of models
→ large scale matrix computation and optimization problems
 - e.g. matrix multiplication, matrix factorization, singular value decomposition, convex optimization, non-convex optimization...

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Can we reduce the data volume with minimal loss of information ?



Matrix Computations

- ▶ Data matrix $A \in R^{n \times d}$ where n, d are extremely large

Matrix Computations

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Examples:

- ▶ Airline dataset (120GB) $n = 120 \times 10^6$, $d = 28$
Flight arrival and departure details from 1987 to 2008

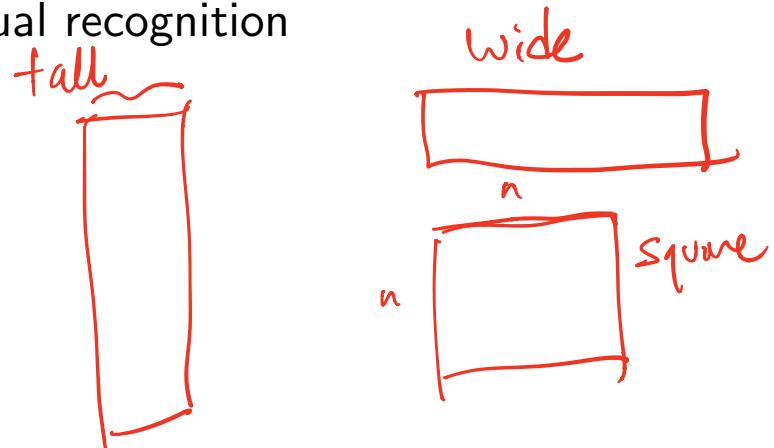
Matrix Computations

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Examples:

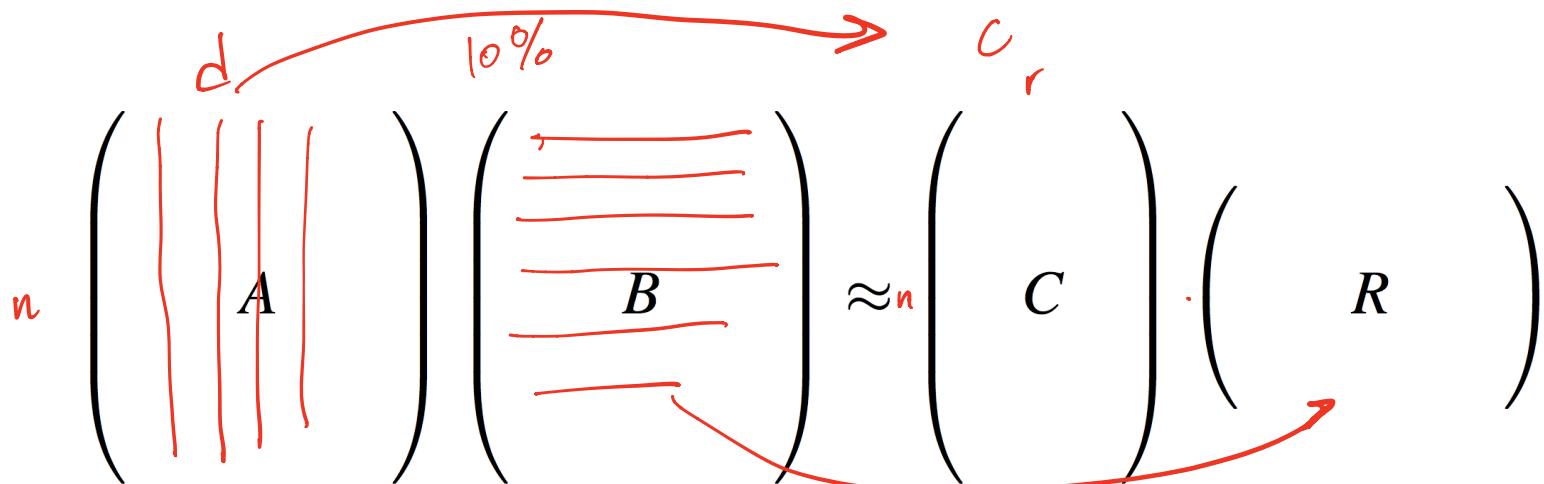
- ▶ Airline dataset (120GB) $n = 120 \times 10^6$, $d = 28$
Flight arrival and departure details from 1987 to 2008
- ▶ Imagenet dataset (1.31TB) $n = 14 \times 10^6$, $d = 2 \times 10^5$
14 Million images for visual recognition

[US Department of Transportation]
[Deng et al. 2009]

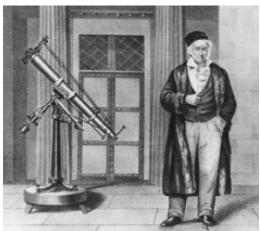


Approximate Matrix Multiplication

- ▶ How to approximate the matrix product AB fast ?



Least Squares Problems



[Gauss, 1795]

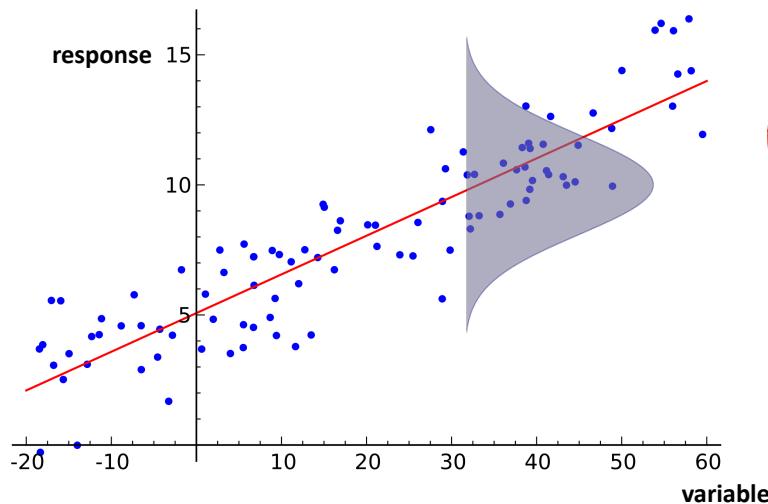
$$\boxed{A}$$

~~$$Ax = y$$~~

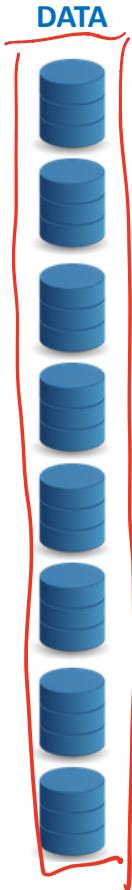
Least squares

$$\min_x \|Ax - y\|^2$$

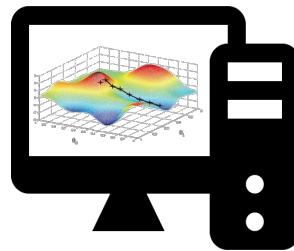
$$\begin{aligned} & \xrightarrow{\quad} A^T A x = A^T y \\ & (\bar{A}^T \bar{A})^{-1} \bar{A}^T y = x \\ & \uparrow \end{aligned}$$

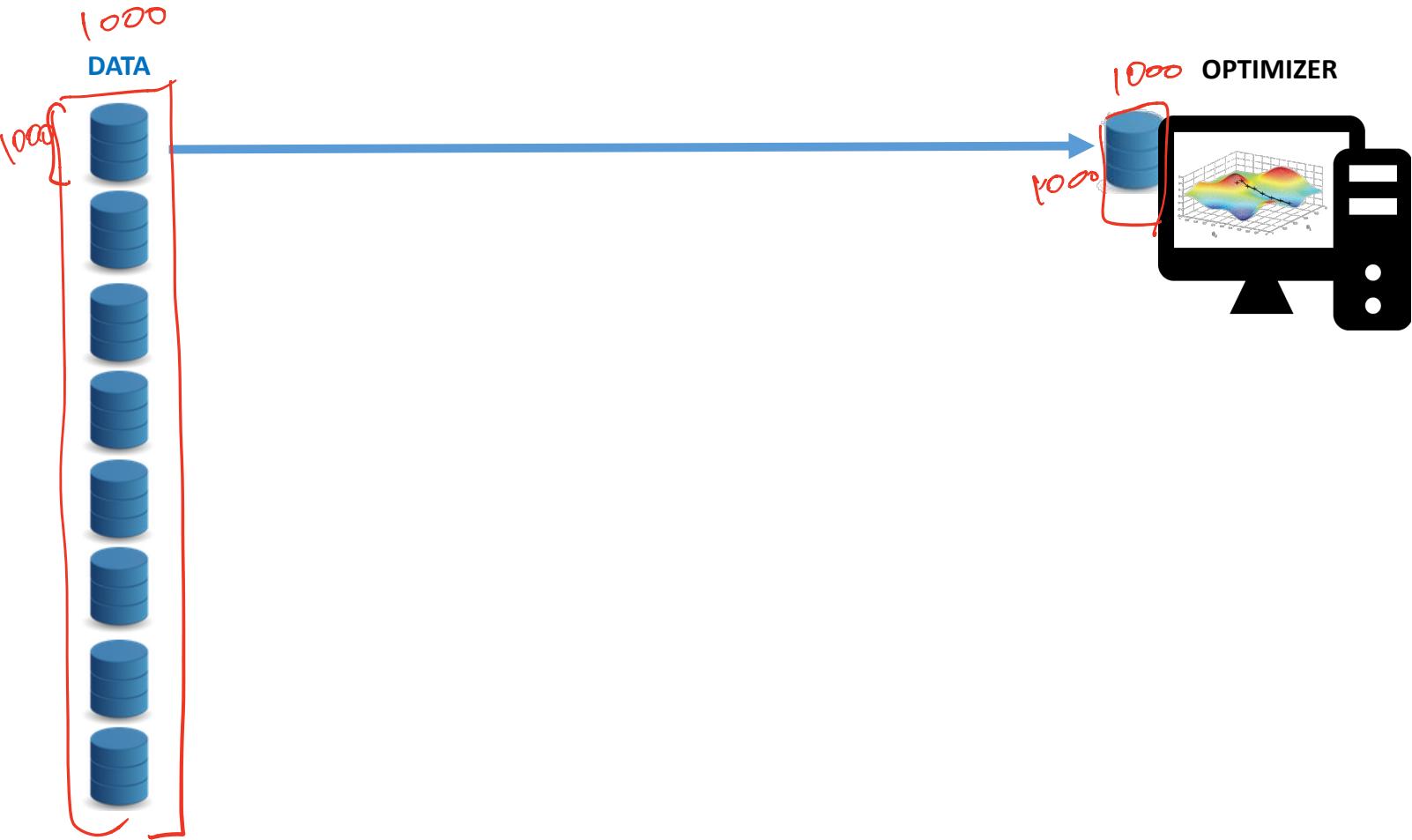


Sketching:



OPTIMIZER

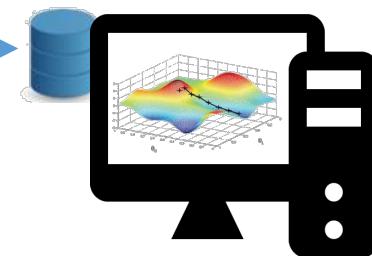




DATA



OPTIMIZER



cost

all data

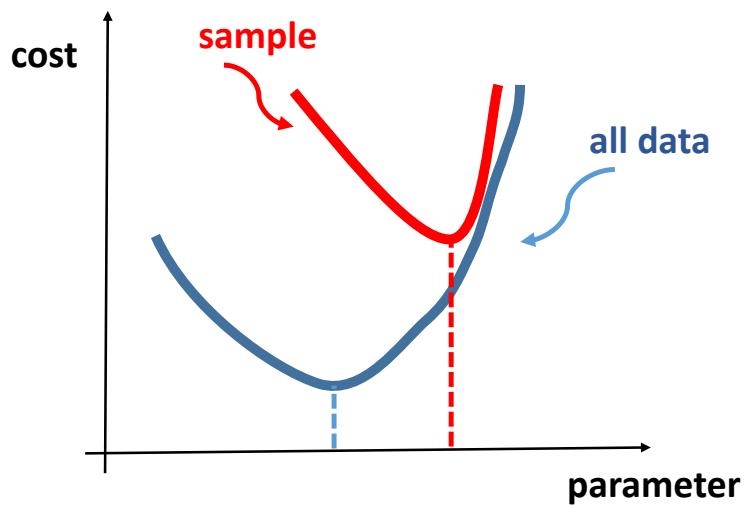
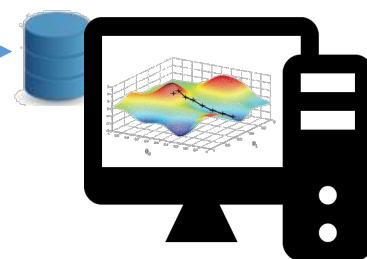
parameter

