High-dimensional prediction: Some computational challenges

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Statistics and EECS

Baker-Kingland Lecture
Predictive Inference and its Applications

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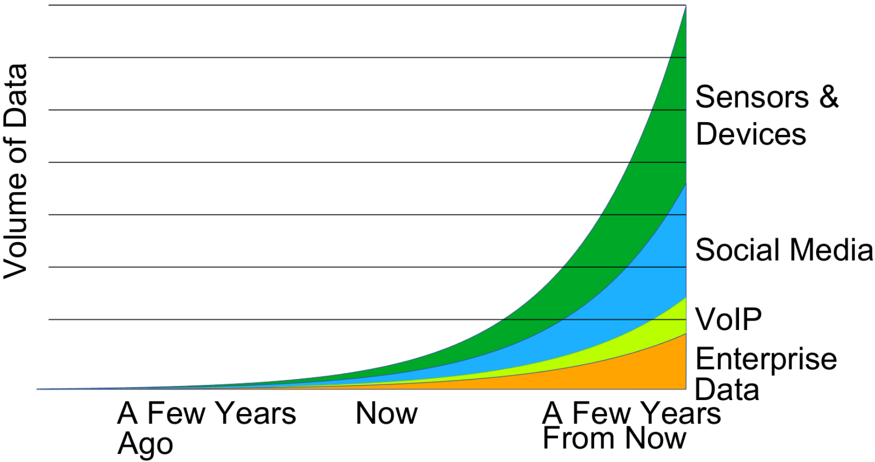
The Data Explosion



- Every day: 2.5 billion gigabytes of data created
- Last two years: creation of 90% of the world's data (source: IBM)
- Data stored grows 4X faster than world economy
  (source: Mayer-Schonberger)

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- Computational considerations need to be considered jointly with statistical ones.
- Interesting trade-offs between computational and statistical efficiency.

Today's talk: Two vignettes

§1 Data sketches: randomized dimensionality reduction

§2 Early stopping of iterative algorithms for prediction

§. 1. Randomized sketches of data

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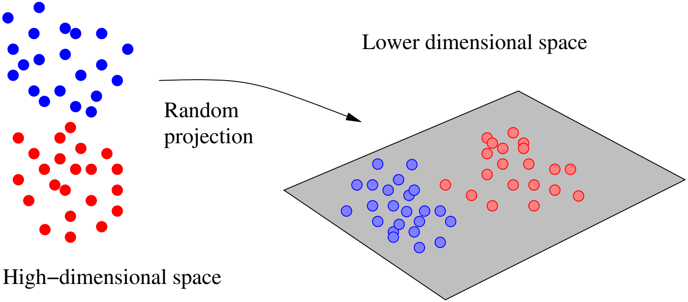
Randomized projection is a general purpose tool:

- Choose a random subspace of "low" dimension m.
- Project data into subspace, and solve reduced dimension problem.



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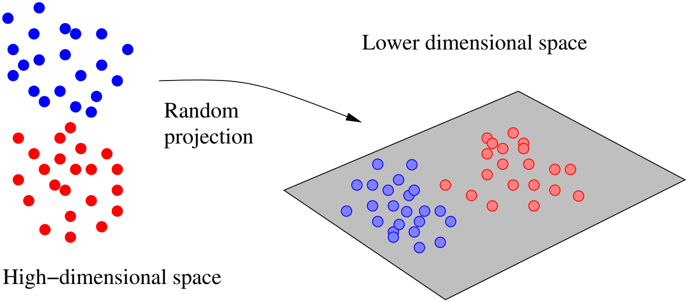


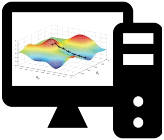
Widely studied and used:

- Johnson & Lindenstrauss (1984): in Banach/Hilbert space geometry
- various surveys and books: Vempala, 2004; Mahoney et al., 2011 Cormode et al., 2012.

Randomized sketches for statistical optimization

DATA

OPTIMIZER



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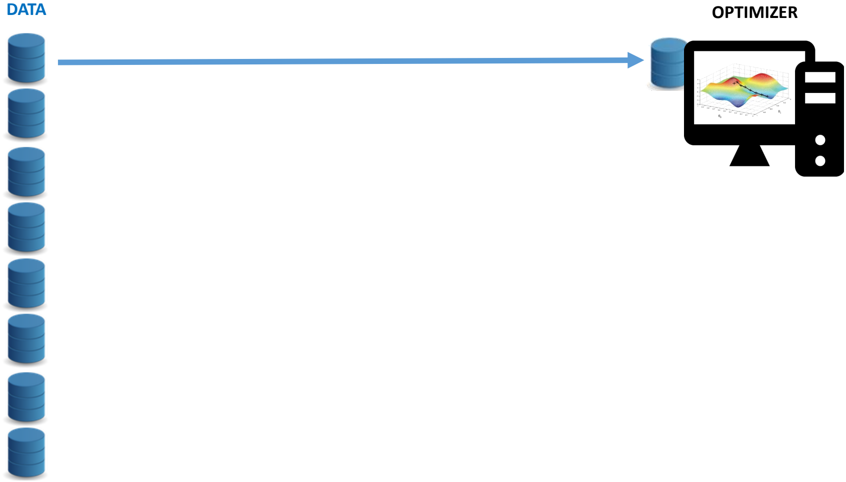

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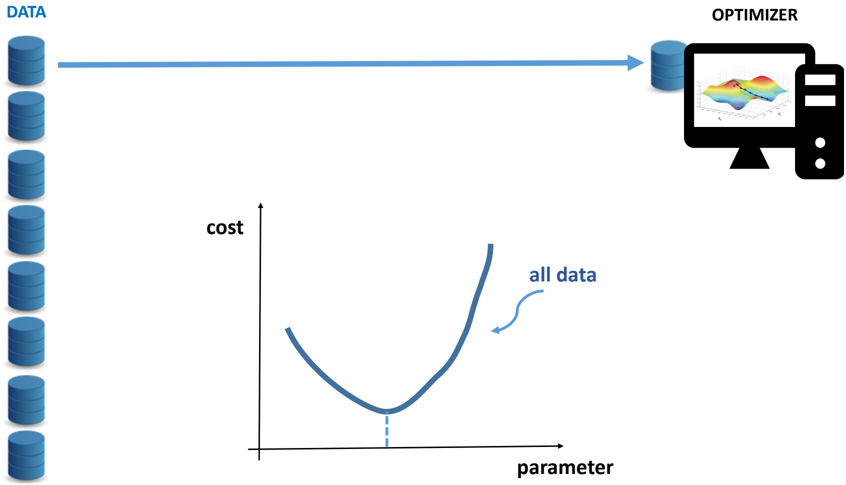

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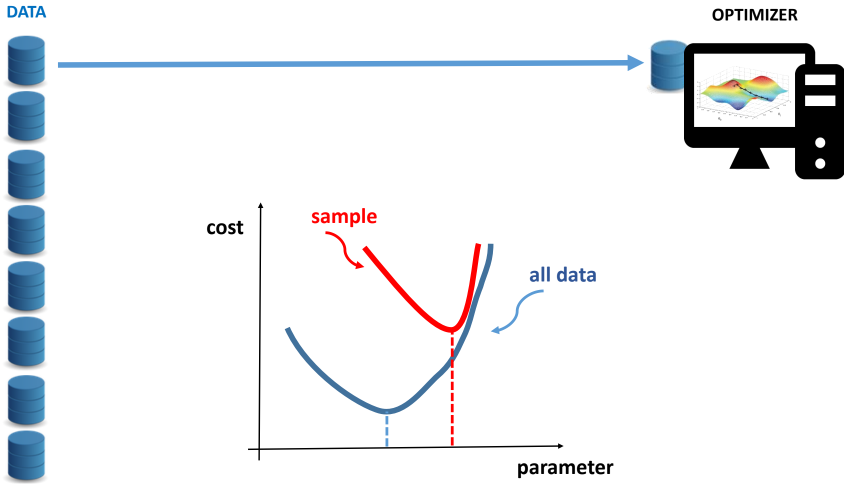

