EE270
Large scale matrix computation, optimization and learning

Instructor : Mert Pilanci

Stanford University

Tuesday, Jan 7 2020

Outline

- Introduction
- Administrative
- Overview of topics and applications

Administrative

Teaching staff

- Instructor: Mert Pilanci
  - Email: pilanci@stanford.edu
  - Office hours: Wednesday 3-5pm in Packard 255

  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:
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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**.

Prerequisites

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

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
  - I will suggest a list of research problems on the course website
  - Proposal (1 page) and progress report (4 pages)
  - Final presentation (last week of classes)

Topics

- randomized linear algebra
  - approximate matrix multiplication
  - tools from probability theory
  - sampling and projection methods
- randomized linear system solvers and regression
  - leverage scores
  - iterative sketching and preconditioning
  - sparse linear systems
  - robust regression
- matrix decompositions
  - randomized QR decomposition
  - randomized low rank factorization
  - column subset selection

Topics

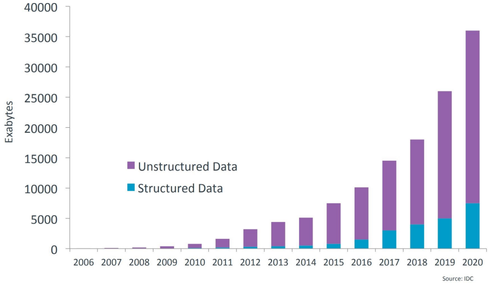
- large-scale optimization
  - empirical risk minimization
  - stochastic gradient methods and variants
  - second order methods and Hessian approximations
  - asynchronous distributed optimization
- kernel methods
  - Reproducing kernel Hilbert spaces
  - Nystrom approximations
  - Random features
  - neural networks and Neural Tangent Kernel
- information-theoretic methods
  - Error-resilient computations via error-correcting codes
  - Lower-bounds on random projections

For details see Canvas!

Any questions?

Overview of topics and applications

Scale of data



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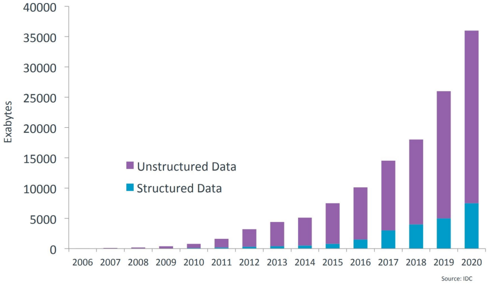
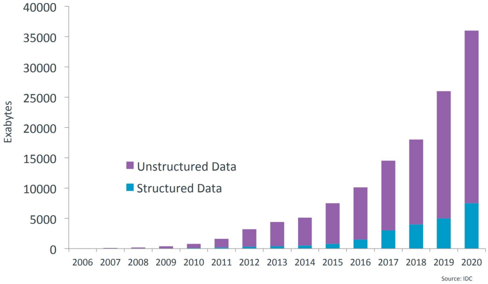


- Every day, we create 2.5 billion gigabytes of data

Scale of data



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- Data stored grows 4x faster than world economy (Mayer-Schonberger)

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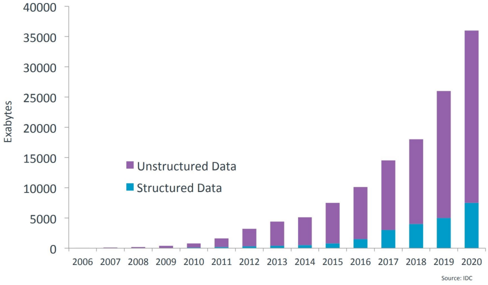

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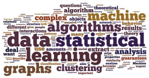
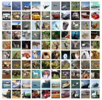
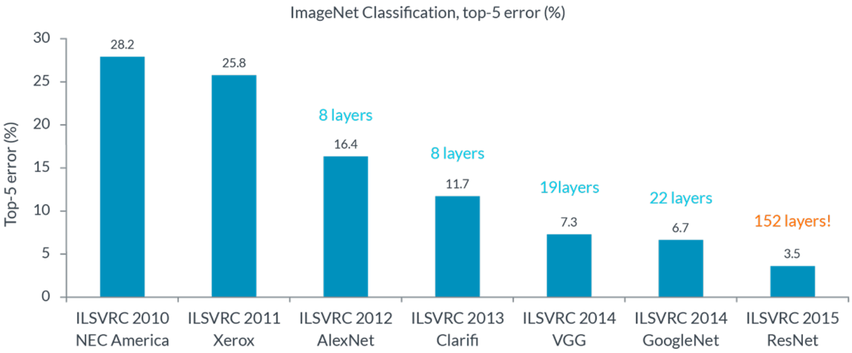


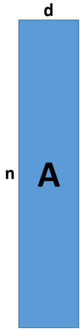


Deep learning revolution



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.

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
- ...

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
⋮						

in machine learning, statistics and signal processing

- More data points typically increase the accuracy of models
  $\rightarrow$ large scale matrix computation and optimization problems

  e.g. matrix multiplication, matrix factorization, singular value decomposition, convex optimization, non-convex optimization...

in machine learning, statistics and signal processing

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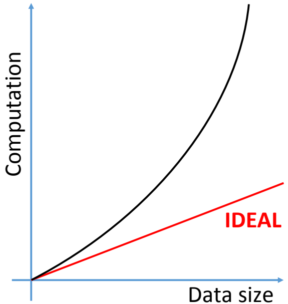
Can we reduce the data volume with minimal loss of information ?



Matrix Computations

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

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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

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

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

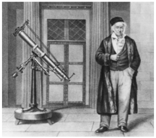
[US Department of Transportation]
[Deng et al. 2009]

Approximate Matrix Multiplication

- How to approximate the matrix product AB fast ?