θ^*

DATA



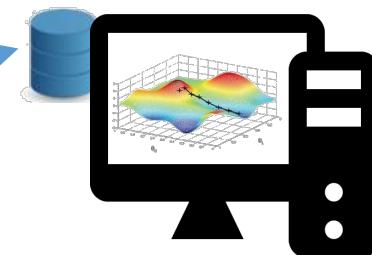
OPTIMIZER



DATA



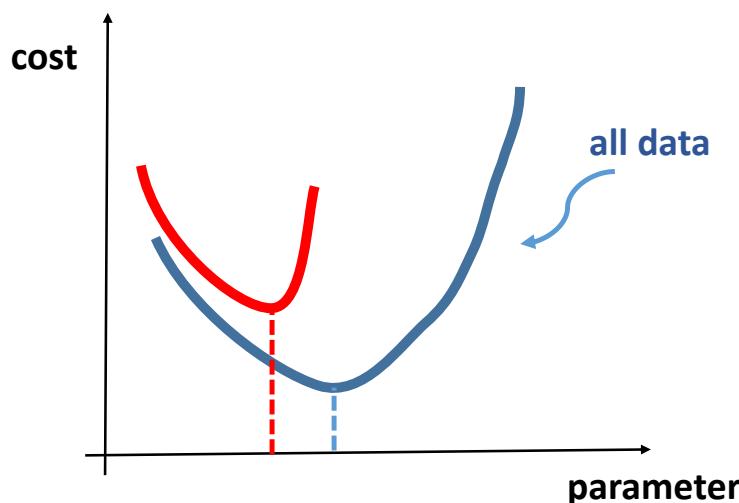
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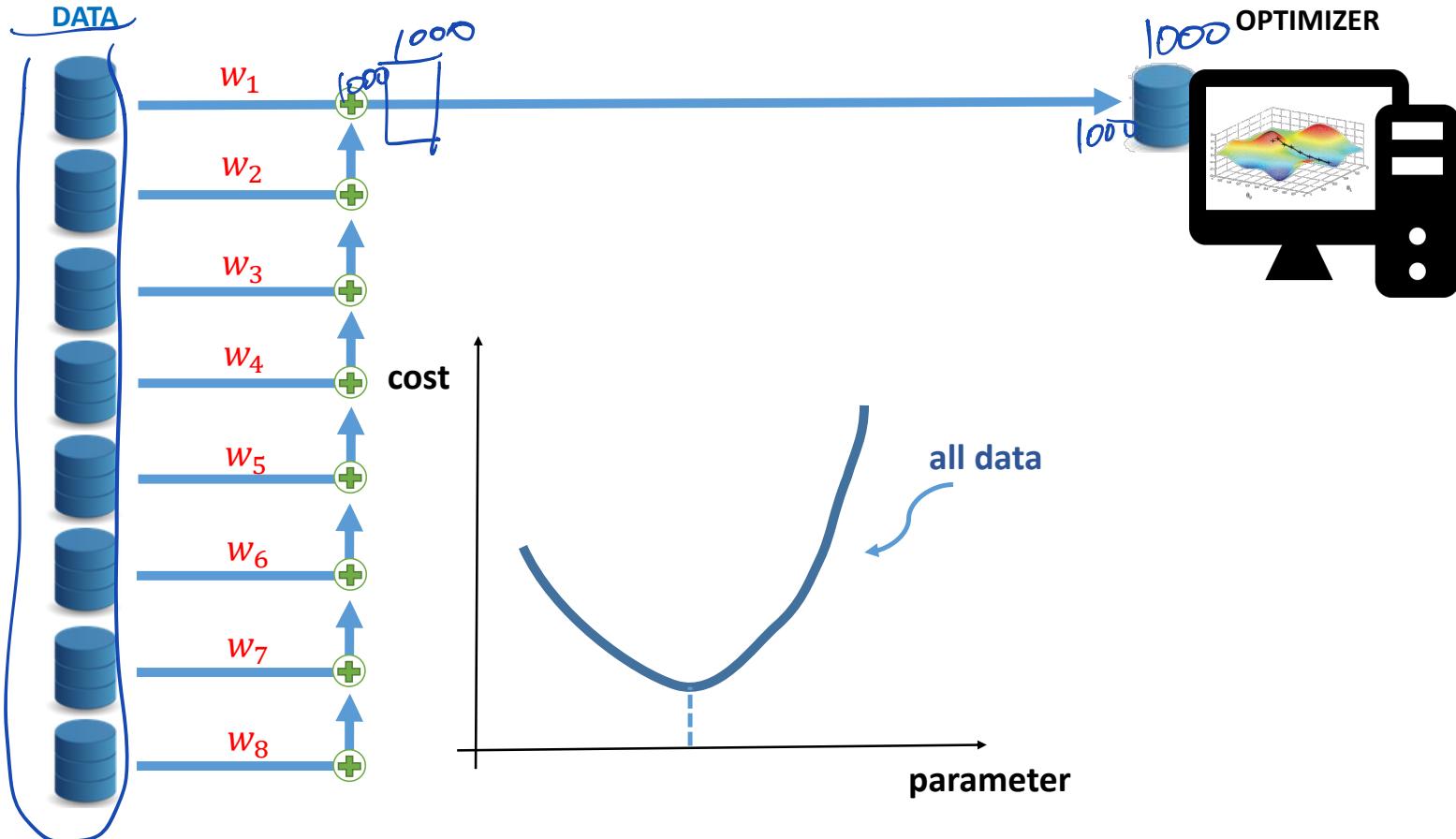


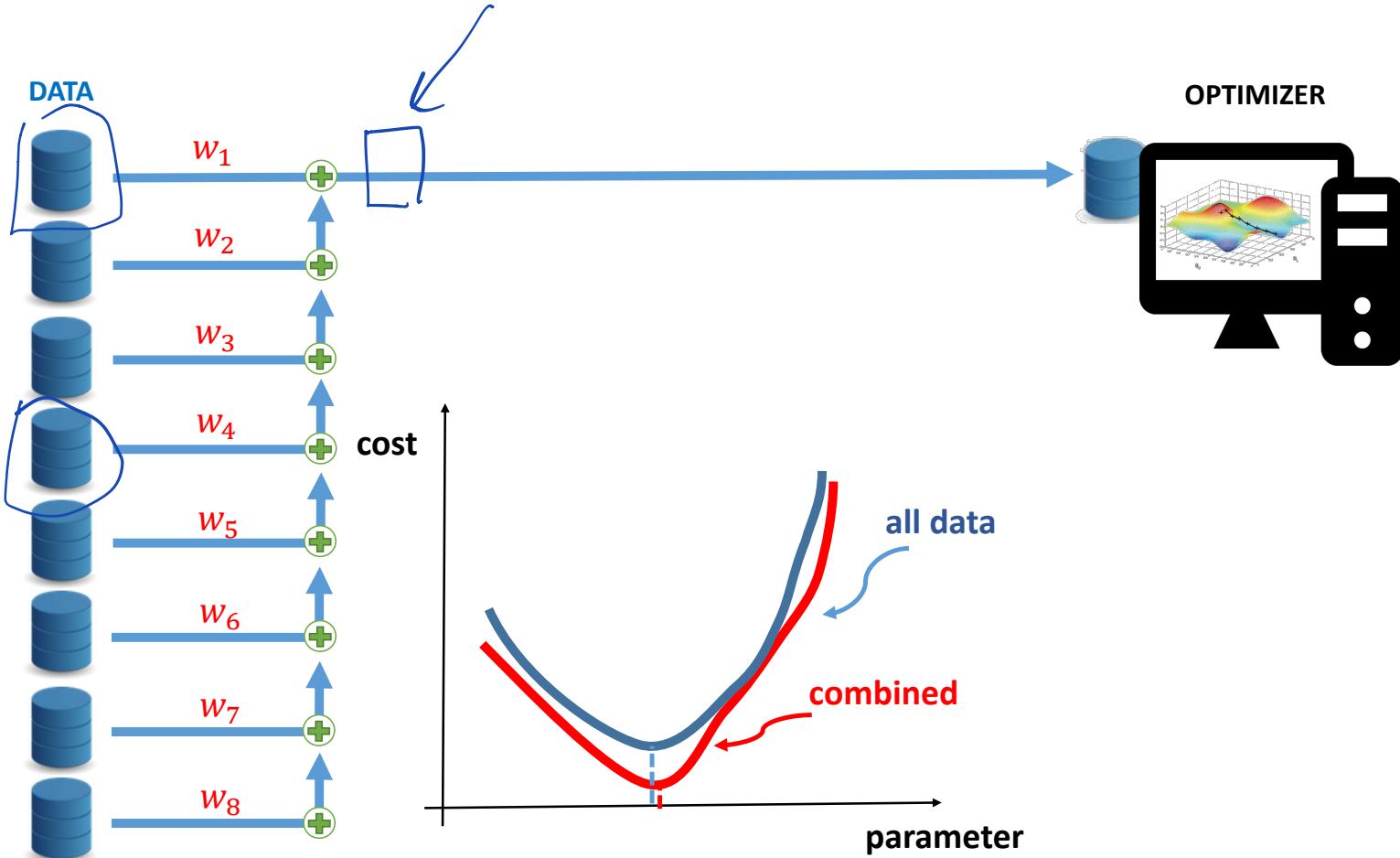
cost

parameter

all data



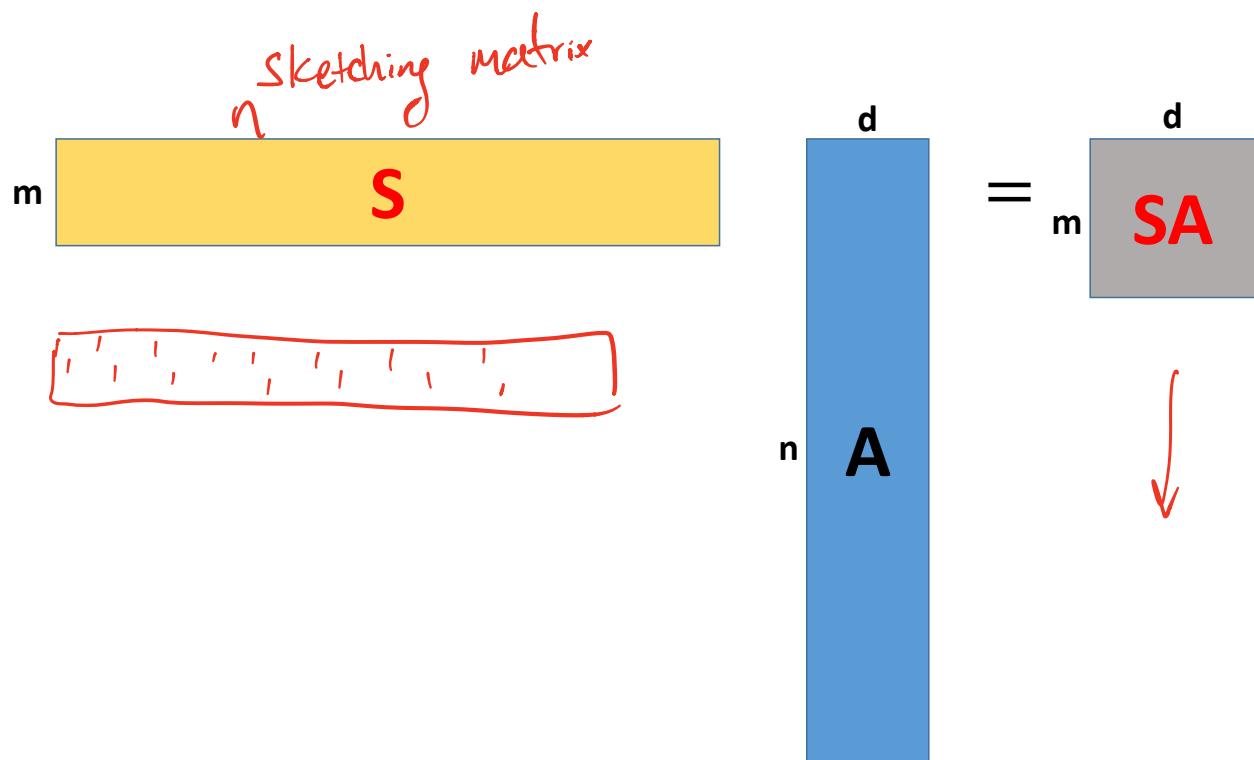




Randomized Sketching



Randomized Sketching



Randomized Least Squares Solvers

$$A = \boxed{\quad}$$

$$\tilde{X} = SA \quad \boxed{\quad} \quad \tilde{y} = Sy$$

- ▶ $A : n \times d$ feature matrix, and $y : n \times 1$ response vector

- ▶ Original problem $\boxed{\text{OPT} = \min_{x \in C} \|Ax - y\|^2}$ $n \times d$

- ▶ Randomized approximation $\min_{x \in C} \underbrace{\|\tilde{A}x - \tilde{y}\|^2}_{m \times d}$

- ▶ \tilde{A} and \tilde{y} are smaller approximations

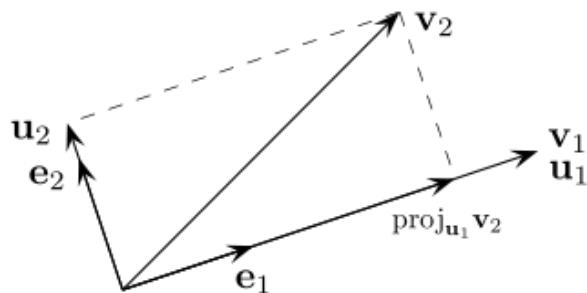
E.g. pick entry of S indep. $N(0, 1)$
↑
Gaussian Distribution

QR decomposition



$\Theta(n \Delta^2)$

- The Gram–Schmidt process takes a finite, linearly independent set of vectors $v_1, \dots, v_n \in \mathbb{R}^d$ generates an orthogonal set $u_1, \dots, u_k \in \mathbb{R}^d$ that spans the same n-dimensional subspace.



$$u_1 = v_1,$$

$$u_2 = v_2 - \text{proj}_{u_1}(v_2),$$

$$u_3 = v_3 - \text{proj}_{u_1}(v_3) - \text{proj}_{u_2}(v_3),$$

$$u_4 = v_4 - \text{proj}_{u_1}(v_4) - \text{proj}_{u_2}(v_4) - \text{proj}_{u_3}(v_4),$$

\vdots

$$e_1 = \frac{u_1}{\|u_1\|}$$

$$e_2 = \frac{u_2}{\|u_2\|}$$

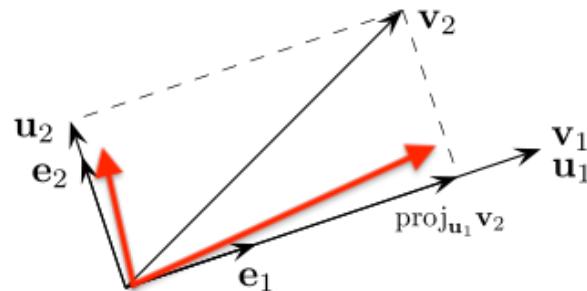
$$e_3 = \frac{u_3}{\|u_3\|}$$

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\vdots

QR decomposition

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- ▶ complexity $O(dn^2)$
- ▶ **randomized** algorithm complexity $\approx O(dn)$
produces an *approximately orthogonal* basis

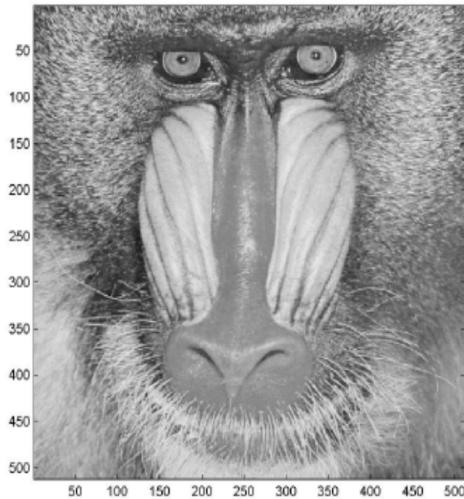
Low-rank matrix approximations

- ▶ Singular Value Decomposition (SVD)
- ▶ $A = U\Sigma V^T$
- ▶ takes $O(nd^2)$ time for $A \in R^{n \times d}$
- ▶ best rank- k approximation is $A_k := U_k \Sigma_k V_k^T = \sum_{i=1}^k \sigma_i u_i v_i^T$
- ▶ $\|A - A_k\|_2 \leq \sigma_{k+1}$