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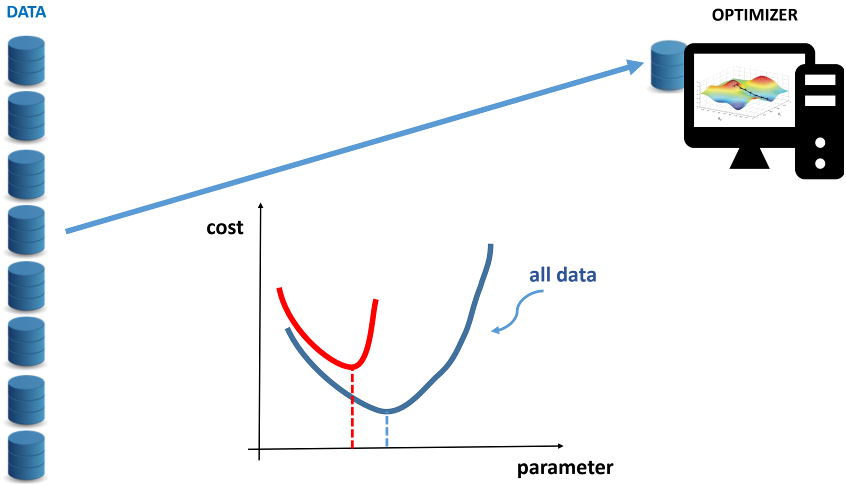

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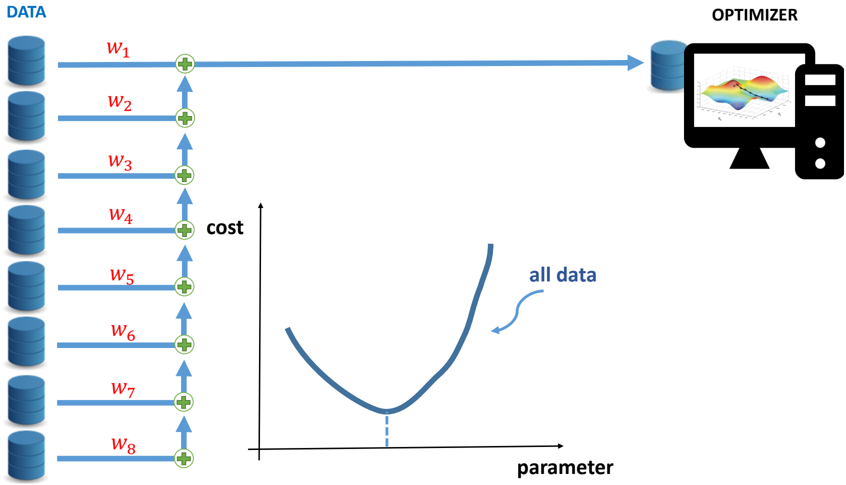

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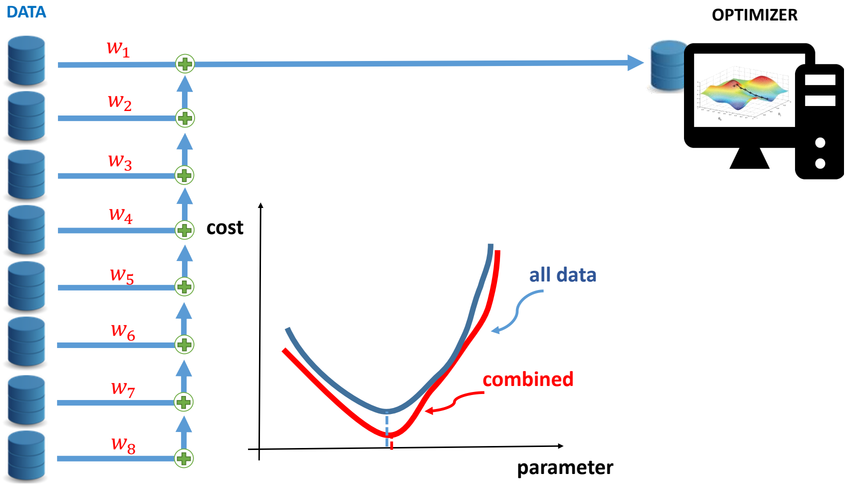

Randomized projection for constrained least-squares

- Given data matrix $A \in \mathbb{R}^{n \times d}$, and response vector $y \in \mathbb{R}^n$
- Least-squares over convex constraint set $\mathcal{C} \subseteq \mathbb{R}^d$:

$$x_{\text{LS}} = \arg\min_{x \in \mathcal{C}} \underbrace{\|Ax - y\|_2^2}_{f(Ax)}$$

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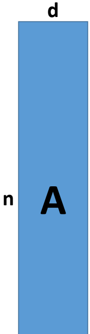

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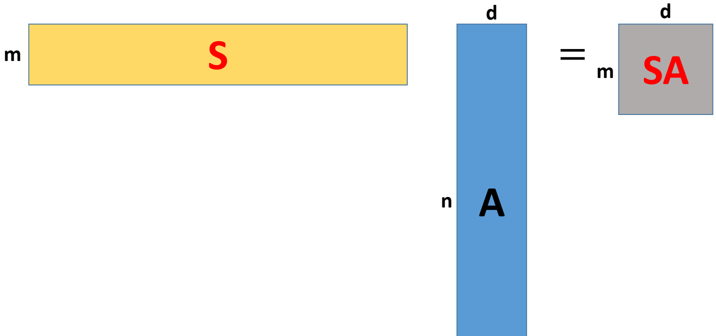
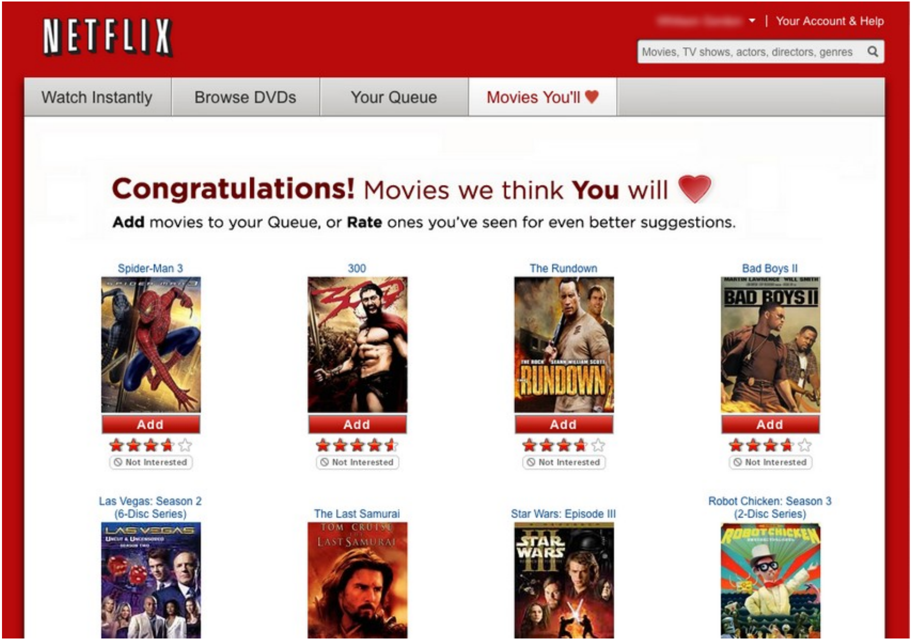
- Randomized approximation: (Sarlos, 2006, Mahoney et al., 2011)

$$\widehat{x} = \arg\min_{x \in \mathcal{C}} \|S(Ax - y)\|_2^2$$

- Random projection matrix $S \in \mathbb{R}^{m \times n}$



Application to Netflix data



Netflix data set

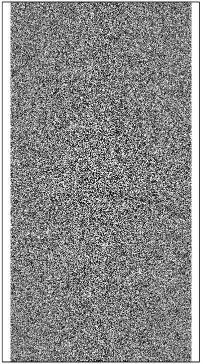
- 2 million $\times$ 17000 matrix A of ratings (users $\times$ movies)
- Predict the ratings of a particular movie
- Least-squares regression with ℓ_2 regularization

$$\min_{x \in \mathbb{R}^{17000}} \left\{ \|Ax - y\|_2^2 + \lambda \|x\|_2^2 \right\}$$