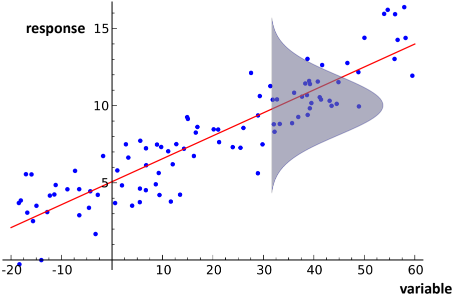
$$\begin{pmatrix} & & \\ & A & \\ & & \end{pmatrix}\begin{pmatrix} & & \\ & B & \\ & & \end{pmatrix} \approx \begin{pmatrix} \\ C \\ \\ \end{pmatrix}\begin{pmatrix} & R & \end{pmatrix}$$

Least Squares Problems



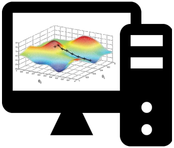
Least squares
$$\min_x \|Ax - y\|^2$$

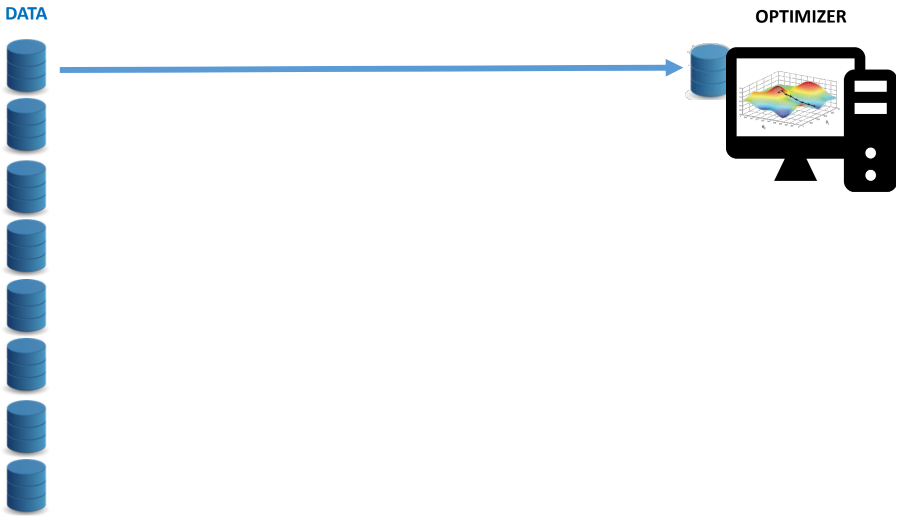
[Gauss, 1795]