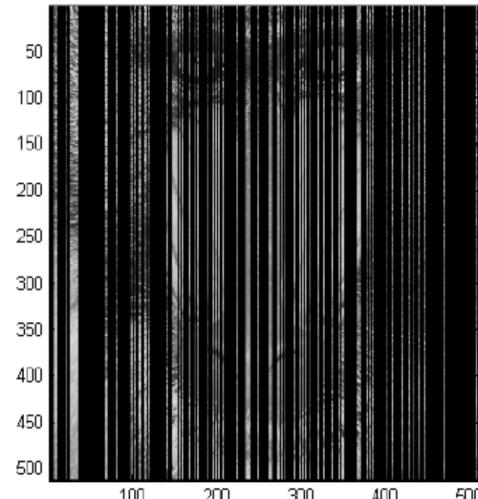
Randomized low-rank matrix approximations

- ▶ Randomized (SVD)
- ▶ approximation C (e.g. a subset of the columns of A)
- ▶ $AA^T \approx CC^T$
- ▶ $\tilde{A}_k = CC^\dagger A$ is a randomized rank-k approximation
- ▶ $\|A - \tilde{A}_k\|_2^2 \leq \sigma_{k+1}^2 + \epsilon \|A\|_2^2$

Randomized low-rank approximation example

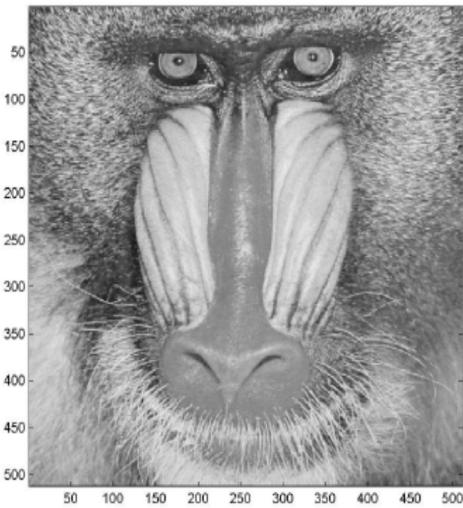


Original matrix

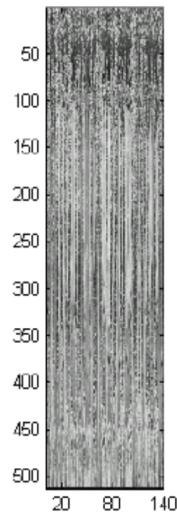


Sampling ($c = 140$ columns)

Randomized low-rank approximation example

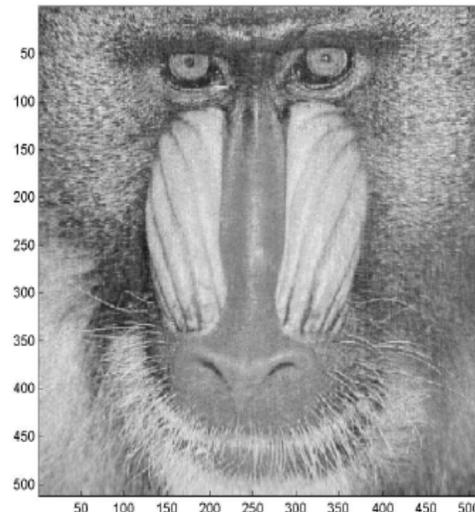
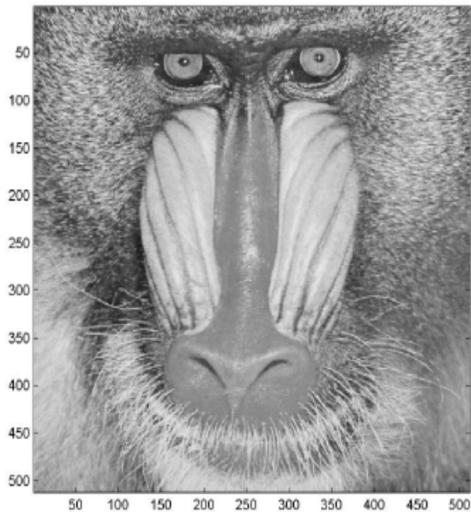


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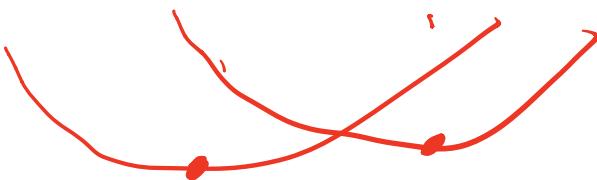
Randomized low-rank approximation example



Iterative Methods

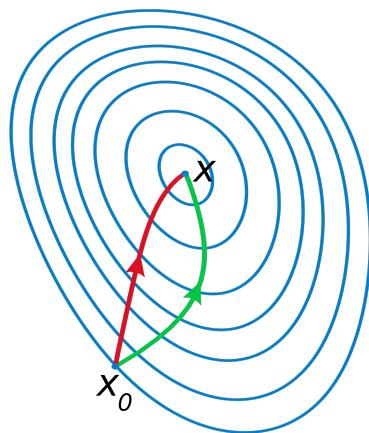
- ▶ Gradient descent and momentum acceleration
- ▶ Iterative sketching methods
- ▶ Conjugate gradient
- ▶ Preconditioning
- ▶ Newton's method
- ▶ Quasi-Newton methods
- ▶ Stochastic Gradient Descent
- ▶ Variance reduction and adaptive gradient methods

Newton's Method



$$\min_{x \in \mathcal{C}} g(x)$$

$$x^{t+1} = \arg \min_{x \in \mathcal{C}} \langle \nabla g(x^t), x - x^t \rangle + \frac{1}{2} (x - x^t)^T \underbrace{\nabla^2 g(x^t)}_{\text{Hessian}} (x - x^t)$$

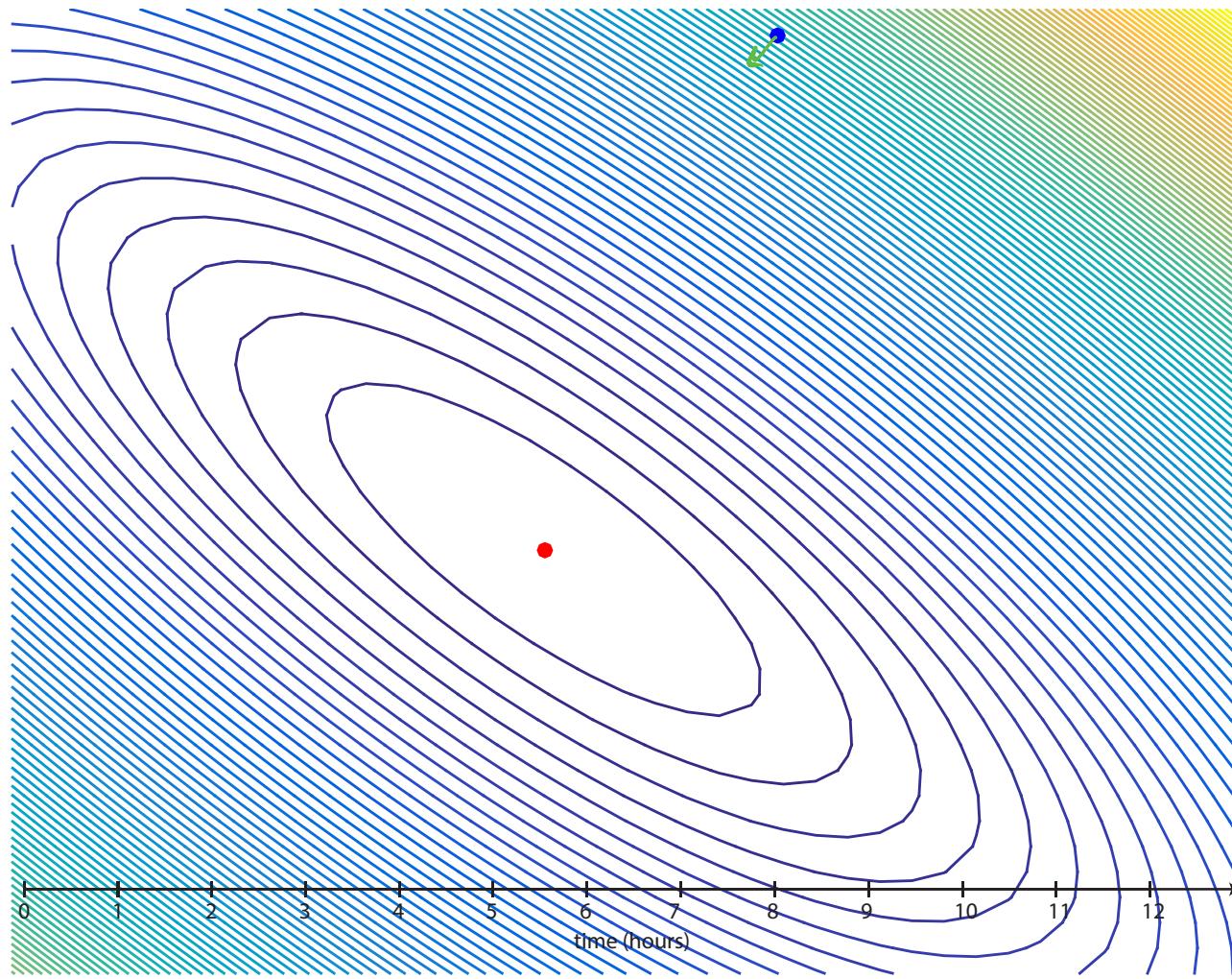


$$[\nabla^2 g(x)]_{k,l} = \frac{\partial}{\partial x_k} \frac{\partial}{\partial x_l} g(x)$$