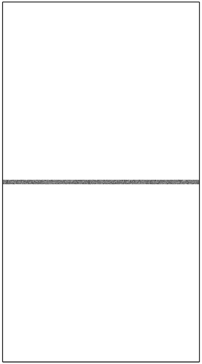
- Partition into test and training sets, solve for all values of $\lambda \in \{1, 2, ..., 100\}$.

Sketching for Netflix movie database

- original data set: 2 million $\times$ 17000 matrix A of ratings (users $\times$ movies)
- perform sketching (randomized dimensionality reduction)



Original data matrix



Sketched data matrix

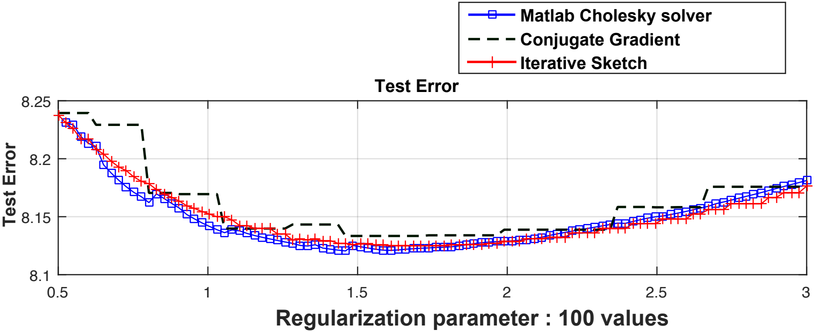
Key fact:

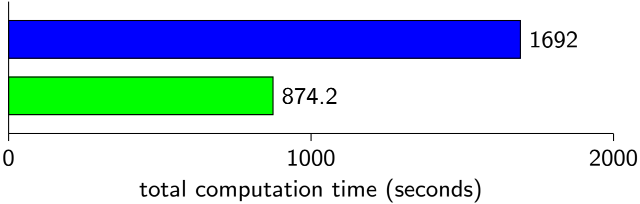
Sketching to dimension 2000 is enough!

Sketch is 2000 $\times$ 17000 : a few Megabytes.

Fitting the full regularization path

(Pilanci & W., 2016, J. Machine Learning Research)





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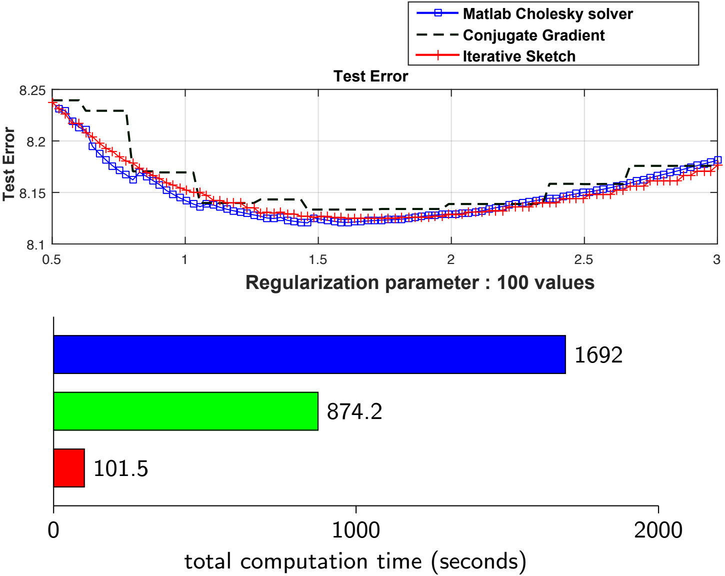
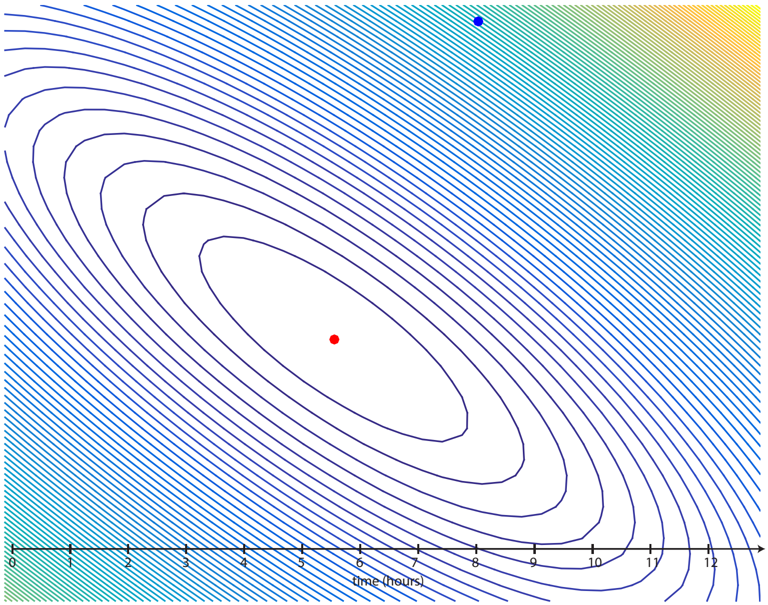


Gradient Descent



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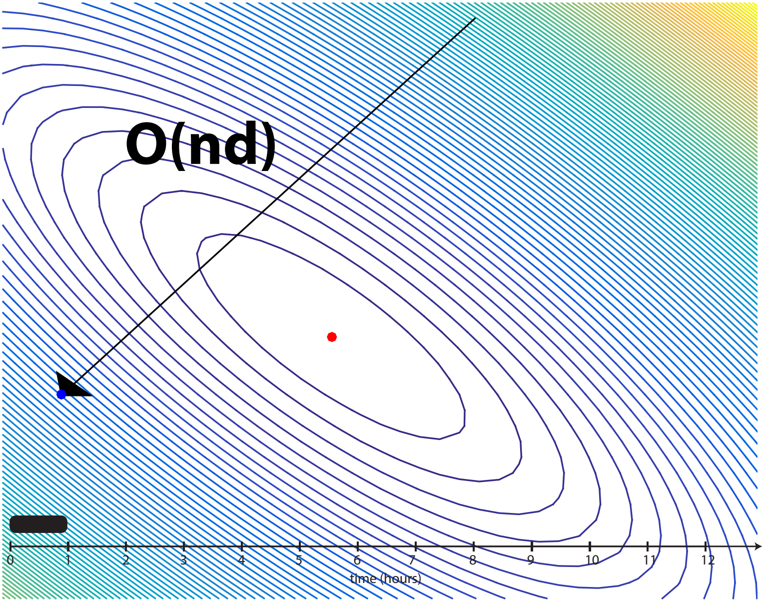