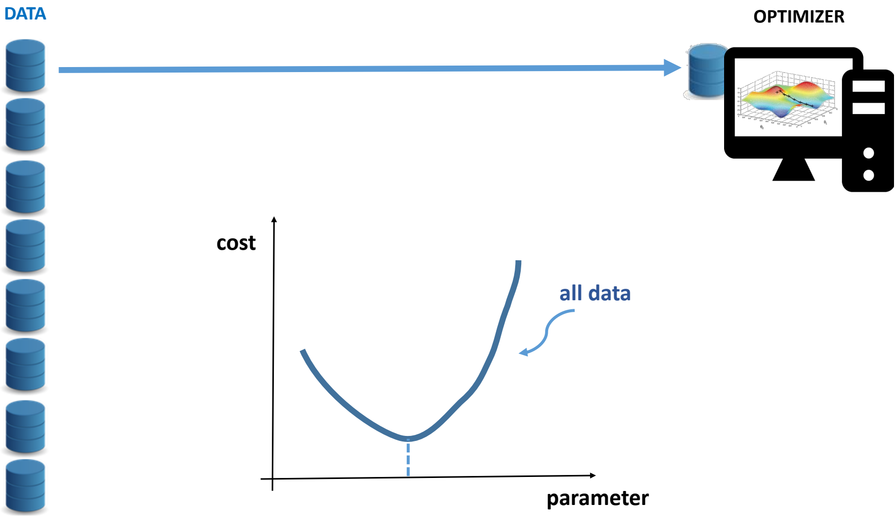


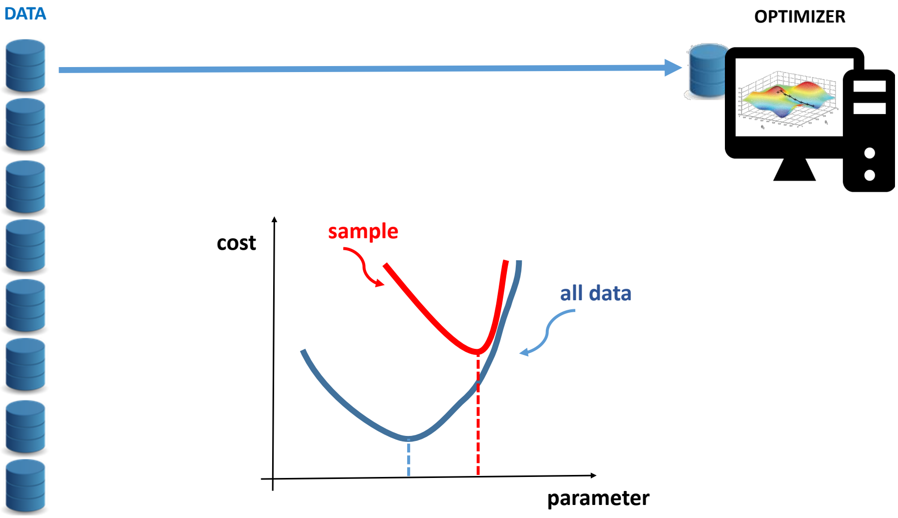
DATA

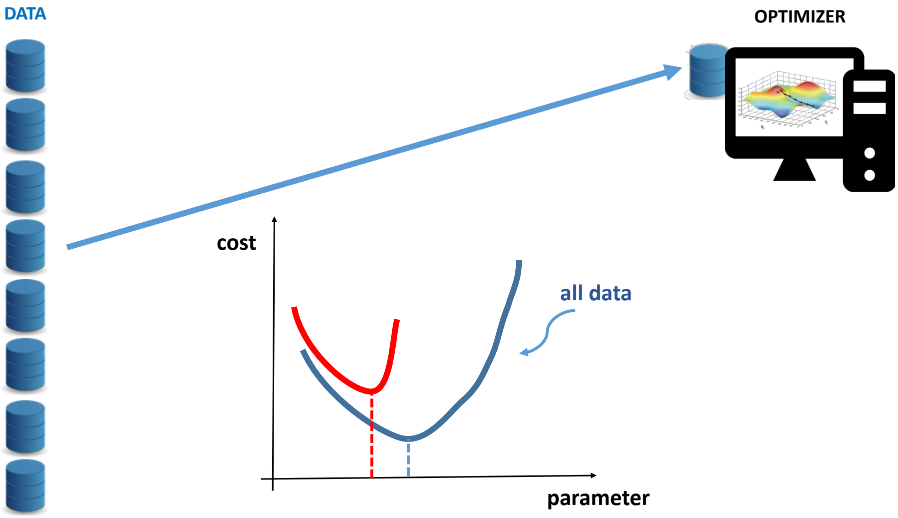
OPTIMIZER

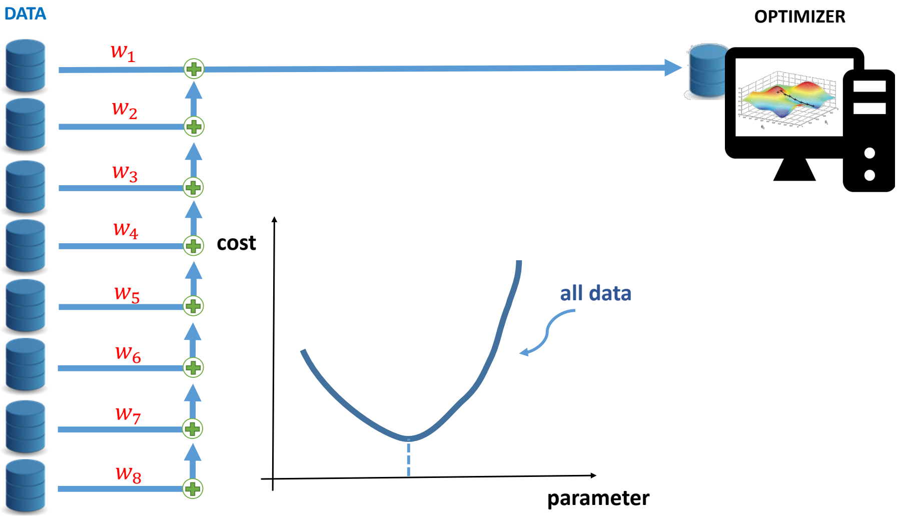


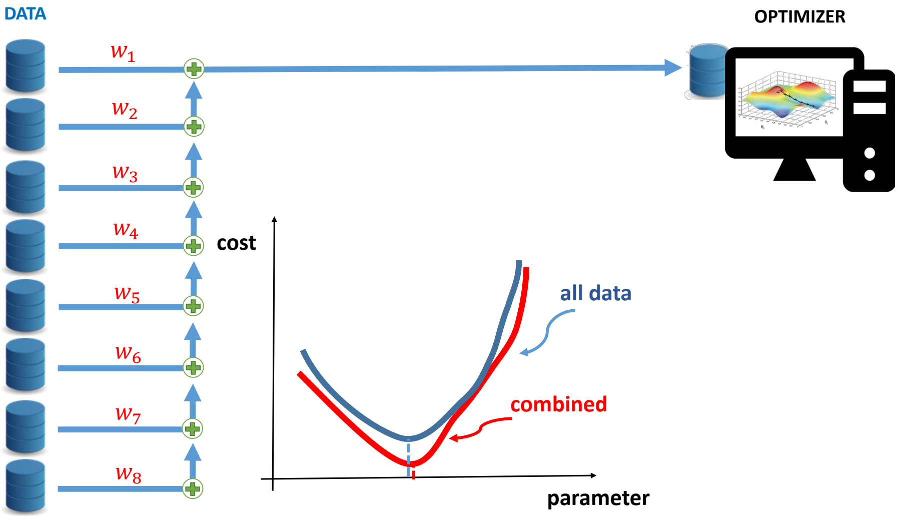

DATA
OPTIMIZER


DATA
OPTIMIZER
cost
all data
parameter

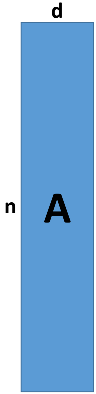

DATA
OPTIMIZER
cost
sample
all data
parameter


DATA
OPTIMIZER
cost
all data
parameter


DATA
OPTIMIZER
w_1
w_2
w_3
w_4
w_5
w_6
w_7
w_8
cost
all data
parameter


DATA
OPTIMIZER
w_1
w_2
w_3
w_4
w_5
w_6
w_7
w_8
cost
all data
combined
parameter

Randomized Sketching



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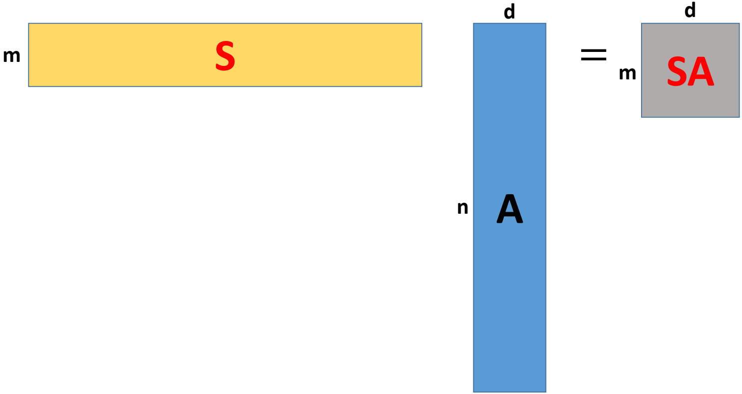
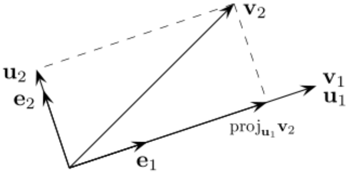


Randomized Least Squares Solvers

- A : $n \times d$ feature matrix, and y : $n \times 1$ response vector
- Original problem $\quad \mathbf{OPT} = \min_{x \in \mathcal{C}} \underbrace{\|Ax - y\|^2}$
- Randomized approximation $\quad \min_{x \in \mathcal{C}} \underbrace{\|\tilde{A}x - \tilde{y}\|^2}$
- $\tilde{A}$ and $\tilde{y}$ are smaller approximations

QR decomposition

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



$$
\begin{aligned}
\mathbf{u}_1 &= \mathbf{v}_1, & \mathbf{e}_1 &= \frac{\mathbf{u}_1}{\|\mathbf{u}_1\|} \\
\mathbf{u}_2 &= \mathbf{v}_2 - \mathrm{proj}_{\mathbf{u}_1}(\mathbf{v}_2), & \mathbf{e}_2 &= \frac{\mathbf{u}_2}{\|\mathbf{u}_2\|} \\
\mathbf{u}_3 &= \mathbf{v}_3 - \mathrm{proj}_{\mathbf{u}_1}(\mathbf{v}_3) - \mathrm{proj}_{\mathbf{u}_2}(\mathbf{v}_3), & \mathbf{e}_3 &= \frac{\mathbf{u}_3}{\|\mathbf{u}_3\|} \\
\mathbf{u}_4 &= \mathbf{v}_4 - \mathrm{proj}_{\mathbf{u}_1}(\mathbf{v}_4) - \mathrm{proj}_{\mathbf{u}_2}(\mathbf{v}_4) - \mathrm{proj}_{\mathbf{u}_3}(\mathbf{v}_4), & \mathbf{e}_4 &= \frac{\mathbf{u}_4}{\|\mathbf{u}_4\|} \\
&\vdots & &\vdots
\end{aligned}
$$