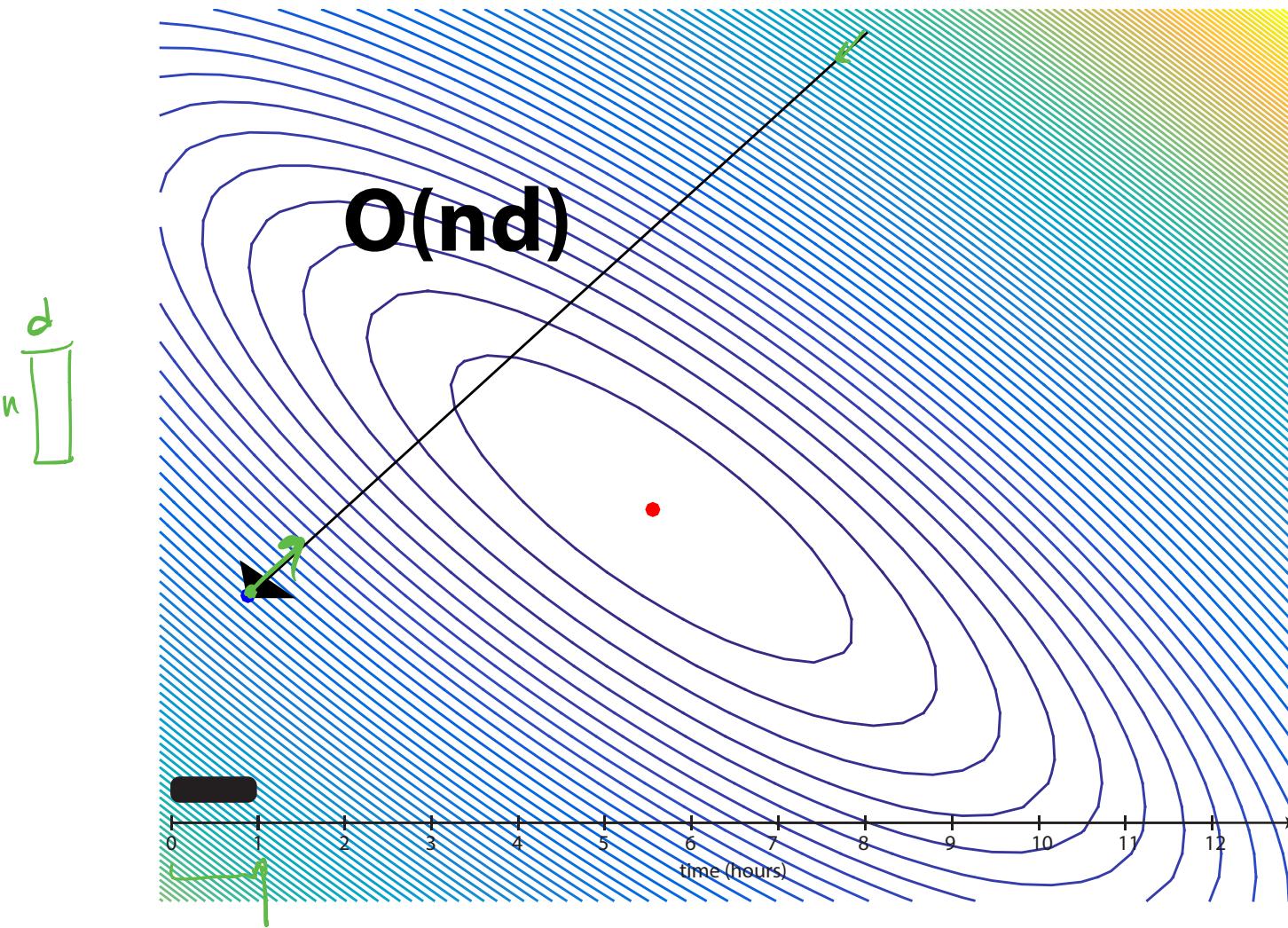
d

$$d \times d \rightarrow O(d^2)$$

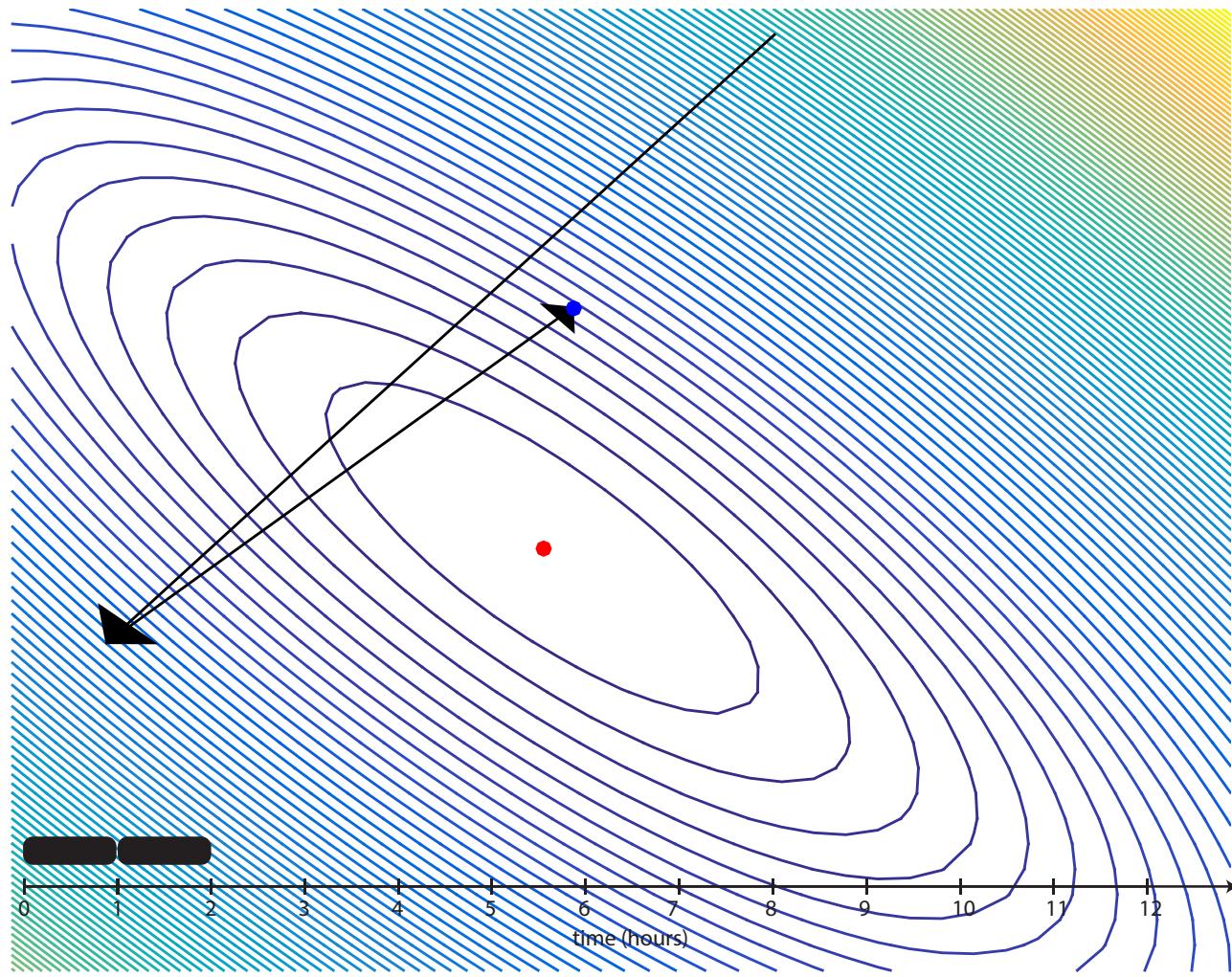
Gradient Descent



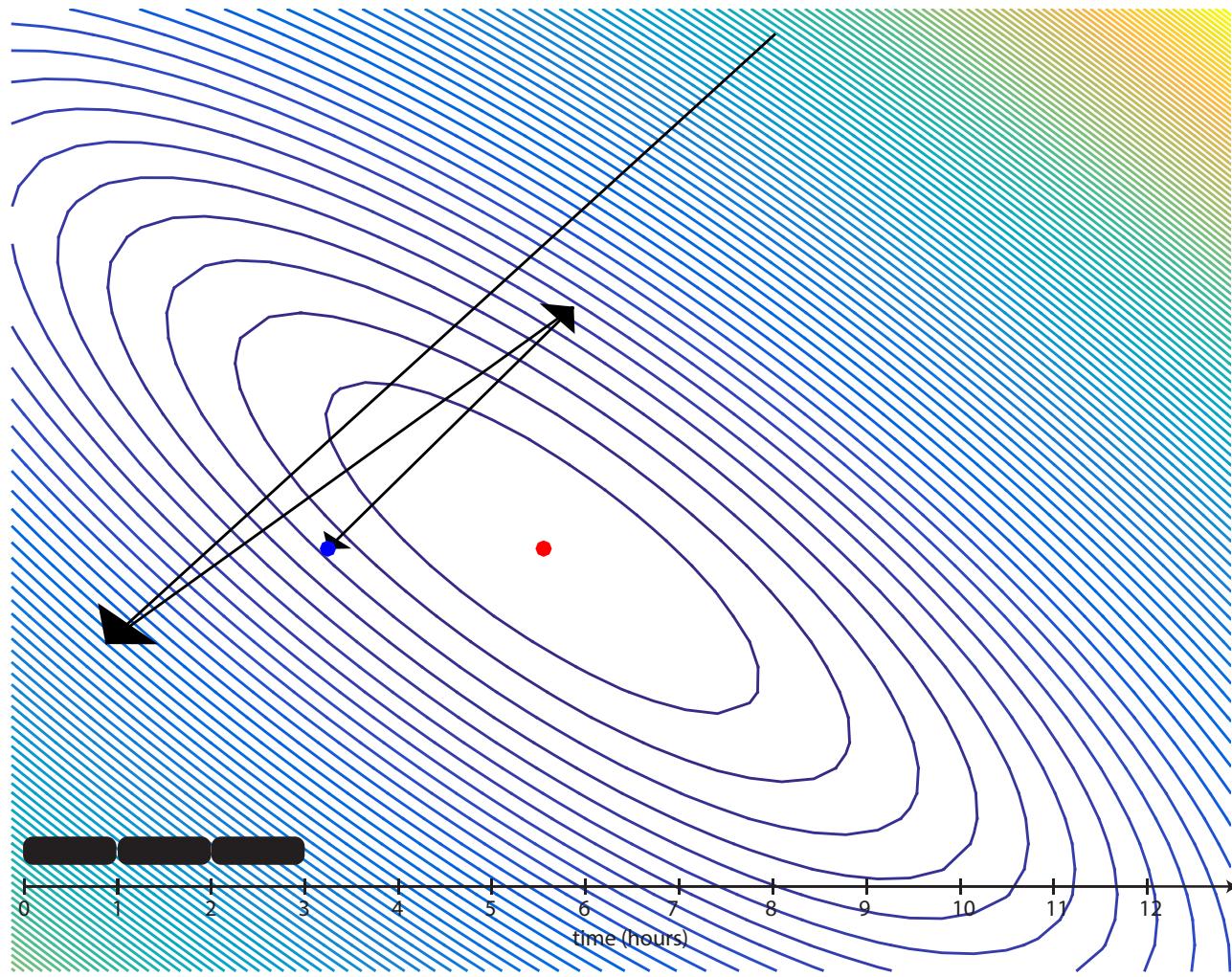
Gradient Descent



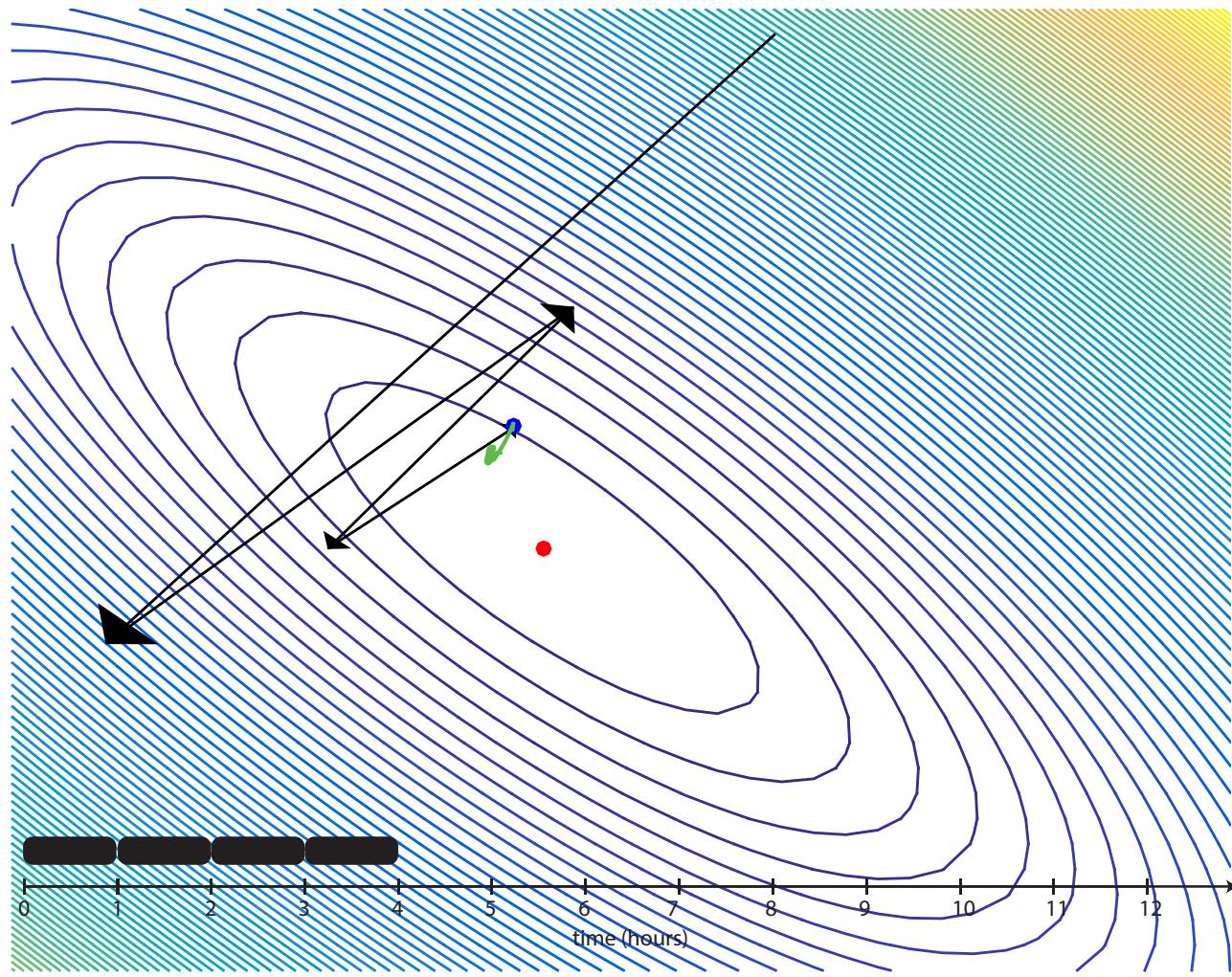
Gradient Descent



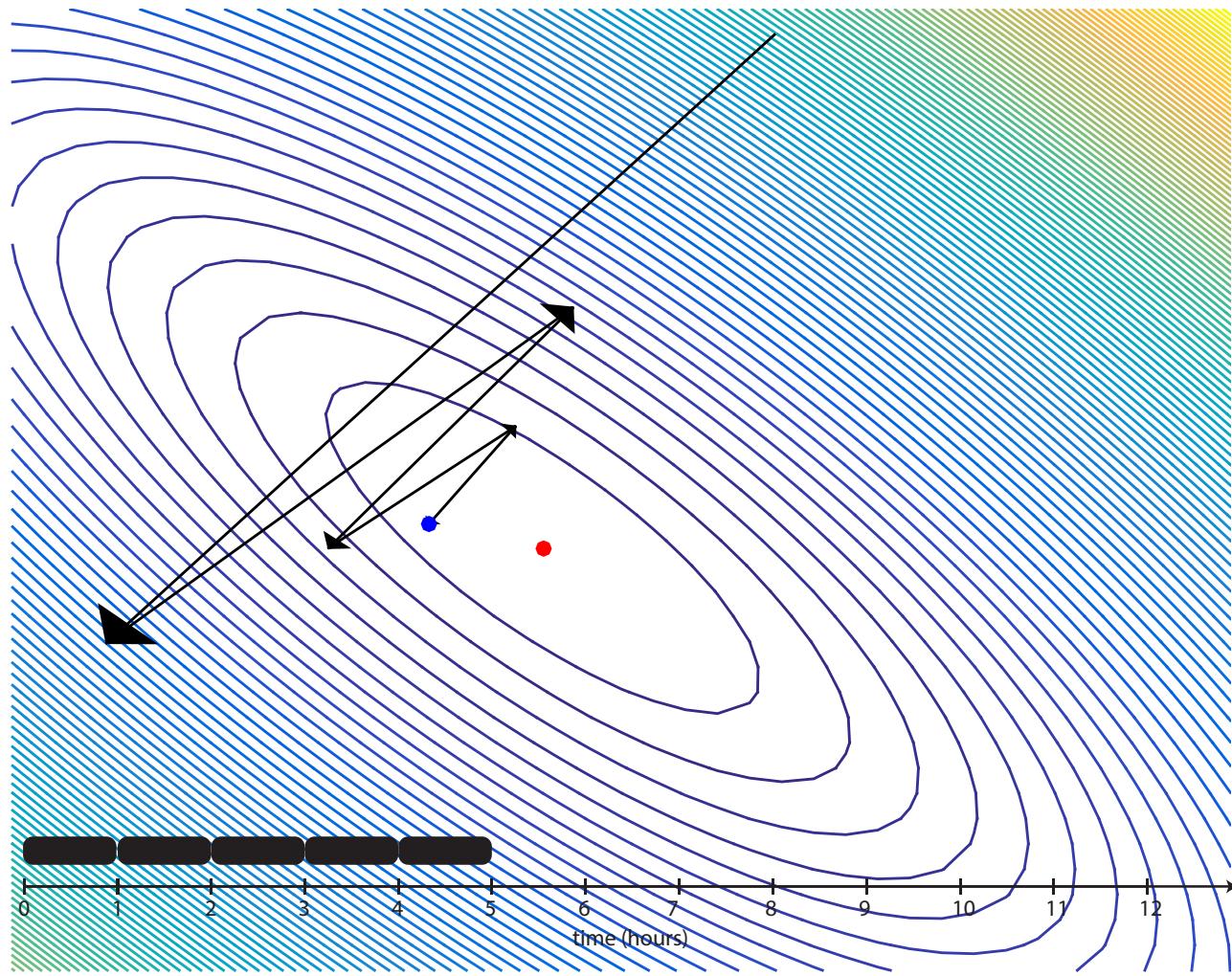
Gradient Descent



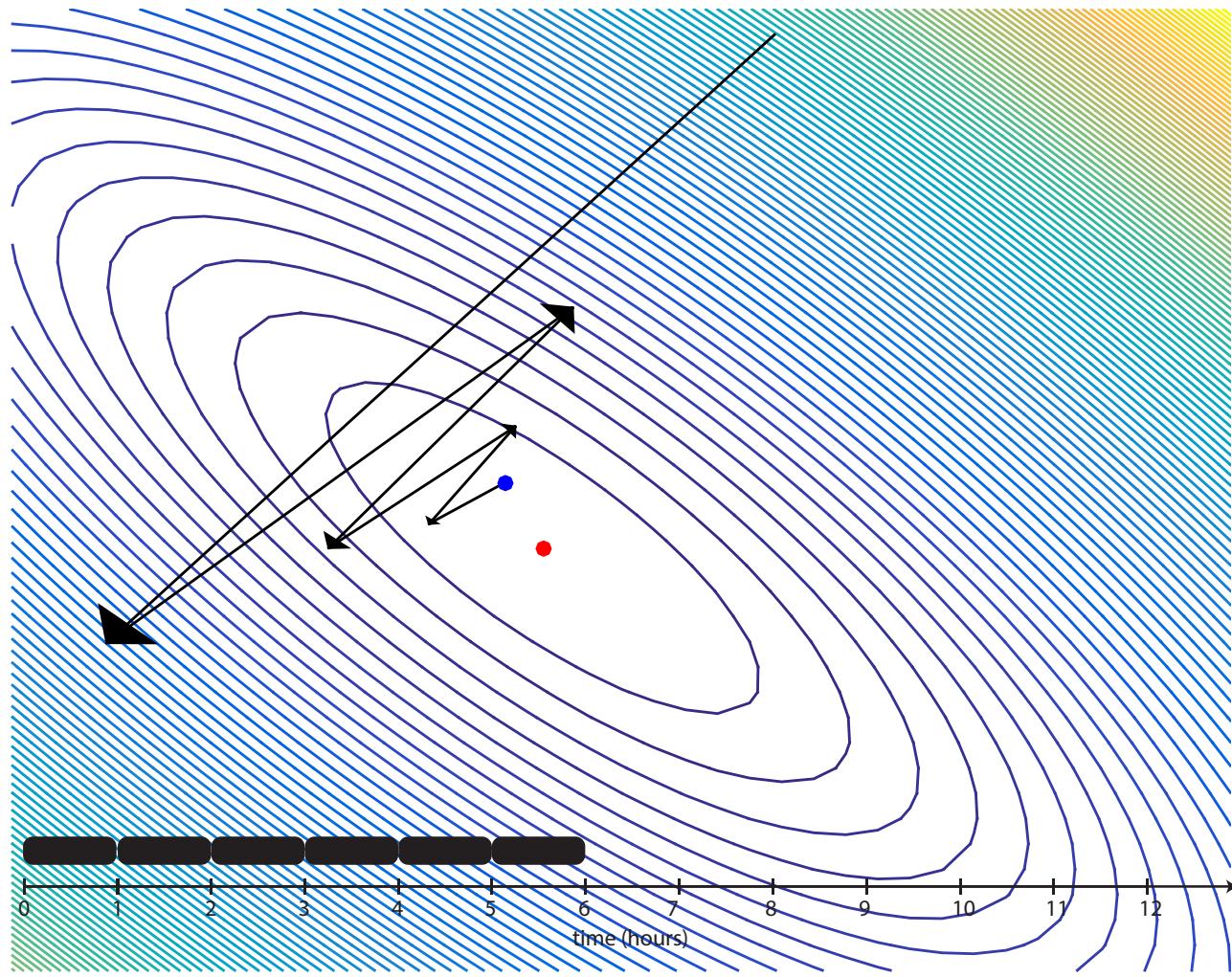
Gradient Descent



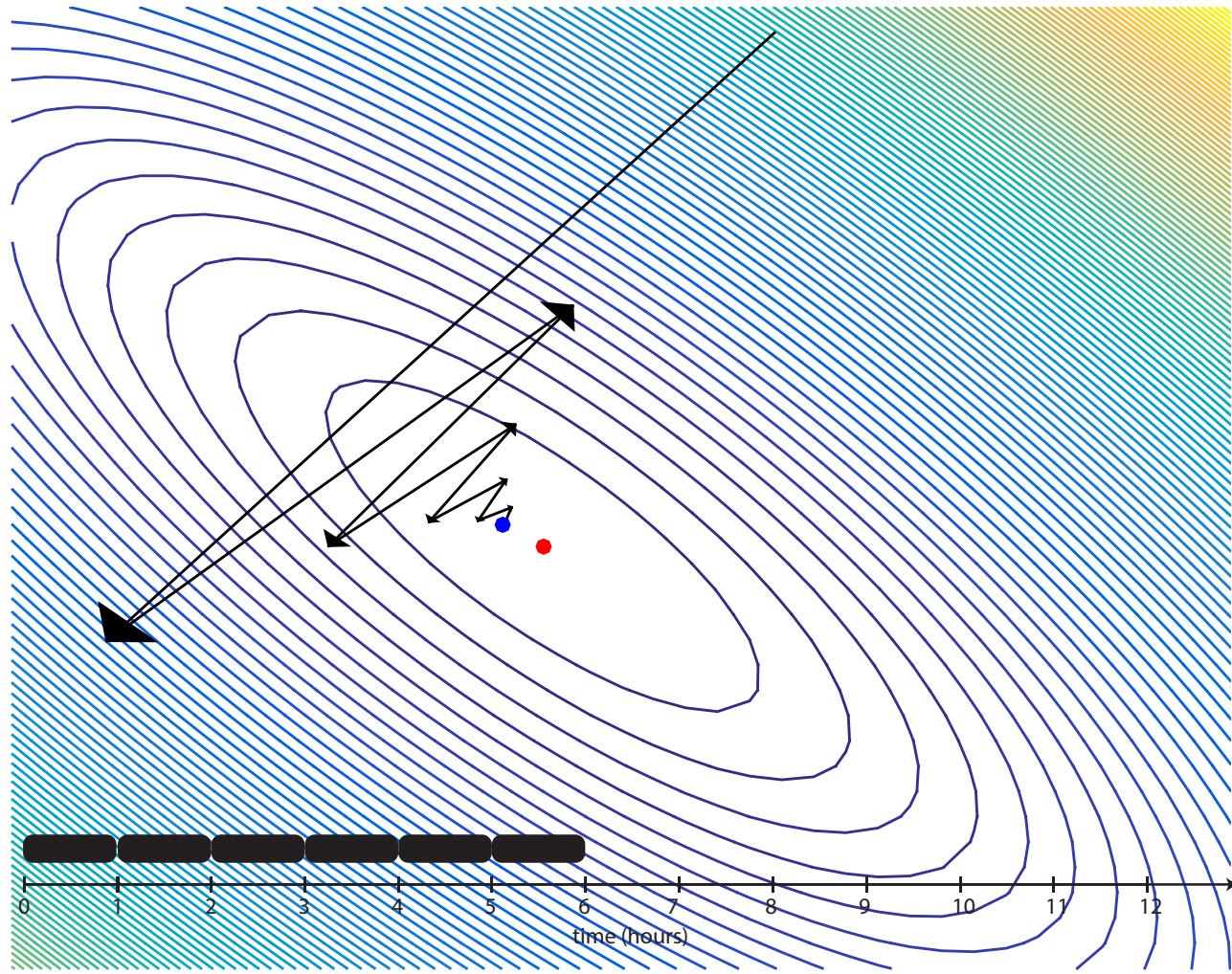
Gradient Descent



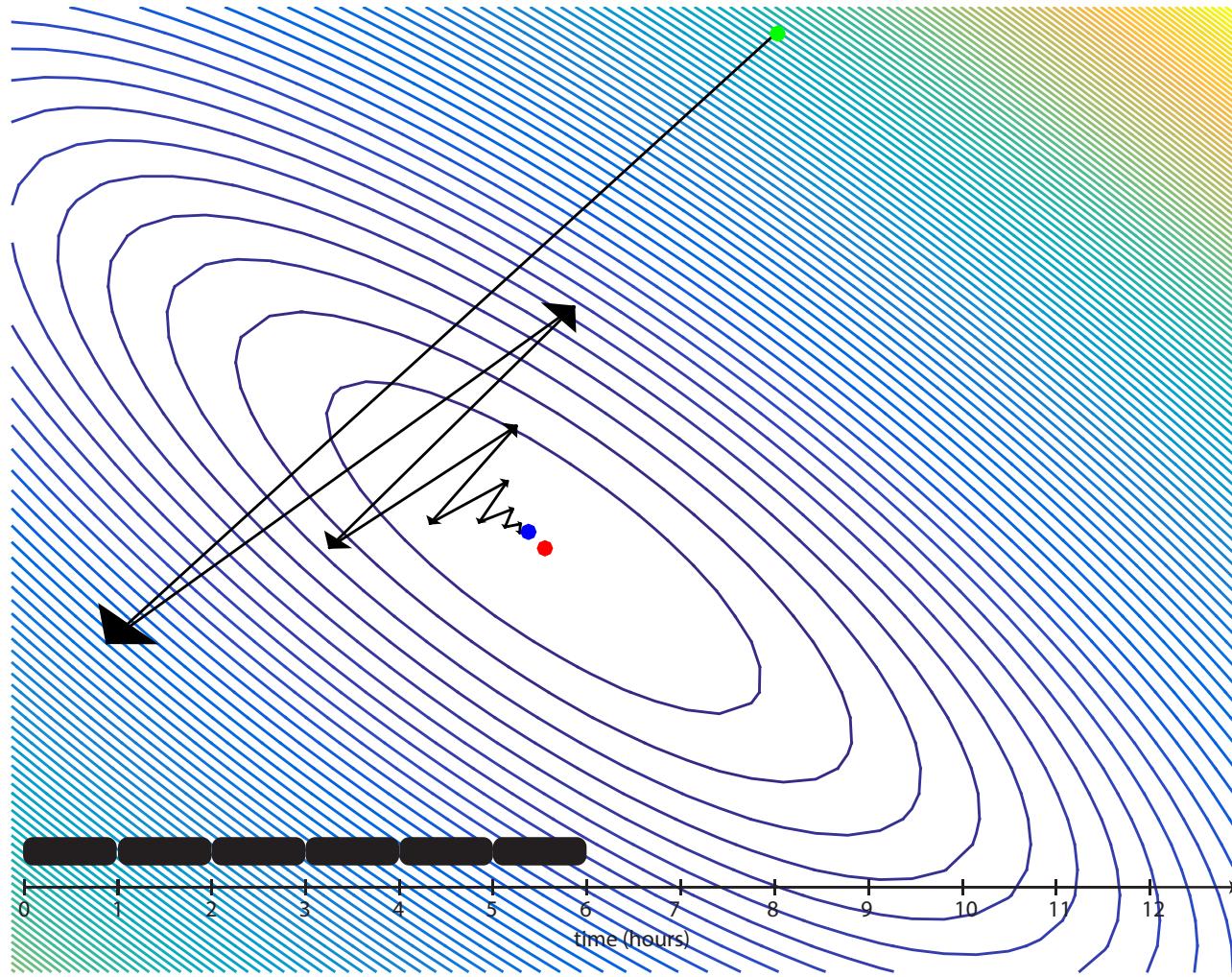
Gradient Descent



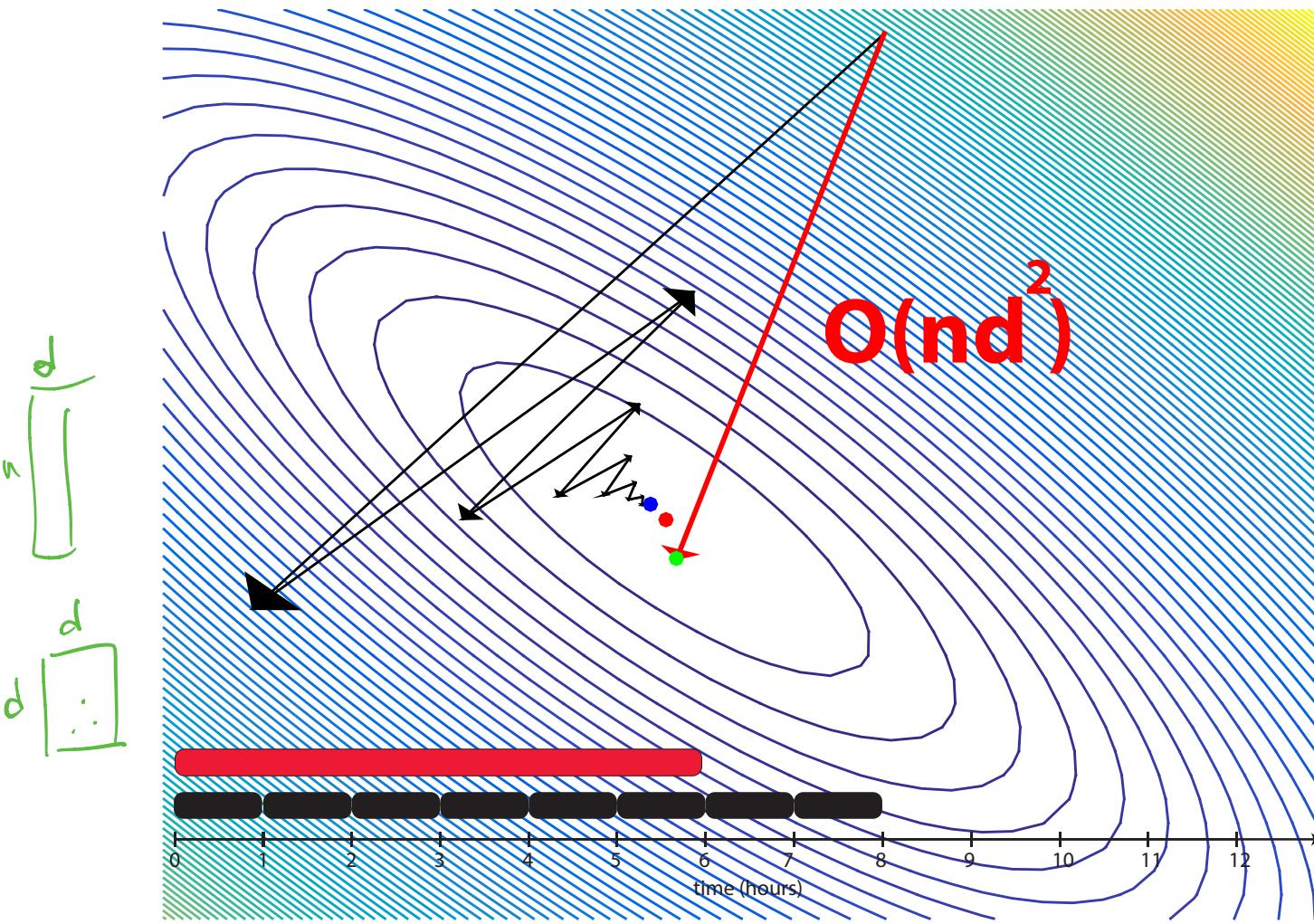