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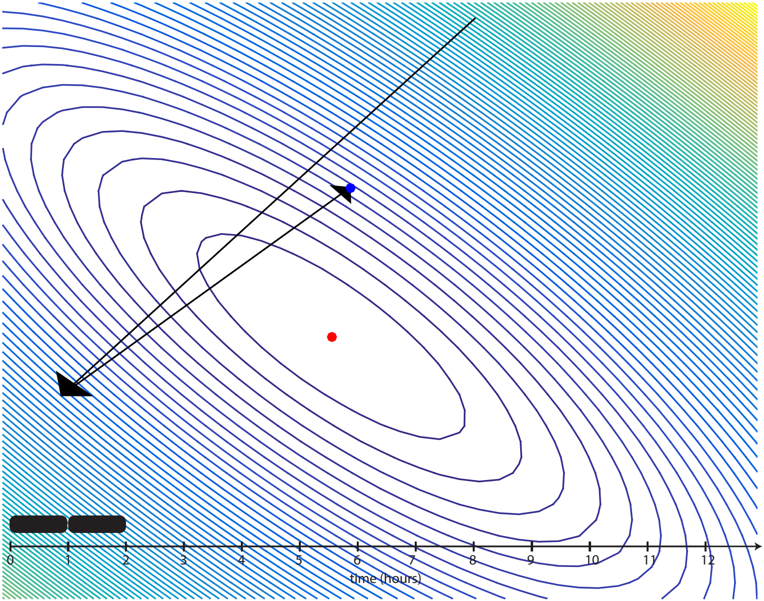

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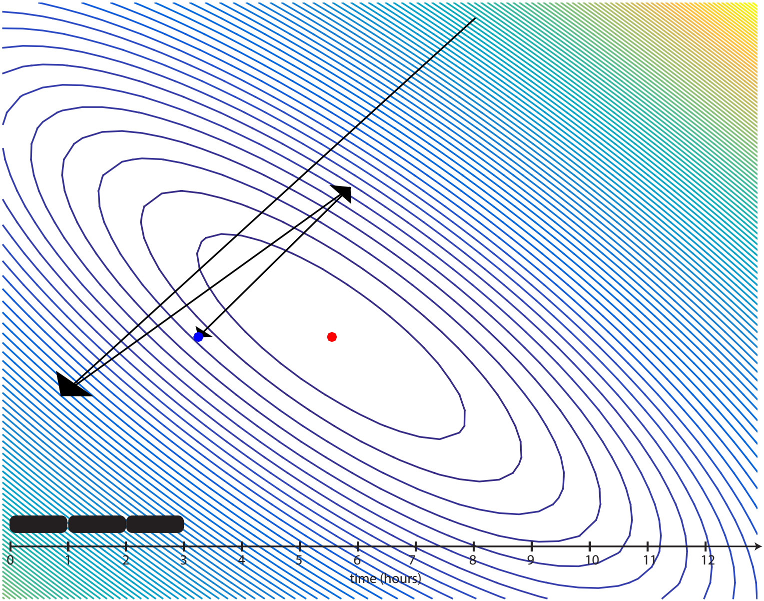

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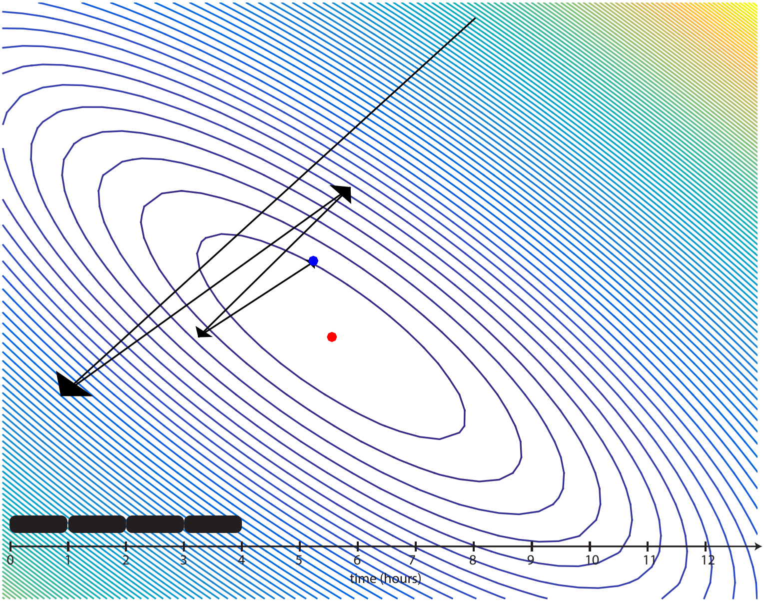

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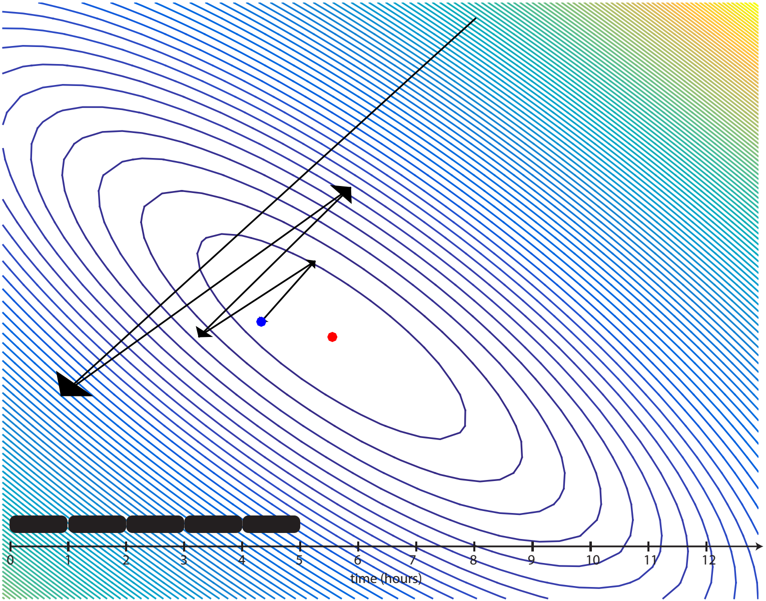