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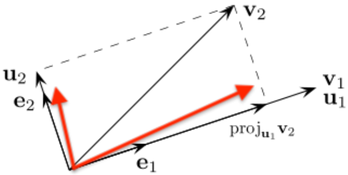


- complexity $O(dn^2)$
- randomized algorithm complexity $\approx O(dn)$

  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
- $\|A - \tilde{A}_k\|_2^2 \leq \sigma_{k+1}^2 + \epsilon\|A\|_2^2$

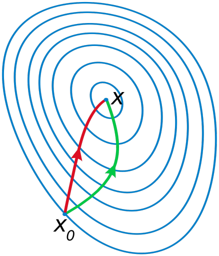
Iterative Methods

- Gradient descent and momentum acceleration
- Iterative sketching methods
- Conjugate gradient
- Preconditioning
- Sparse linear systems
- Stochastic Gradient Descent
- Variance reduction
- Adaptive gradient methods: Adagrad, ADAM

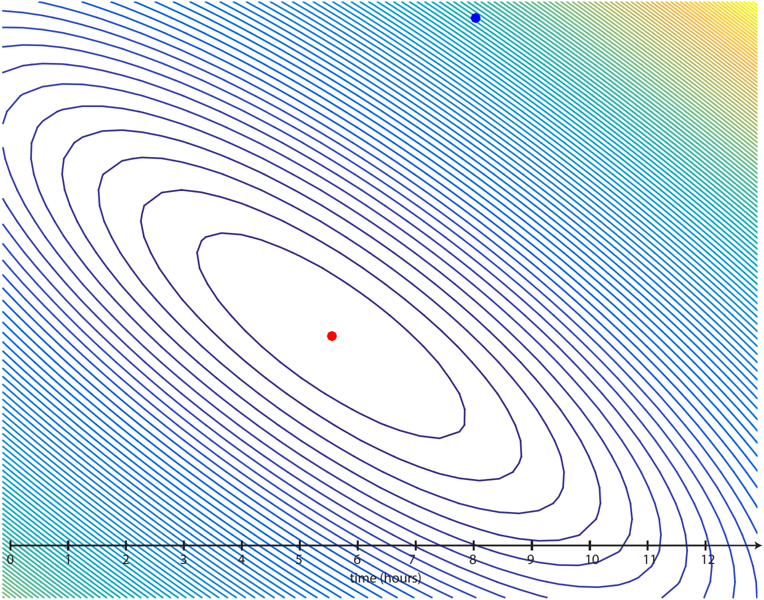
Newton's Method

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

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



Gradient Descent



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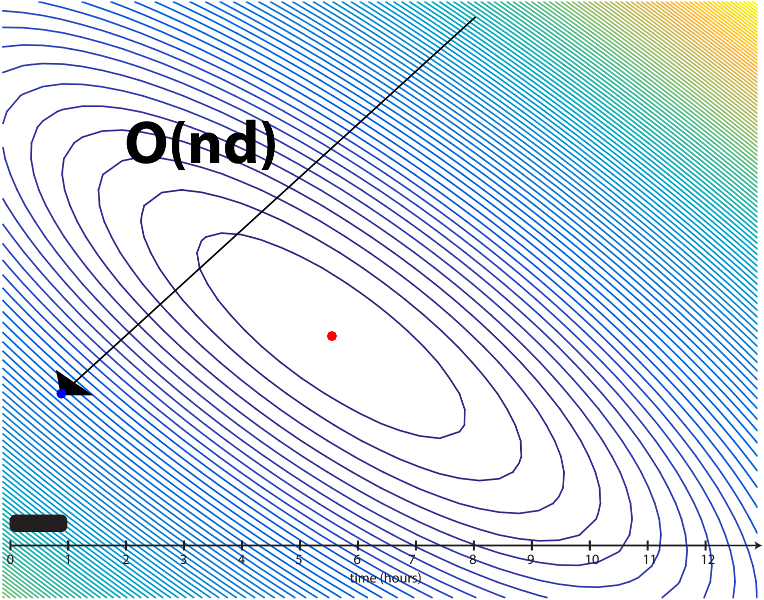

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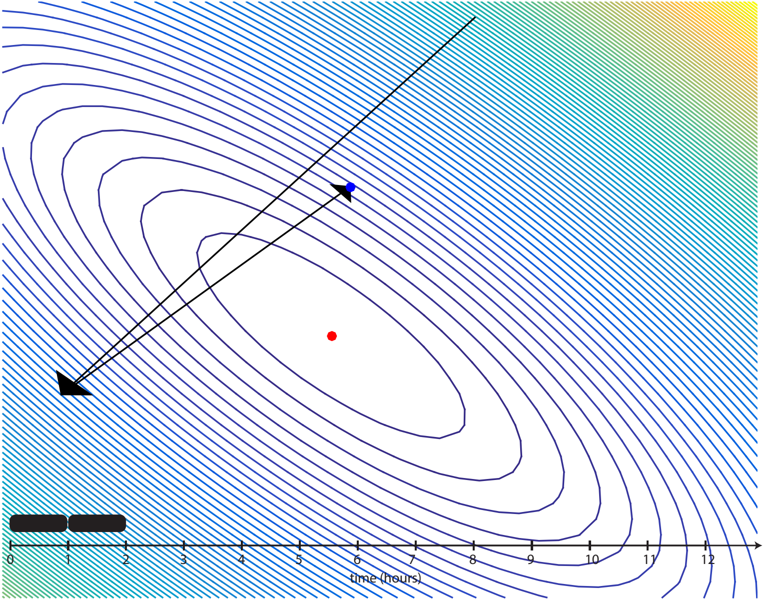