Gradient Descent vs



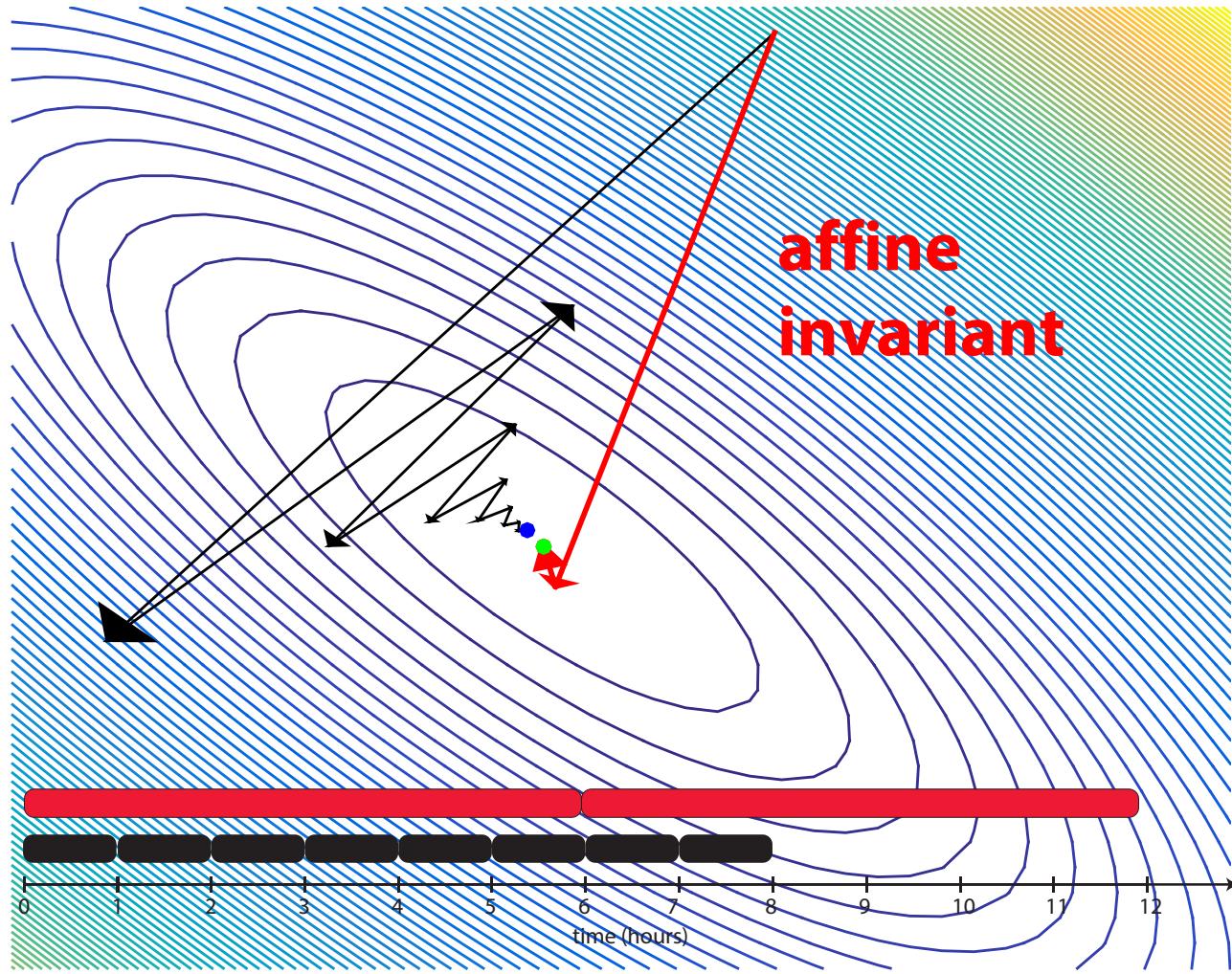
Gradient Descent vs Newton's Method



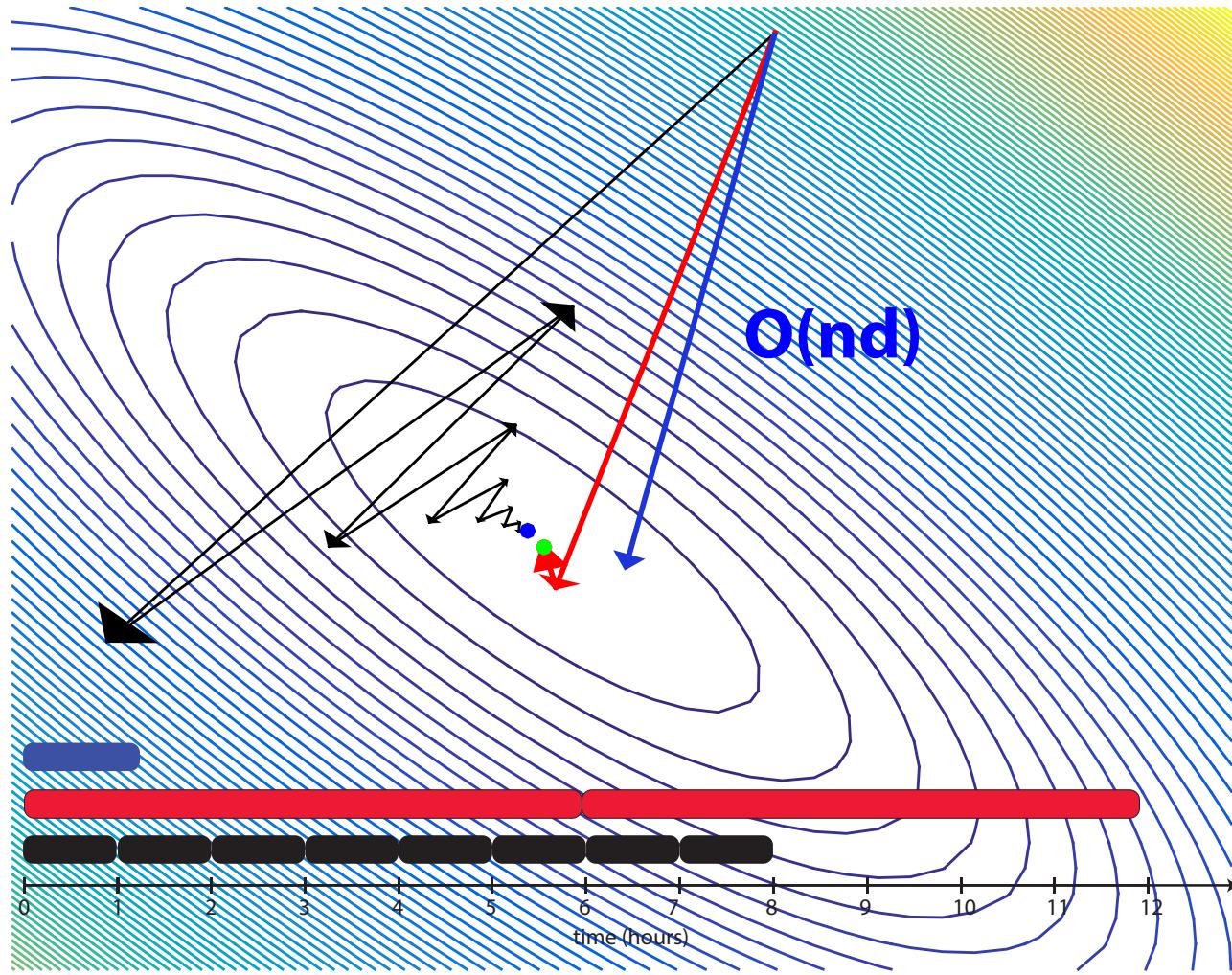
Gradient Descent vs Newton's Method



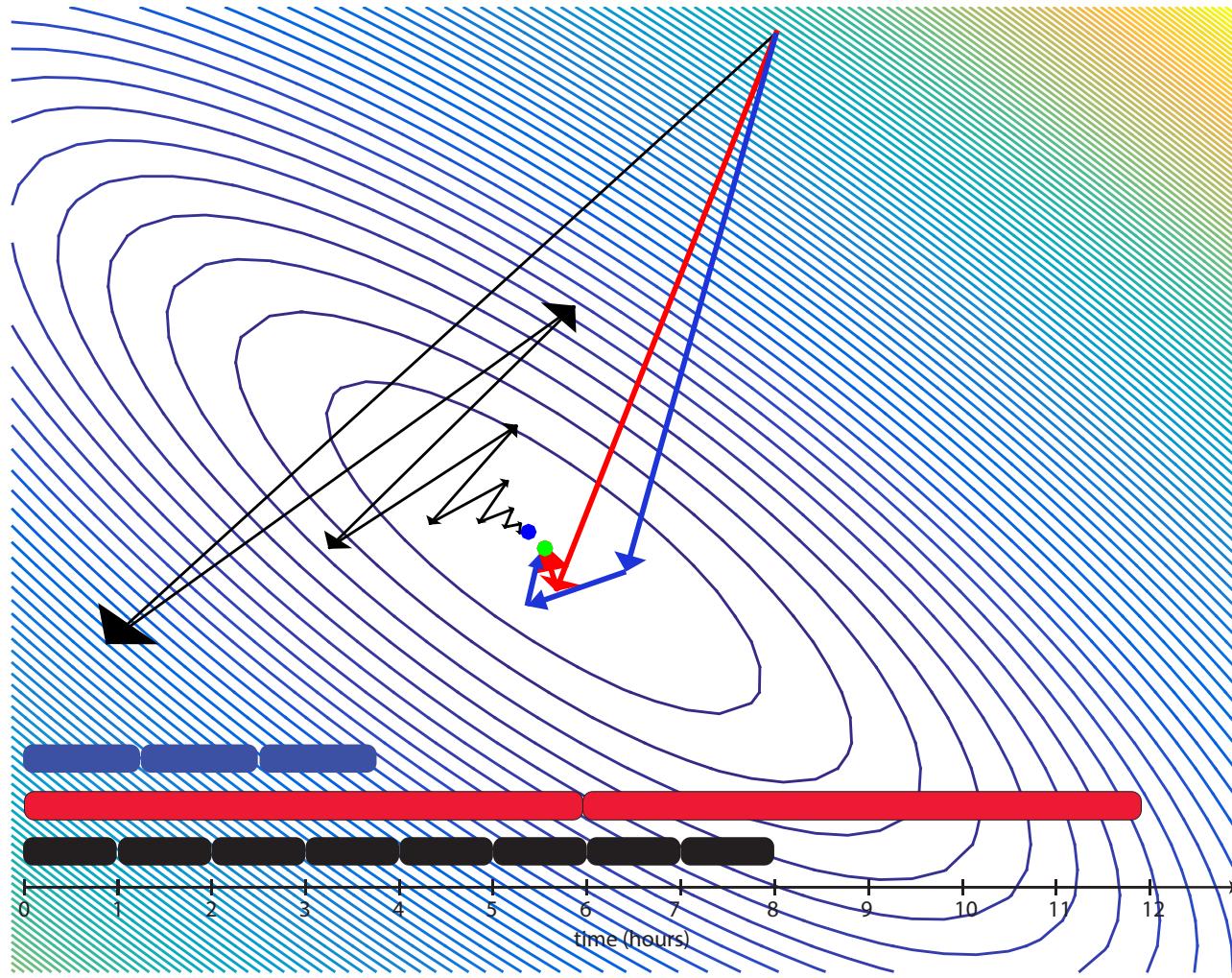
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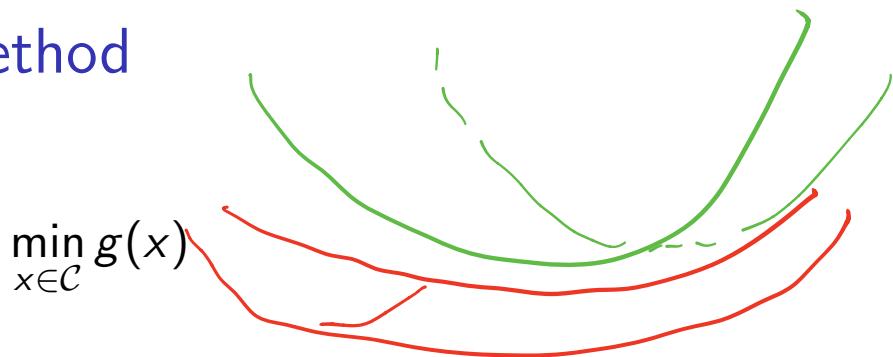
Gradient Descent vs Newton's Method



Gradient Descent vs Newton's Method

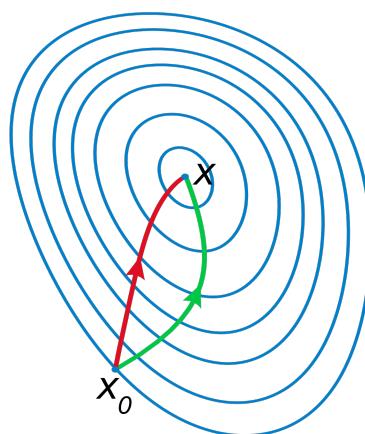


Randomized Newton's Method



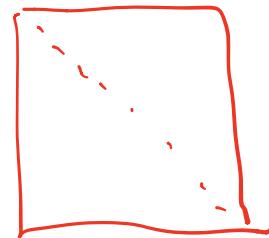
$$x^{t+1} = \arg \min_{x \in C} \langle \nabla g(x^t), x - x^t \rangle + \frac{1}{2}(x - x^t)^T \tilde{\nabla}^2 g(x^t)(x - x^t)$$

- $\tilde{\nabla}^2 g(x^t) \approx \nabla^2 g(x^t)$ is an approximate Hessian



Randomized Newton's Method

$$\min_{x \in \mathcal{C}} g(x)$$



$$x^{t+1} = \arg \min_{x \in \mathcal{C}} \langle \nabla g(x^t), x - x^t \rangle + \frac{1}{2}(x - x^t)^T \tilde{\nabla}^2 g(x^t)(x - x^t)$$

- ▶ $\tilde{\nabla}^2 g(x^t) \approx \nabla^2 g(x^t)$ is a randomly projected Hessian matrix

Other diagonal, subsampled, low-rank approximations:

- ▶ Adagrad, ADAM
- ▶ Stochastic Variance Reduced Gradient (SVRG)
- ▶ Broyden–Fletcher–Goldfarb–Shanno (BFGS) algorithm

Linear Programming

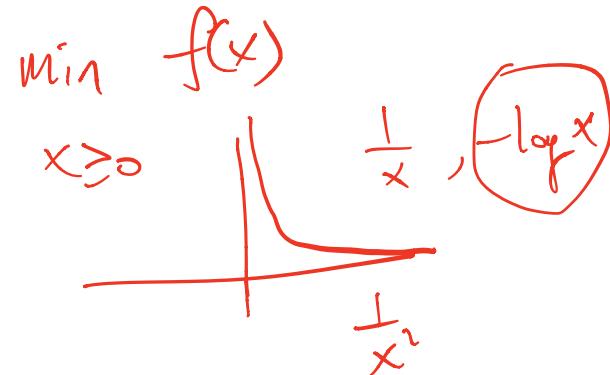
- ▶ LP in standard form where $A \in R^{n \times d}$

$$\min_{Ax \leq b} c^T x$$

- ▶ Log barrier

$$\min_x \mu c^T x - \sum_{i=1}^n \log(b_i - a_i^T x)$$

Linear Programming



- ▶ LP in standard form where $A \in R^{n \times d}$

$$\min_{Ax \leq b} c^T x$$

Self-concordance

- ▶ Log barrier

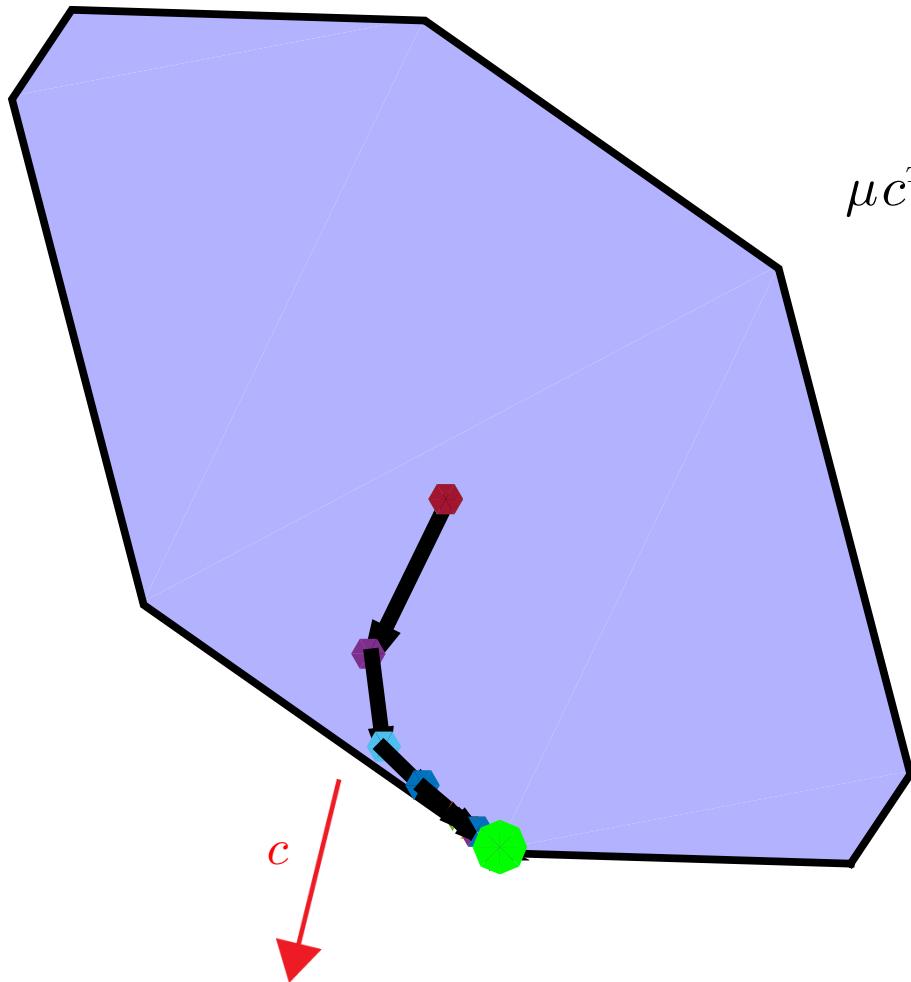
$$\min_x \mu c^T x - \sum_{i=1}^n \log(b_i - a_i^T x)$$

- ▶ Hessian $A^T \text{diag} \left(\frac{1}{(b_i - a_i^T x)^2} \right) A$ takes $O(nd^2)$ operations

$$\begin{array}{l} \min c^T x \\ Ax \leq b \end{array}$$

— Exact Newton

$$\mu c^T x - \sum_{i=1}^n \log(b_i - a_i^T x)$$



Interior Point Methods for Linear Programming

- ▶ Hessian of $f(x) = c^T x - \sum_{i=1}^n \log(b_i - a_i^T x)$

$$\nabla^2 f(x) = A^T \text{diag} \left(\frac{1}{(b_i - a_i^T x)^2} \right) A ,$$

Interior Point Methods for Linear Programming

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- ▶ Root of the Hessian

$$(\nabla^2 f(x))^{1/2} = \text{diag} \left(\frac{1}{|b_i - a_i^T x|} \right) A ,$$

Interior Point Methods for Linear Programming

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- ▶ Root of the Hessian

$$(\nabla^2 f(x))^{1/2} = \text{diag} \left(\frac{1}{|b_i - a_i^T x|} \right) A ,$$

- ▶ Sketch of the Hessian

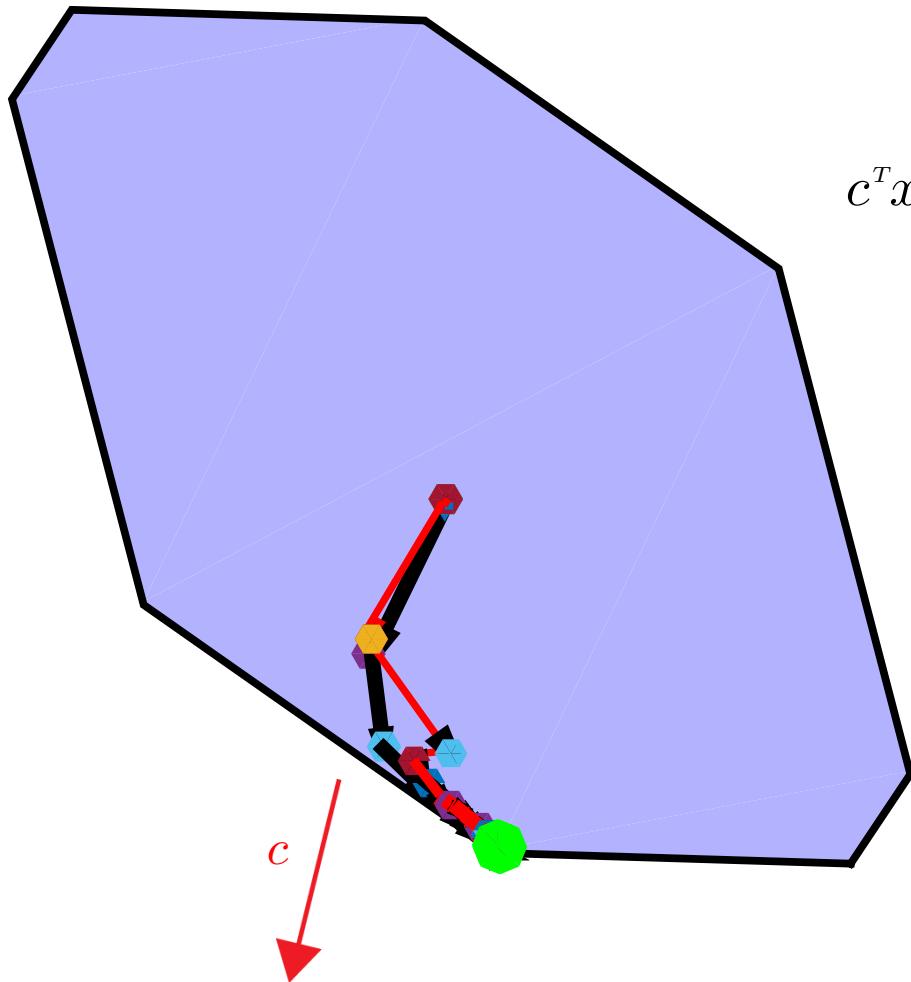
$$S^t (\nabla^2 f(x))^{1/2} = S^t \text{diag} \left(\frac{1}{|b_i - a_i^T x|} \right) A$$

takes $O(md^2)$ operations

$$\begin{array}{ll}\min & c^T x \\ Ax \leq & b\end{array}$$

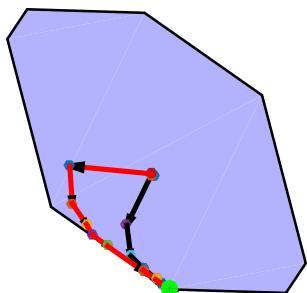
— Exact Newton
— Newton Sketch

$$c^T x - \mu \sum_{i=1}^n \log(b_i - a_i^T x)$$

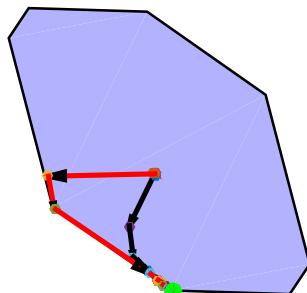


— Exact Newton
— Newton Sketch

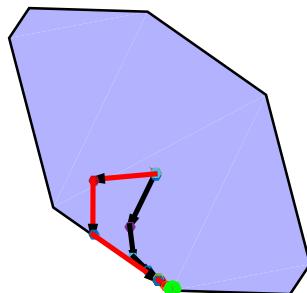
Trial 1



Trial 2



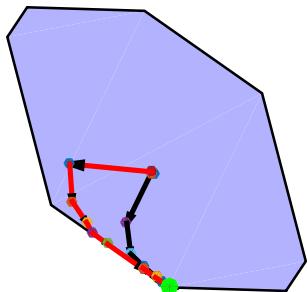
Trial 3



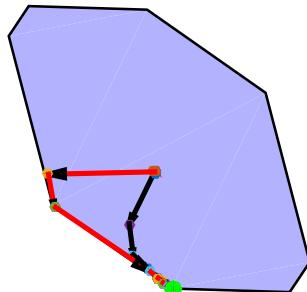
(a) sketch size $m = d$

— Exact Newton
— Newton Sketch

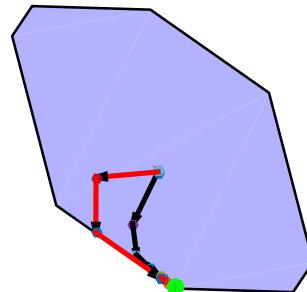
Trial 1



Trial 2



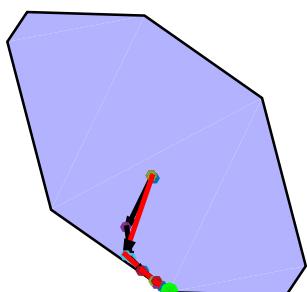
Trial 3



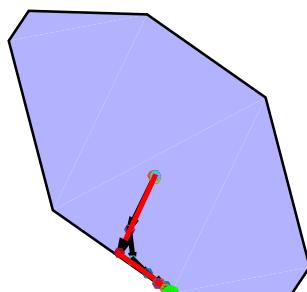
(a) sketch size $m = d$

— Exact Newton
— Newton Sketch

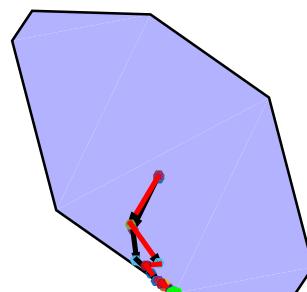
Trial 1



Trial 2

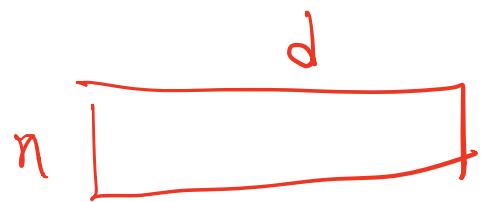


Trial 3



(b) sketch size $m = 4d$

High dimensional problems $n \ll d$



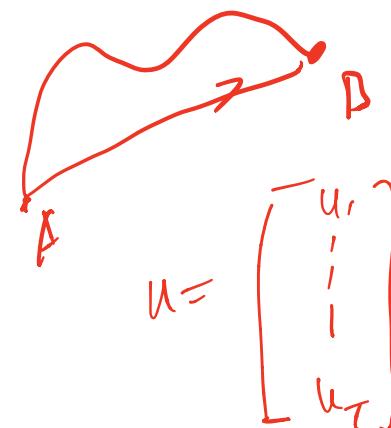
- ▶ $x^{t+1} = Ax_t + Bu_t, \quad t = 1, \dots, T$

High dimensional problems $n \ll d$

- ▶ $x^{t+1} = Ax_t + Bu_t, \quad t = 1, \dots, T$
- ▶ minimum fuel control from $0 \rightarrow x_f$

$$\min_u \|u\|_1$$

$$\text{s.t. } [B \ AB \ A^2B \ \dots]u = x_f$$



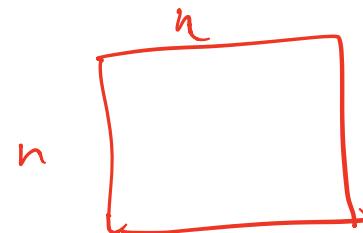
- ▶ nT decision variables
- ▶ We can apply sampling and sketching for the variables
 $u \in \mathbb{R}^{nT}$
- ▶ Basic idea: dual linear program has nT constraints



Kernel methods

- ▶ Kernel matrices

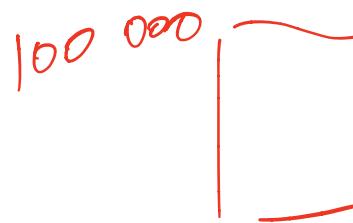
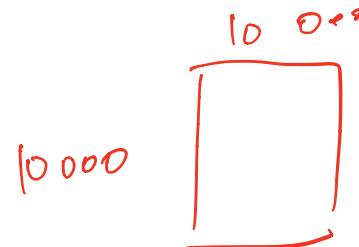
given data points $x_1, \dots, x_n \in \mathbb{R}^d$