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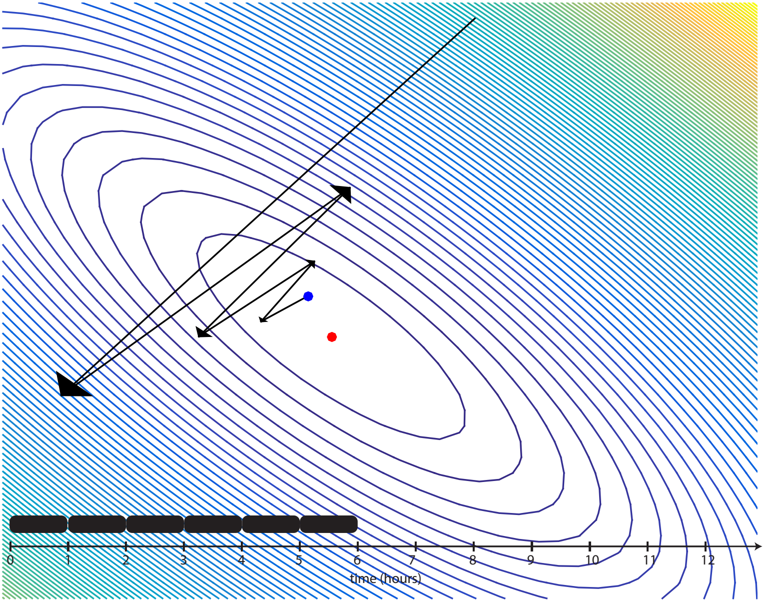
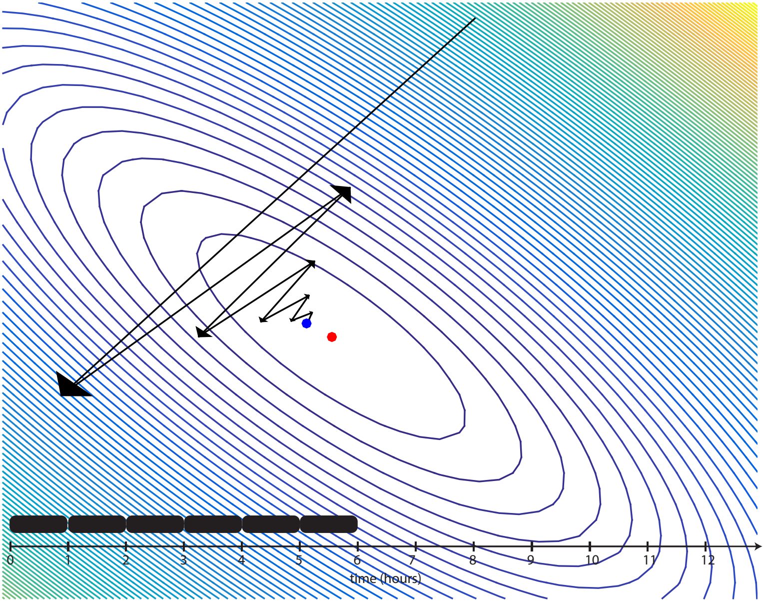
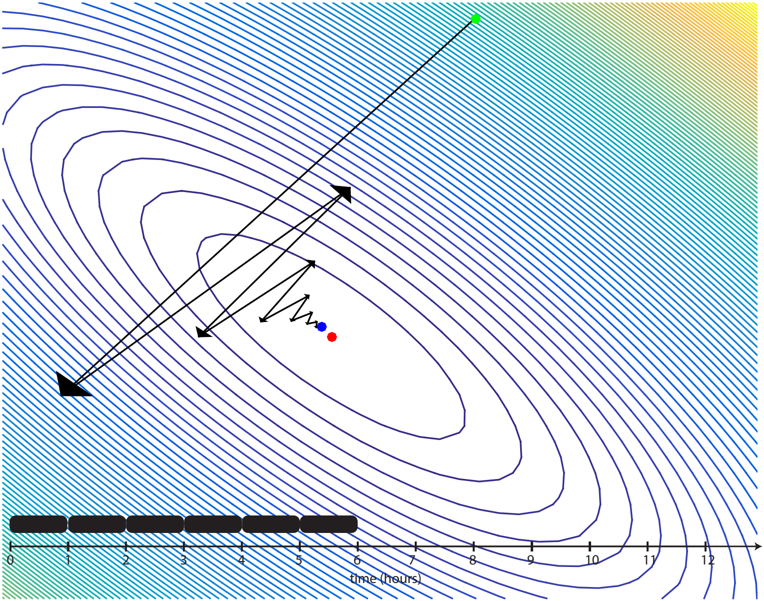


Gradient Descent vs



Gradient Descent vs Newton's Method



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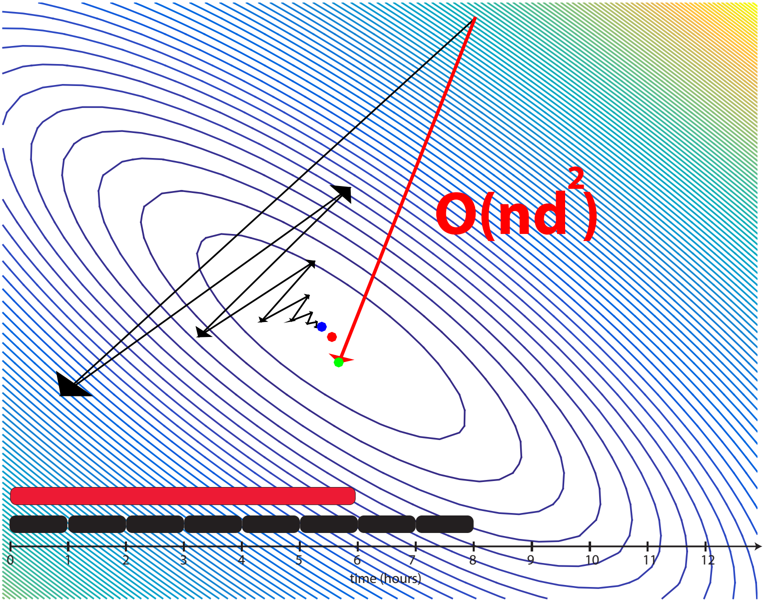

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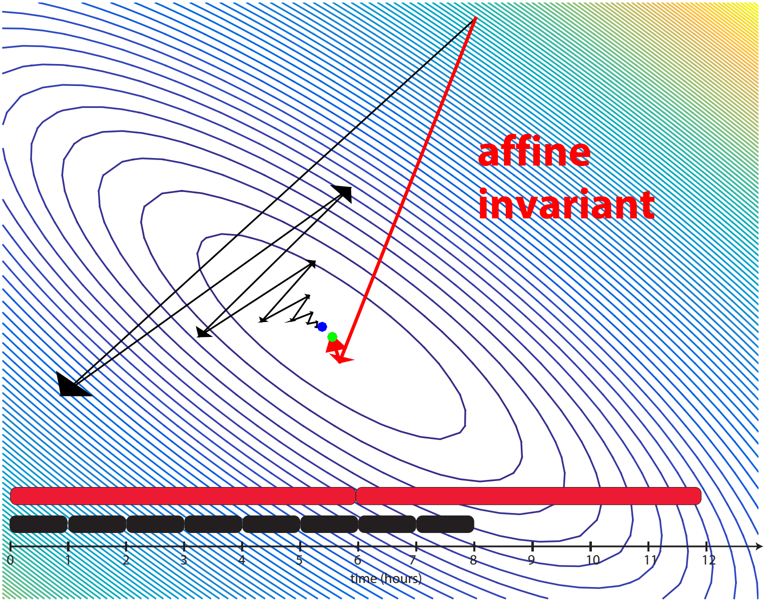

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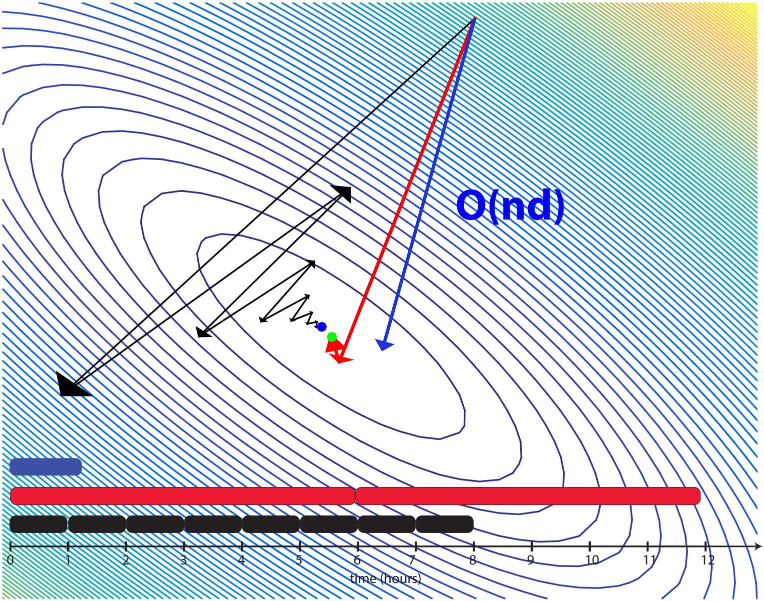