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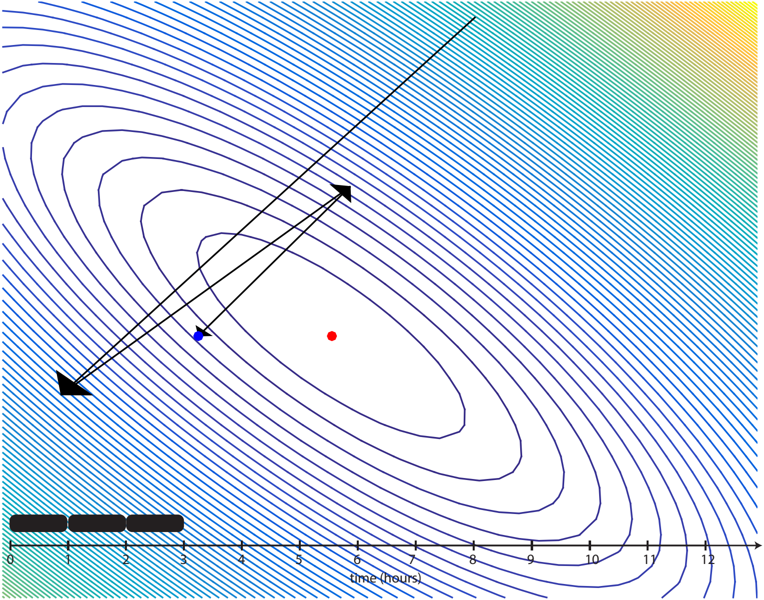

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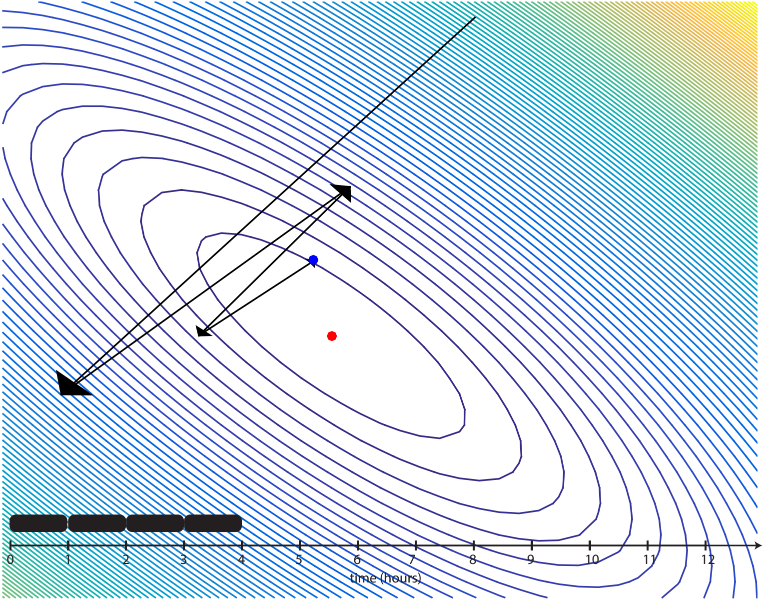

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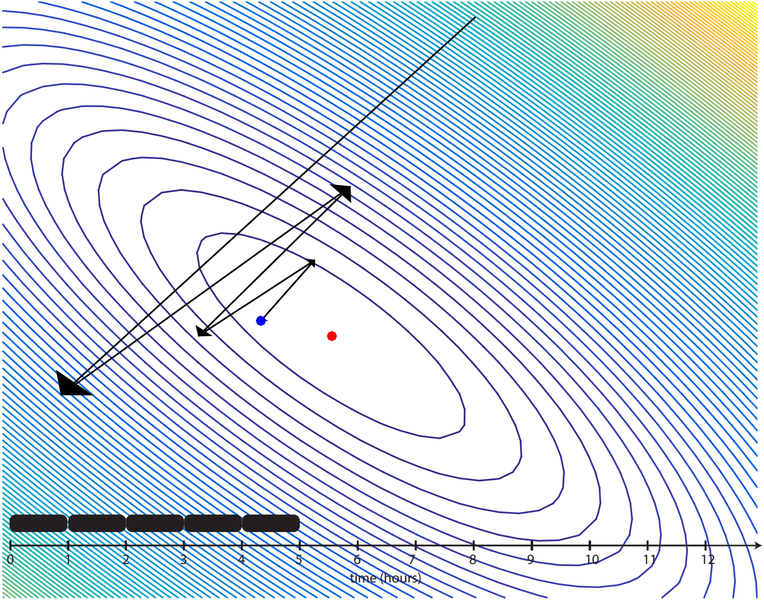