RDF

e.g., Gaussian kernel $K_{ij} = e^{-\frac{1}{\sigma^2} \|x_i - x_j\|_2^2}$

- ▶ large $n \times n$ square matrices



Kernel methods

N.T.L

Neural Tangent Kernel

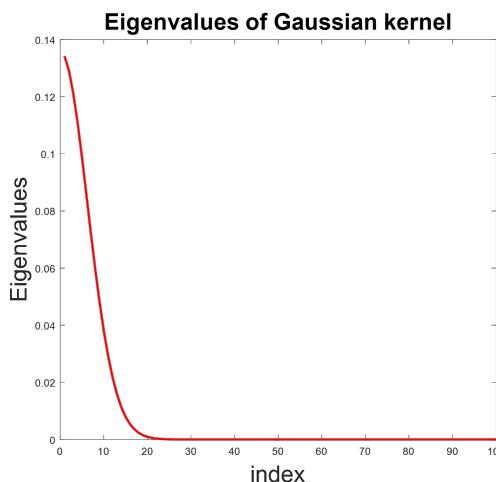
- ▶ Kernel matrices

given data points $x_1, \dots, x_n \in \mathbb{R}^d$

e.g., Gaussian kernel $K_{ij} = e^{-\frac{1}{\sigma^2} \|x_i - x_j\|_2^2}$

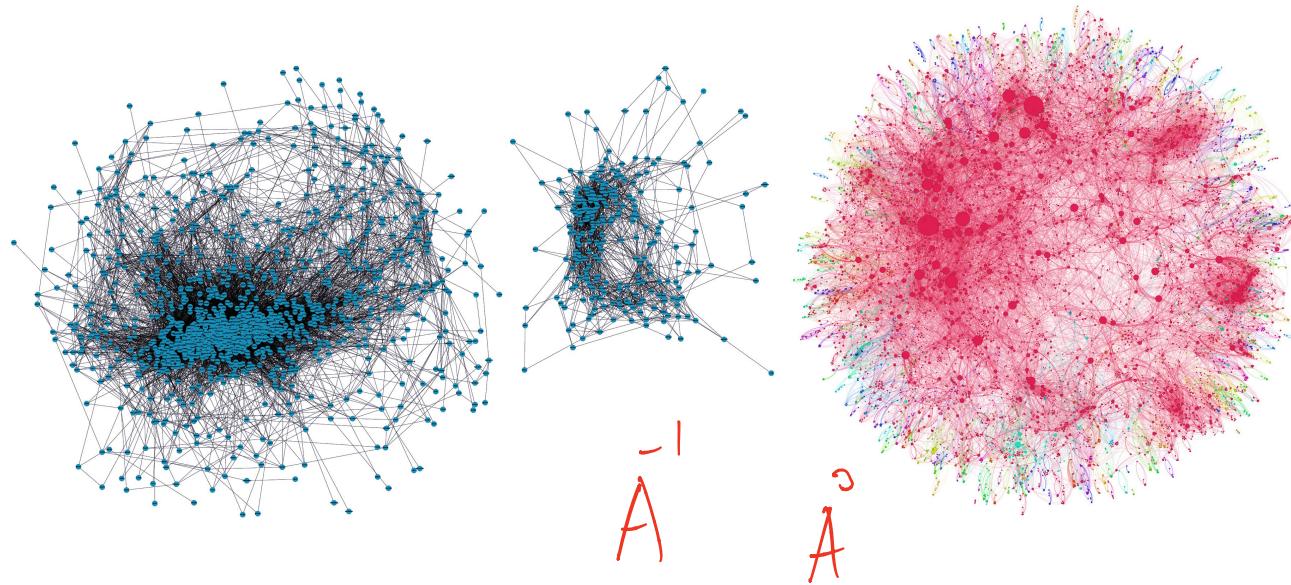
- ▶ large $n \times n$ square matrices

$$\sqrt{\log n} \begin{matrix} n \\ S \end{matrix} = \begin{matrix} n \\ K \end{matrix} \begin{matrix} n \\ SK \end{matrix}$$

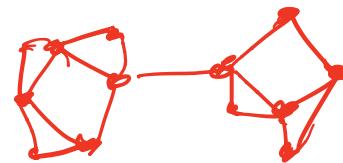


Large Graphs

- ▶ Adjacency matrix or Laplacian
- ▶ Examples: a gene network and a co-authorship network graph



Sampling Graphs

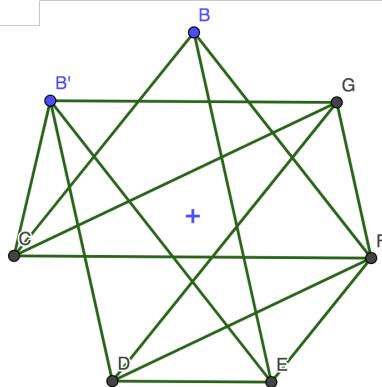


► Random sampling graphs

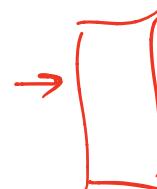
14 edges

Adjacency Matrix:

$$\begin{pmatrix} 0 & 0 & 1 & 0 & 1 & 1 & 0 \\ 0 & 0 & 1 & 1 & 1 & 0 & 1 \\ 1 & 1 & 0 & 0 & 0 & 1 & 1 \\ 0 & 1 & 0 & 0 & 1 & 1 & 1 \\ 1 & 1 & 0 & 1 & 0 & 1 & 0 \\ 1 & 0 & 1 & 1 & 1 & 0 & 1 \\ 0 & 1 & 1 & 1 & 0 & 1 & 0 \end{pmatrix}$$



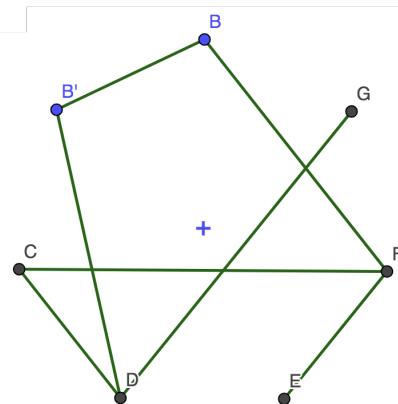
→ | Average Score



7 edges

Adjacency Matrix:

$$\begin{pmatrix} 0 & 1 & 0 & 0 & 0 & 1 & 0 \\ 1 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 1 & 0 \\ 0 & 1 & 1 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 1 & 0 & 1 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 \end{pmatrix}$$



Non-convex Optimization Problems

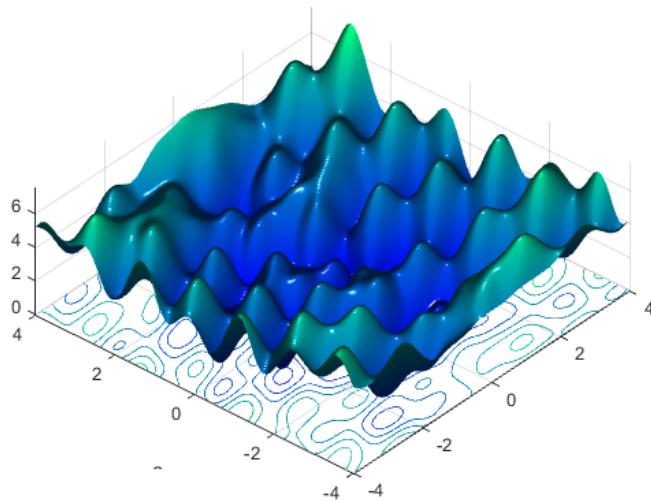
- ▶ In general, very difficult to solve globally
- ▶ Need to make further assumptions

$$\min_{\mathbf{x} \in \mathbb{R}^n} \mathbf{x}^\top \mathbf{Q} \mathbf{x}$$

$0 \leq x_i \leq 1$

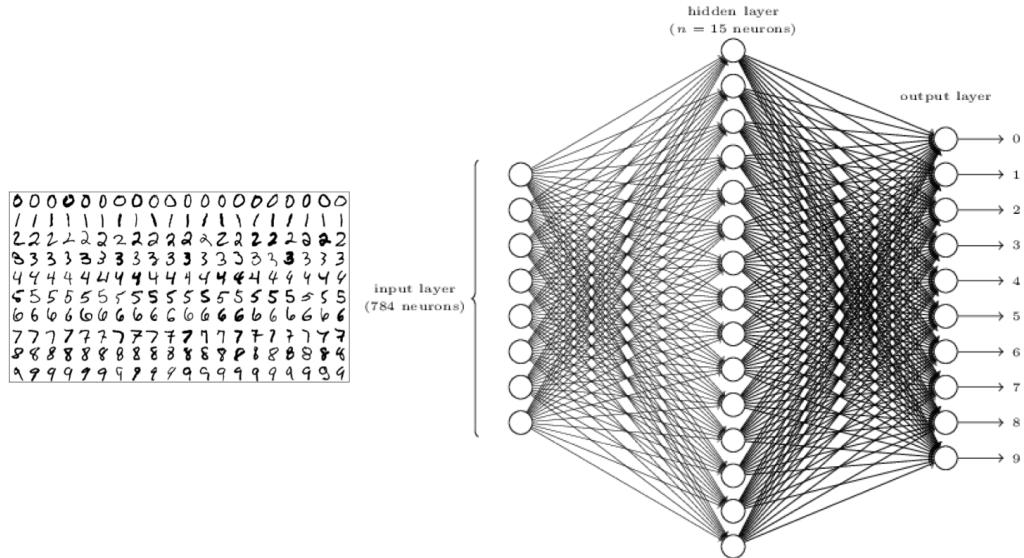
\sim SDP

MAXCUT



Non-convex Optimization Problems

$$\min_x \sum_{i=1}^n (f_x(a_i) - y_i)^2$$



Non-convex Optimization Problems

$$\min_x \sum_{i=1}^n (f_x(a_i) - y_i)^2$$

→ Heuristic: Gauss-Newton method

$$x_{t+1} = \arg \min_x \| \underbrace{f_{x_t}(A) + J_t x}_{\text{Taylor's approx for } f_x} - y \|_2^2$$

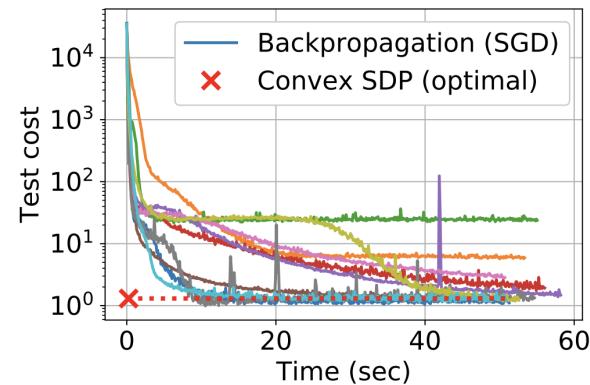
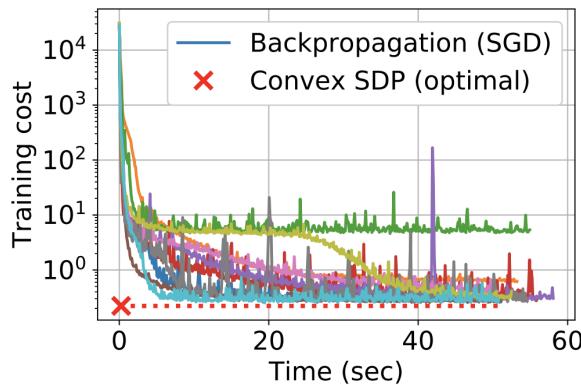
where $(J_t)_{ij} = \frac{\partial}{\partial x_j} f_x(a_i)$ is the Jacobian matrix

- ▶ Jacobian can be sampled for faster computations

Convex Optimization for Neural Networks

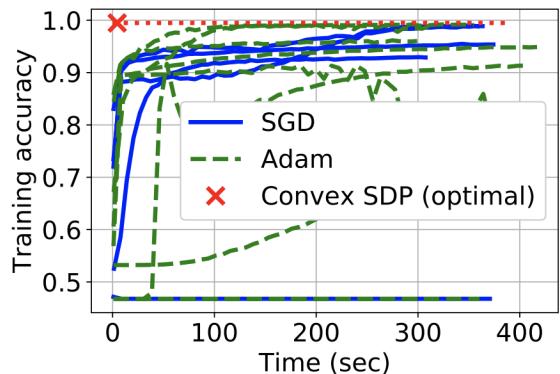


- ▶ Neural Network problems can be formulated as convex optimization problems in higher dimensions by *lifting*
- ▶ enables global optimization in polynomial time

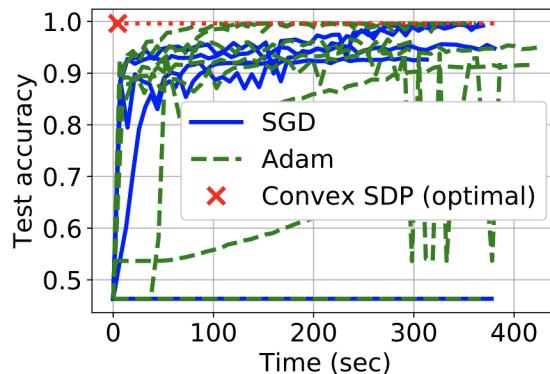


Convex Optimization for Neural Networks

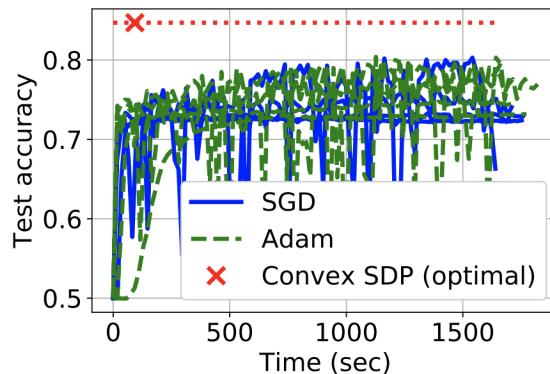
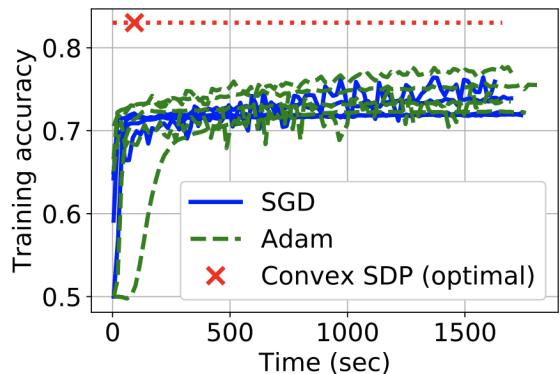
0.0001



(a) CNN, MNIST, training accuracy



(b) CNN, MNIST, test accuracy



Questions?