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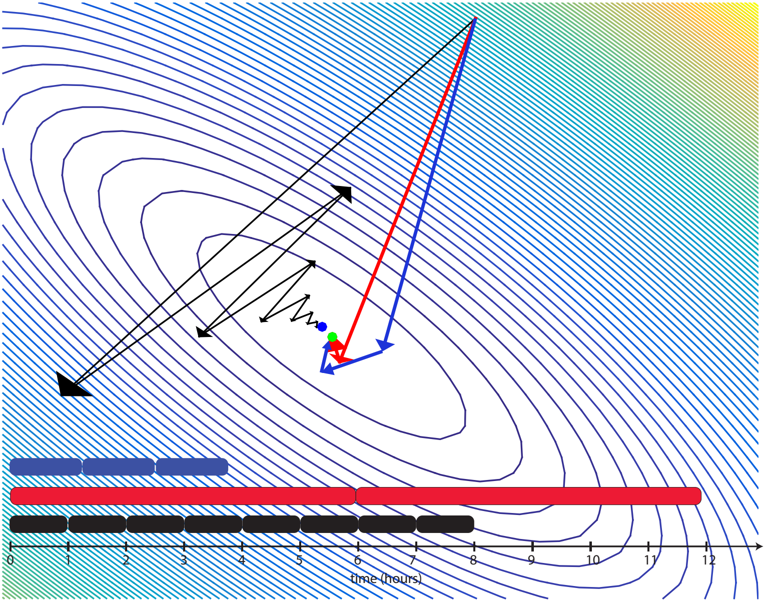

Iterative sketching for general data-based objectives

Goal: Minimize $g(x) = f(Ax)$ over convex set $\mathcal{C} \subseteq \mathbb{R}^d$:

$$x_{\text{opt}} = \arg\min_{x \in \mathcal{C}} g(x), \quad \text{where } g : \mathbb{R}^d \to \mathbb{R} \text{ is twice-differentiable.}$$

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Ordinary Newton steps:

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Sketched Newton steps: Using random sketch matrix S^t:

$$\tilde{x}^{t+1} = \arg\min_{x \in \mathcal{C}} \Big\{ \frac{1}{2} \|S^t \nabla^2 g(x^t)^{1/2}(x - \tilde{x}^t)\|_2^2 + \langle \nabla g(\tilde{x}^t), \, x - \tilde{x}^t \rangle \Big\}.$$

Cost per step: $\widetilde{\mathcal{O}}(nd)$ in unconstrained case.

Convergence of Newton sketch

Run algorithm with sketch dimension $m \asymp d$ on a self-concordant function $g(x) = f(Ax)$, and data matrix $A \in \mathbb{R}^{n \times d}$ with $n \gg d$.

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Theorem (Pilanci & W, SIAM J. Opt, 2017)

With probability at least $1 - c_0 e^{-c_1 m}$, number of iterations required for ϵ accuracy is less than

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Dependence on sample size n, dimension d; conditioning κ; and tolerance ϵ

Algorithm	Computational cost
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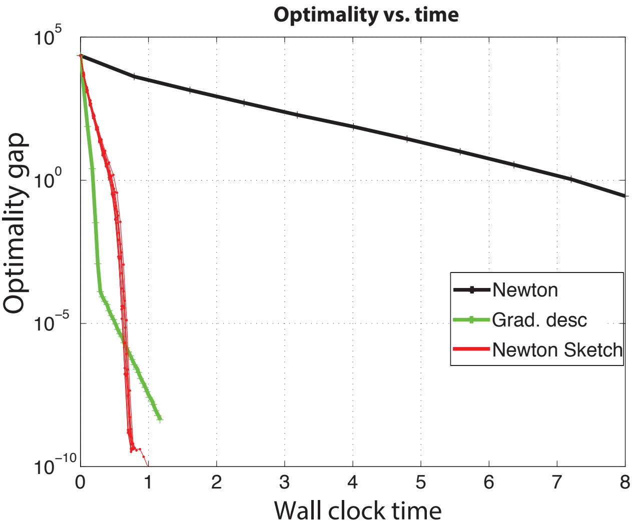
Note: Dependence on condition number κ unavoidable among 1st-order methods (Nesterov, 2004)

Logistic regression: uncorrelated features



Sample size $n = 500,000$ with $d = 5,000$ features

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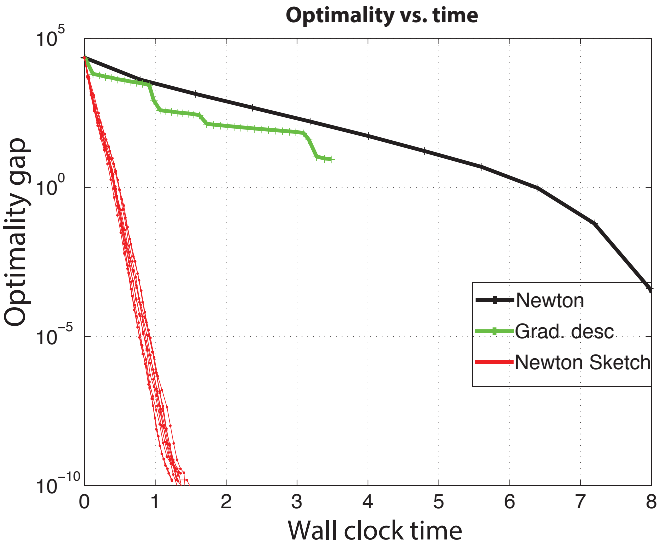

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Given step sizes $\alpha^t > 0$:

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[Freund & Schapire, 1997; Mason et al., 1999; Friedman et al., 2000]

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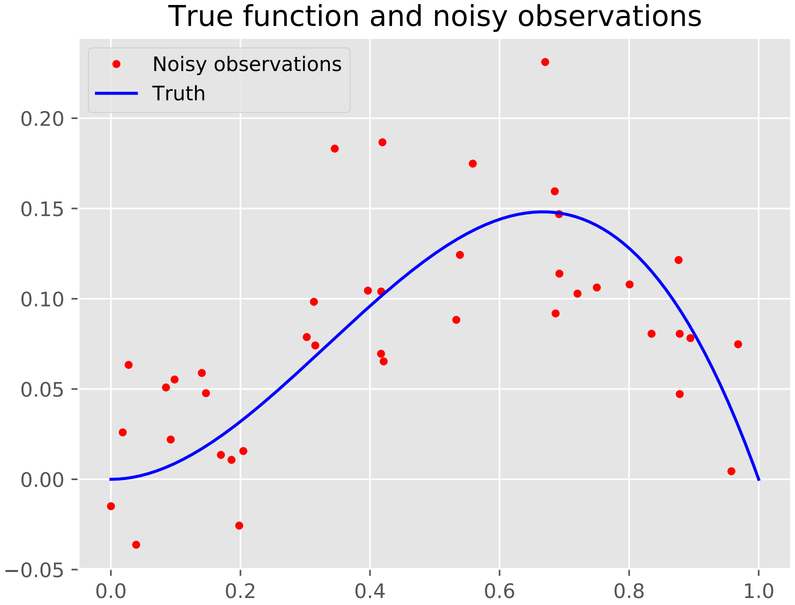
[Freund & Schapire, 1997; Mason et al., 1999; Friedman et al., 2000]

Example: L^2-Boosting with $\mathcal{L}_n(f) = \frac{1}{2n} \sum_{i=1}^n \big[y_i - f(x_i)\big]^2$.
Gradient boosting update takes form

$$g^t = \arg\max_{\|g\|_{\mathscr{F}} \leq 1} \left\{ \frac{1}{n} \sum_{i=1}^n g(x_i) \underbrace{\big[f^t(x_i) - y_i\big]}_{\text{Current residual}} \right\}.$$