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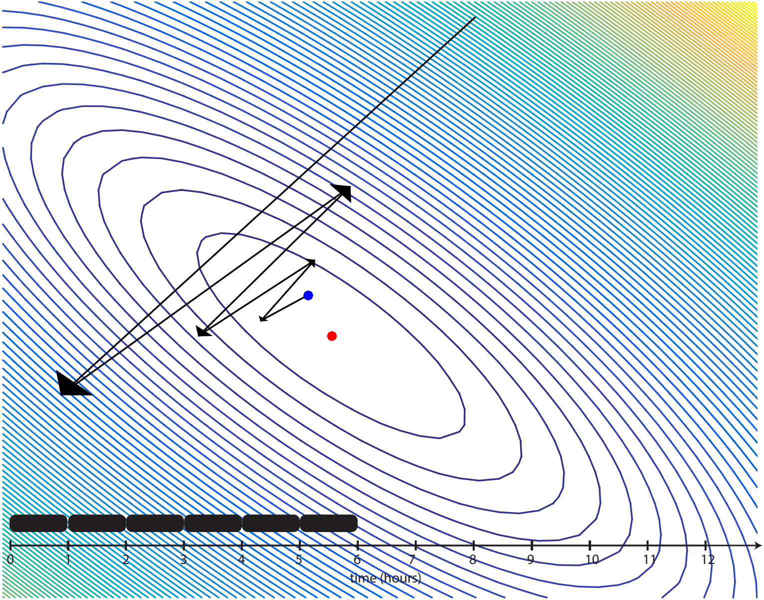
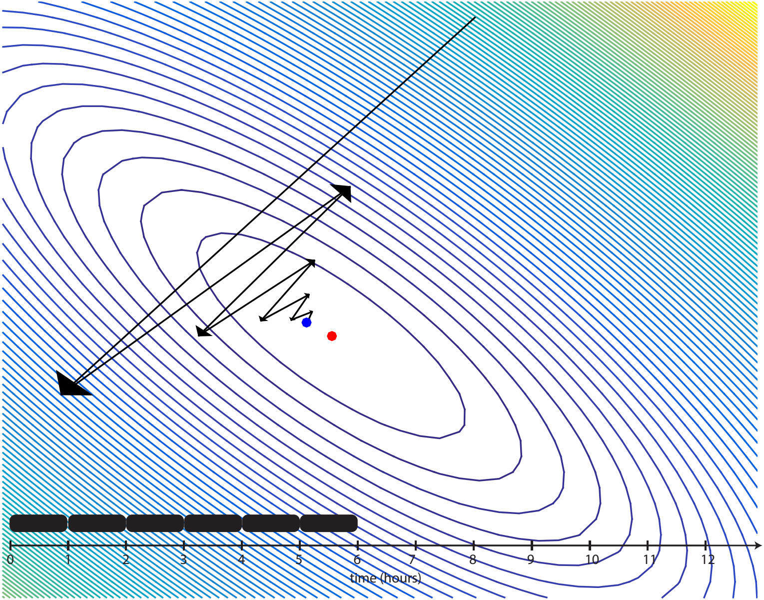
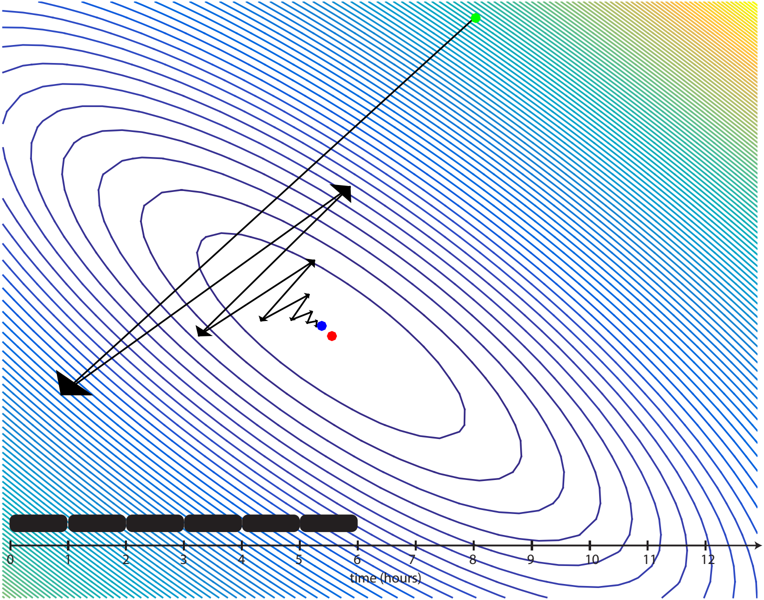


Gradient Descent vs



Gradient Descent vs Newton's Method



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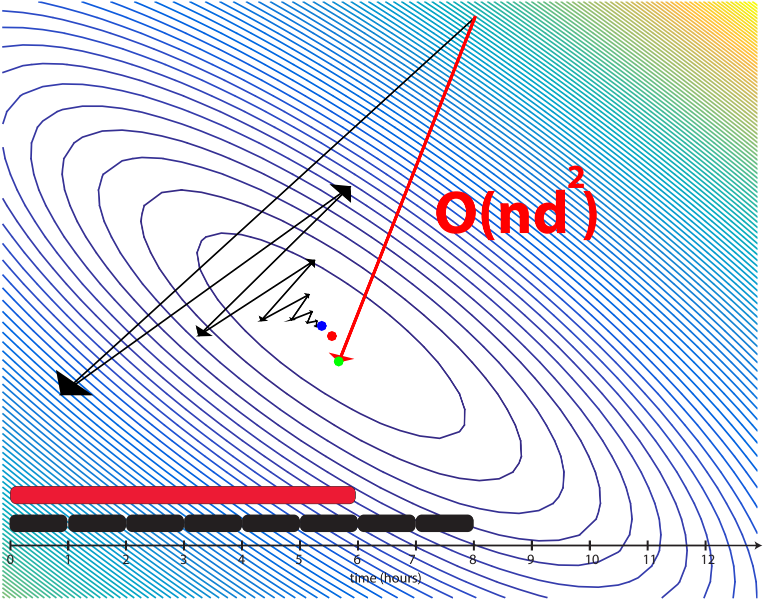

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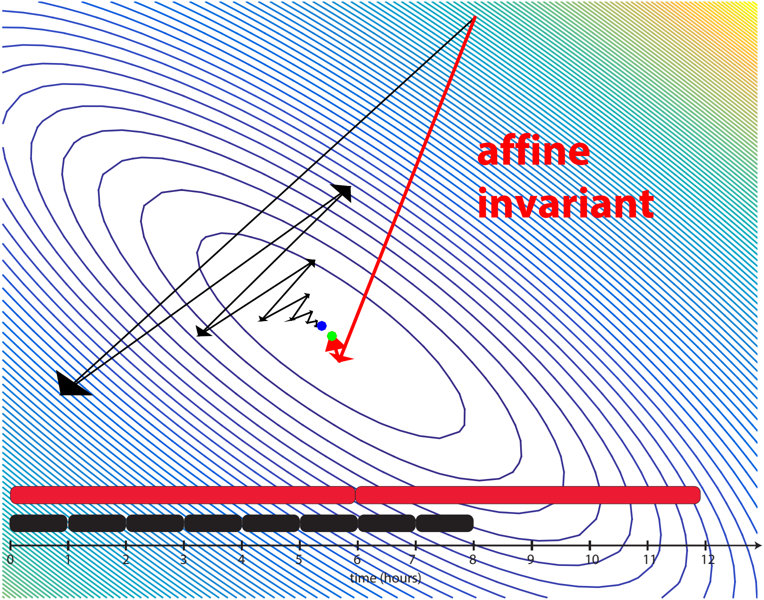

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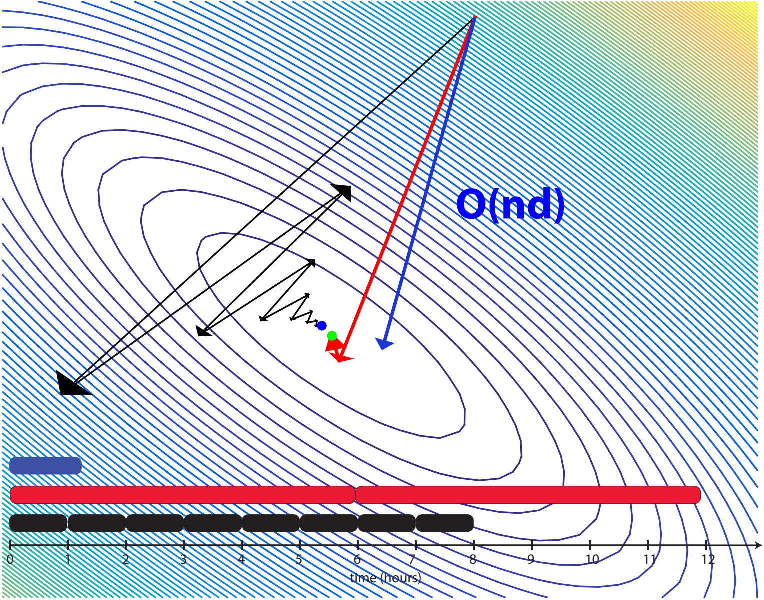