Boosting with a Gaussian kernel



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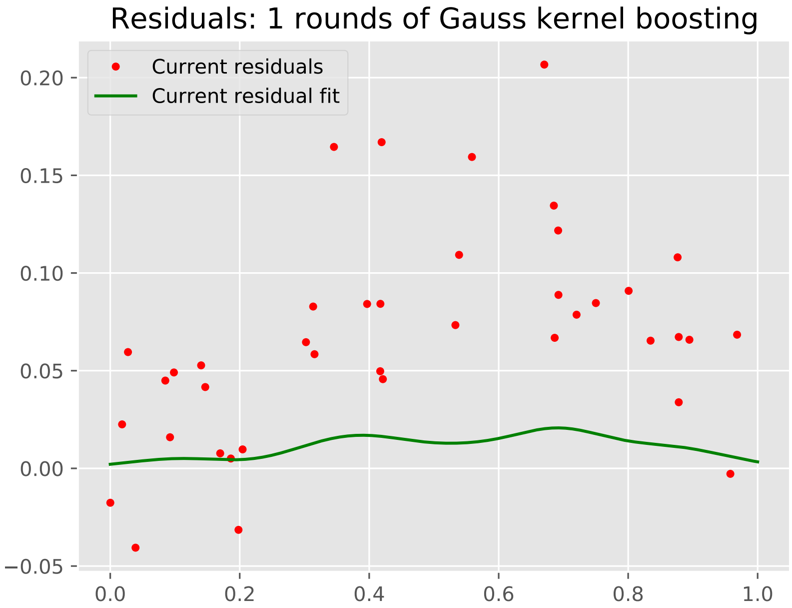

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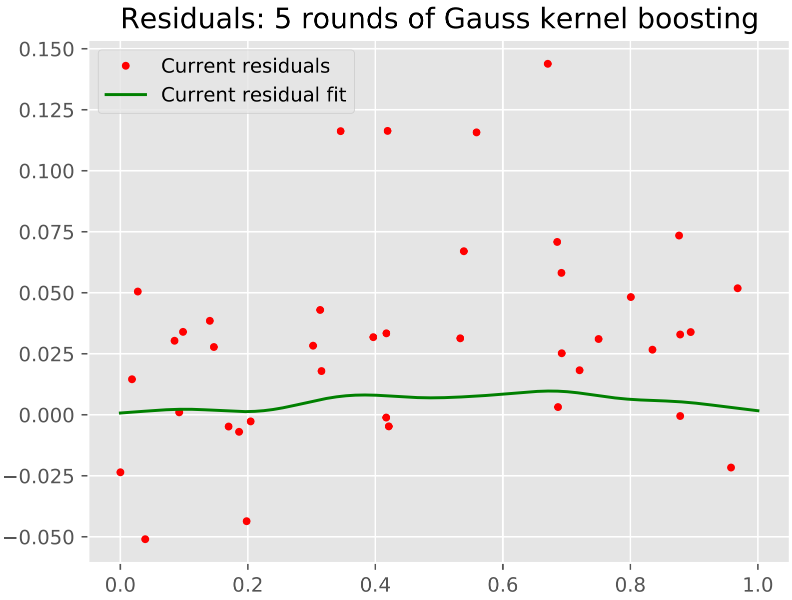

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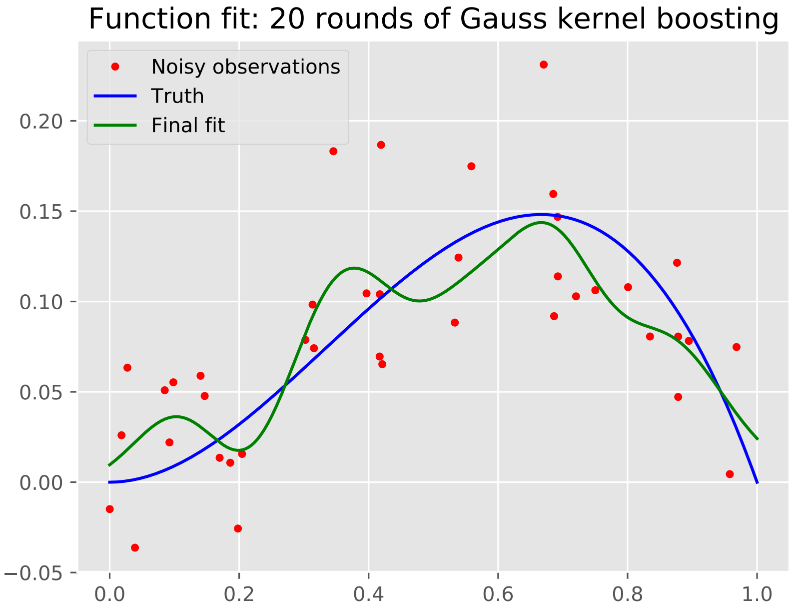

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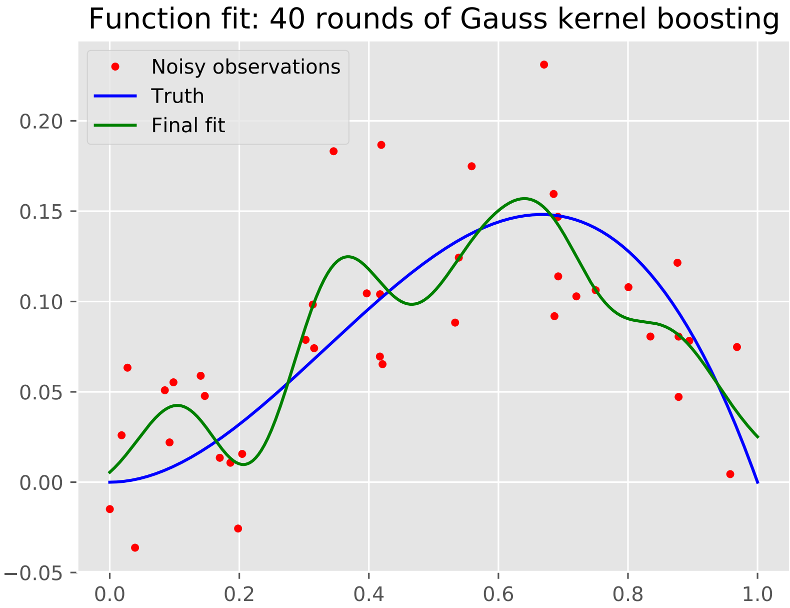
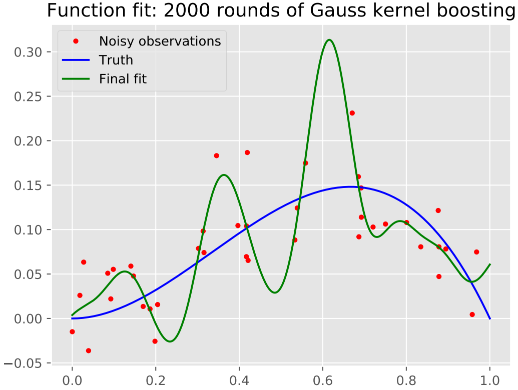