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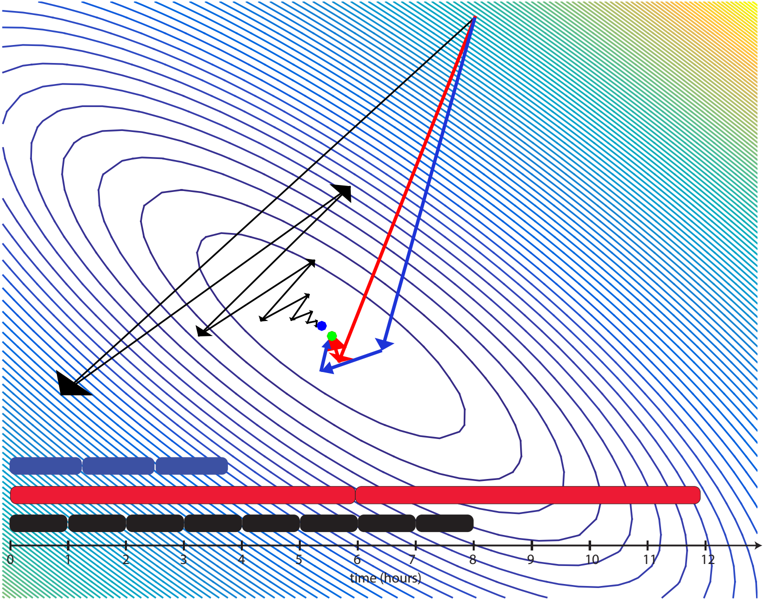
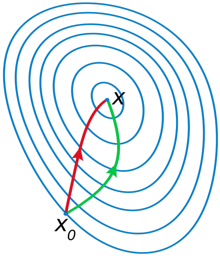


Randomized Newton's Method

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

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

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

Diagonal, subsampled, low-rank approximations yield

- 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 $A \in R^{n \times d}$

$$\min_{Ax \le b} \; c^T x$$

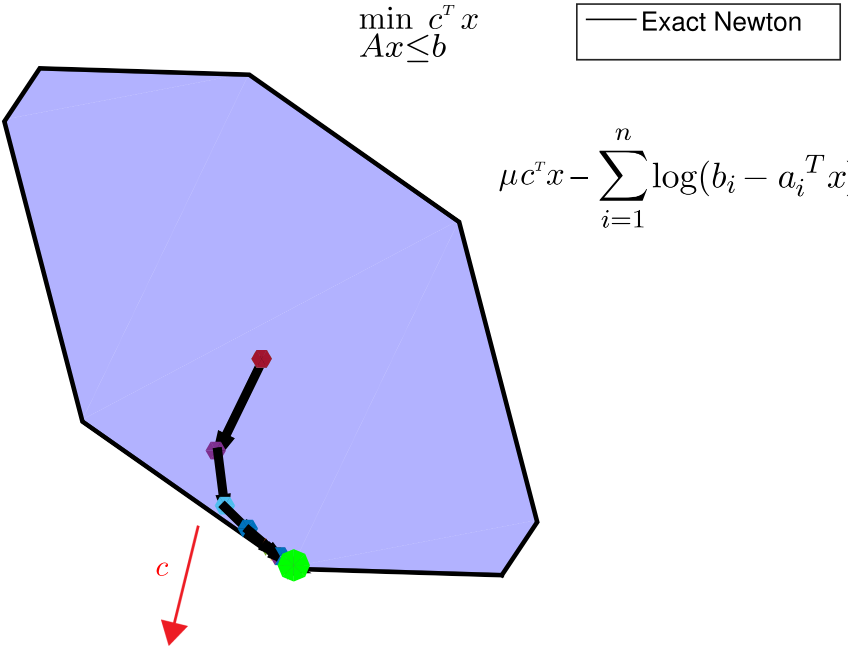
- Log barrier

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

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

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

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



Interior Point Methods for Linear Programming

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

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

Interior Point Methods for Linear Programming

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

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

- Root of the Hessian

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

Interior Point Methods for Linear Programming

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

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

- Root of the Hessian

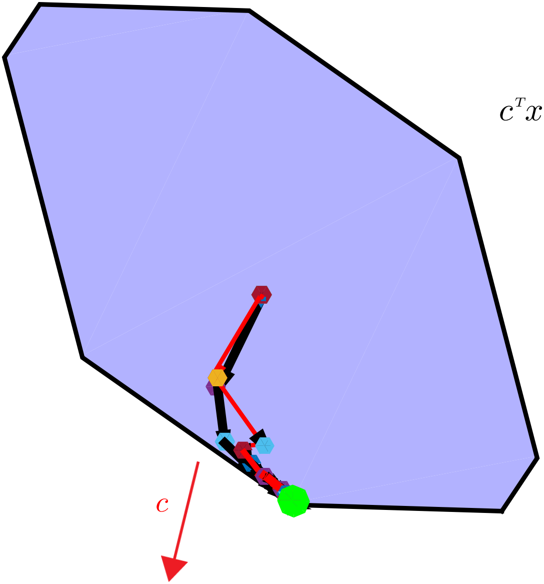
$$(\nabla^2 f(x))^{1/2} = diag\left(\frac{1}{|b_i - a_i^T x|}\right) A \;,$$

- Sketch of the Hessian

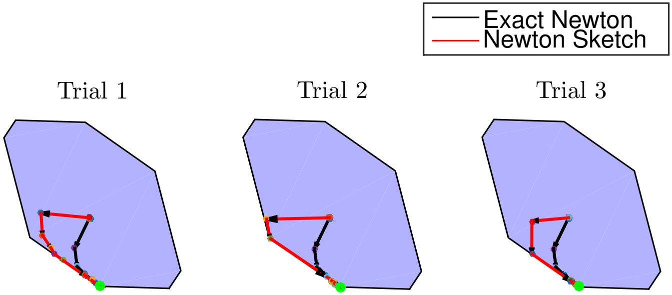
$$S^t (\nabla^2 f(x))^{1/2} = S^t diag\left(\frac{1}{|b_i - a_i^T x|}\right) A$$

takes $O(md^2)$ operations

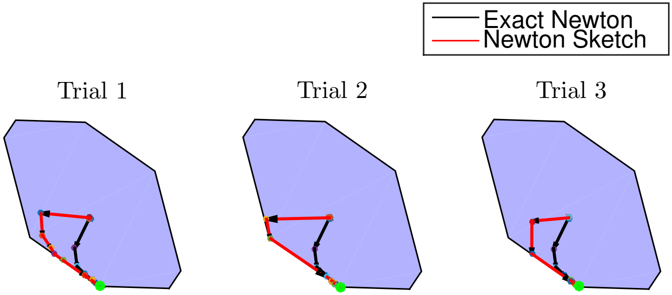
$$\min_{Ax \leq b} \; c^T x$$



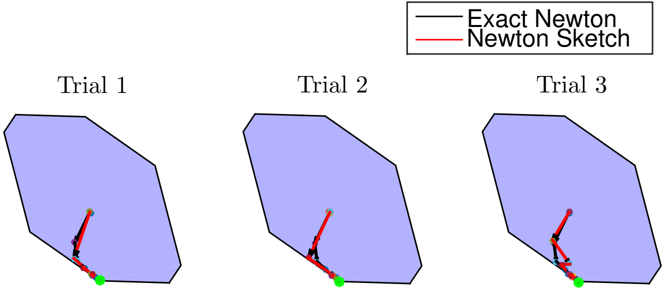
$$c^T x - \mu \sum_{i=1}^{n} \log(b_i - a_i^T x)$$



(a) sketch size $m = d$



(a) sketch size $m = d$



(b) sketch size $m = 4d$

High dimensional problems $n \ll d$

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

High dimensional problems $n \ll d$

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

$$\begin{aligned} &\min_u \ \|u\|_1 \\ &\text{s.t.} \ [\ B \quad AB \quad A^2B \quad \cdots \ ]u = x_f \end{aligned}$$

- 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 $x_1, \ldots, x_n \in \mathbb{R}^d$
  e.g., Gaussian kernel $K_{ij} = e^{-\frac{1}{\sigma^2}\|x_i - x_j\|_2^2}$
- large $n \times n$ square matrices

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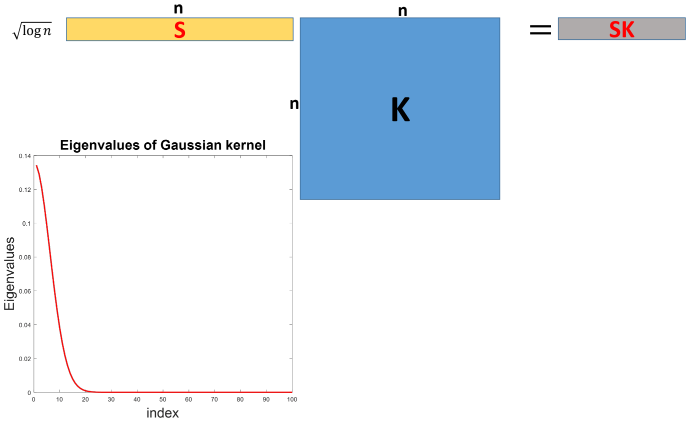
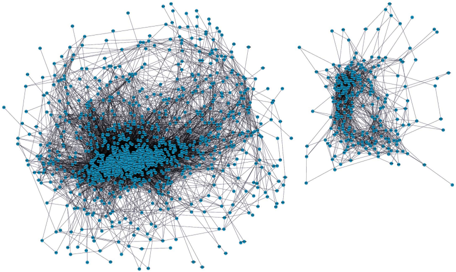
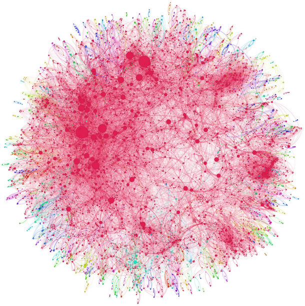


Large Graphs

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





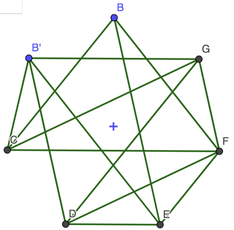
Sampling Graphs

- Random sampling graphs

14 edges

Adjacency Matrix:

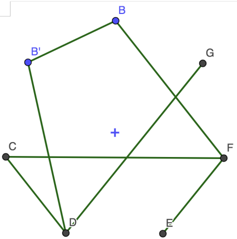
$$\begin{pmatrix} 0 & 0 & 1 & 0 & 1 & 1 & 0 \\ 0 & 0 & 1 & 1 & 1 & 0 & 1 \\ 1 & 1 & 0 & 0 & 0 & 1 & 1 \\ 0 & 1 & 0 & 0 & 1 & 1 & 1 \\ 1 & 1 & 0 & 1 & 0 & 1 & 0 \\ 1 & 0 & 1 & 1 & 1 & 0 & 1 \\ 0 & 1 & 1 & 1 & 0 & 1 & 0 \end{pmatrix}$$



7 edges

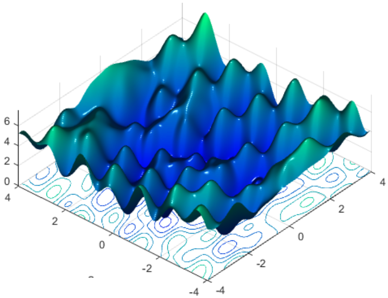
Adjacency Matrix:

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



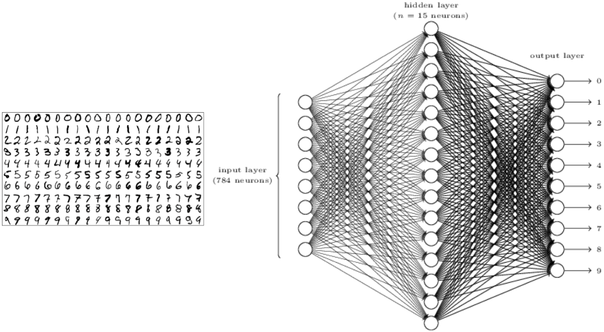
Non-convex Optimization Problems

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



Non-convex Optimization Problems

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



Non-convex Optimization Problems

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

$\rightarrow$ 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

Questions?