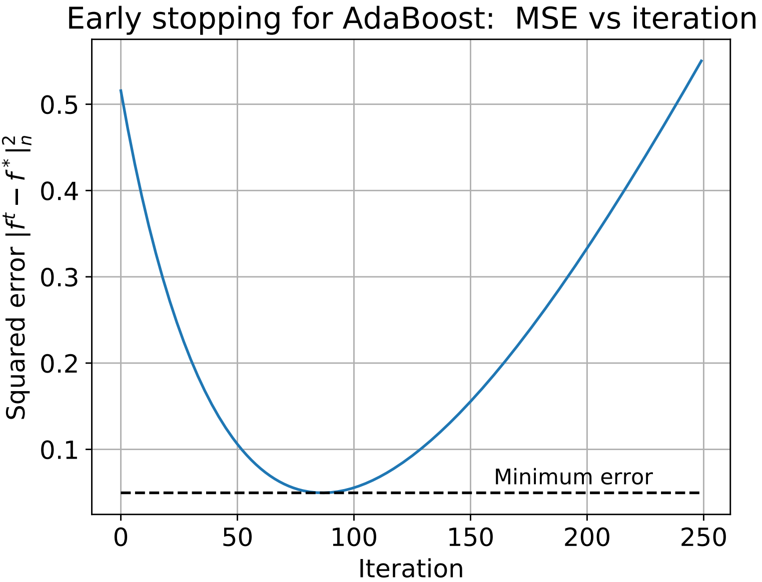
Visualization of over-fitting



I shall not today attempt further to define the kinds of material I understand to be embraced within that shorthand description "overfitting", and perhaps I could never succeed in intelligibly doing so. But I know it when I see it.

Paraphrased from US Supreme Court Justice Potter Stewart, 1964

How to stop at the “right time”?



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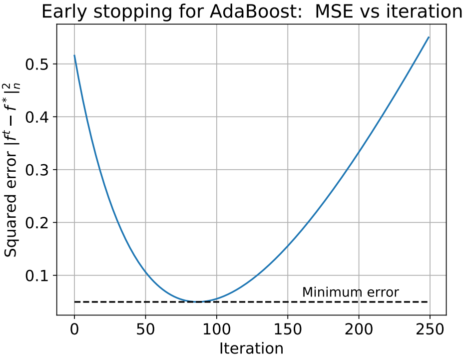

Desiderata:

- a data-dependent stopping rule $\{x_i, y_i\}_{i=1}^n \mapsto T \in \{1, 2, \ldots,\}$
- function estimate at iteration t has optimal mean-squared error

$$\|f^T - f^*\|_n^2 \asymp \min_{k=1,2,\ldots} \|f^k - f^*\|_n^2$$

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Desiderata:

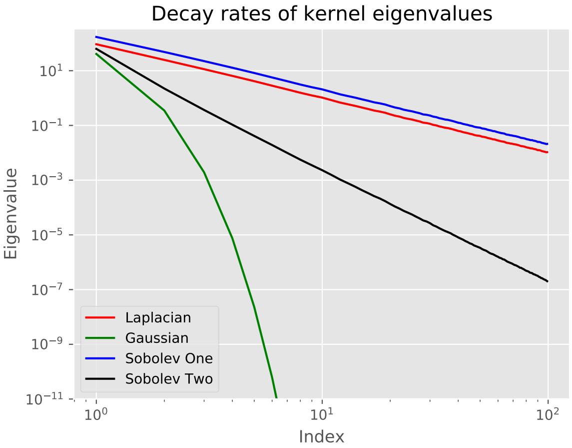
- a data-dependent stopping rule $\{x_i, y_i\}_{i=1}^n \mapsto T \in \{1, 2, \ldots, \}$
- function estimate at iteration t has optimal mean-squared error

$$\|f^T - f^*\|_n^2 \asymp \min_{k=1,2,\ldots} \|f^k - f^*\|_n^2$$

Some past work:

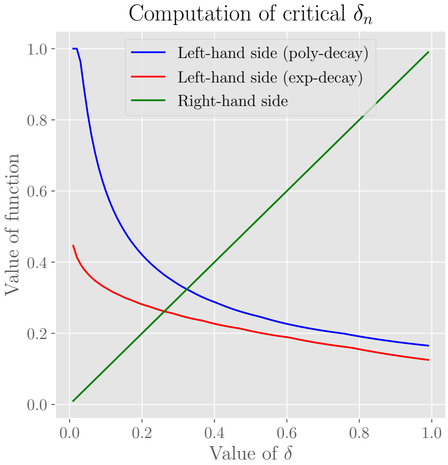
- optimal but not data-dependent rule for spline kernel L^2-boosting: Bühlmann & Yu, 2003
- some results on L^2-boosting with spline kernels: Caponetto et al., 2007, Roscasco et al., 2009
- optimal rates for L^2-boosting, data-dependent any reproducing kernel: Raskutti, W. & Y., 2013

Kernel eigenvalues control "richness"



Kernel	Gaussian	Laplacian	Sobolev One
Form	$\exp(-\frac{1}{2\gamma}(x-y)^2)$	$\exp(-\frac{1}{\gamma}\lvert x-y\rvert)$	$1+\min\{x,y\}$

Statistical error determined by fixed point equation



Fixed point equation:

$$\frac{1}{\sqrt{n}} \sqrt{\sum_{j=1}^{n} \min \left\{ 1, \; \frac{\widehat{\mu}_j^2}{\delta^2} \right\}} = \frac{\delta}{\sigma}$$

where

- $\{\widehat{\mu}_j\}_{j=1}^{n}$ are eigenvalues of kernel matrix
- $\sigma > 0$ is noise level

Required number of iterations scales inversely...

Kernel	Stat. error	Number of iterations
Polynomial (Degree D)	$\frac{D}{n}$	$\frac{n}{D}$
Gaussian	$\frac{\sqrt{\log n}}{n}$	$\frac{n}{\sqrt{\log n}}$
First-order spline	$\left(\frac{1}{n}\right)^{\frac{2}{3}}$	$n^{2/3}$
Second-order spline	$\left(\frac{1}{n}\right)^{\frac{4}{5}}$	$n^{4/5}$

Minimax-optimal bounds for kernel boosting

Kernel boosting sequence:

$$f^{t+1} = f^t - \alpha g^t \qquad \text{where } g^t = \arg \max_{\|g\|_{\mathscr{F}} \leq 1} \langle g, \nabla \mathcal{L}_n(f^t) \rangle$$

Theorem (Wei, Yang & W., 2017)

For any kernel class $\mathscr{F}$, any (m, L)-regular loss function and any step size $\alpha \in (0, \frac{m}{L}]$, and any iterate $t = 1, \ldots, \lfloor \frac{1}{\delta_n^2} \rfloor$:

$$\underbrace{\mathcal{L}(\bar{f}^t) - \mathcal{L}(f^*)}_{\textit{Excess loss}} \quad \precsim \quad \underbrace{\frac{1}{\alpha t}}_{\textit{Opt. error}} \quad + \quad \underbrace{\delta_n^2}_{\textit{Stat. error}}$$

with high probability over the randomized realization.

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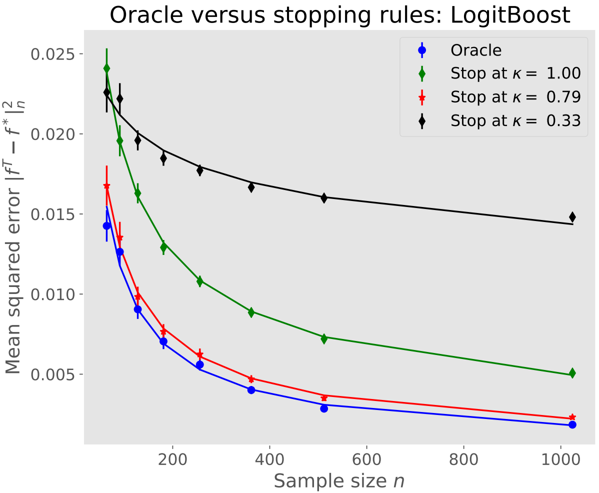
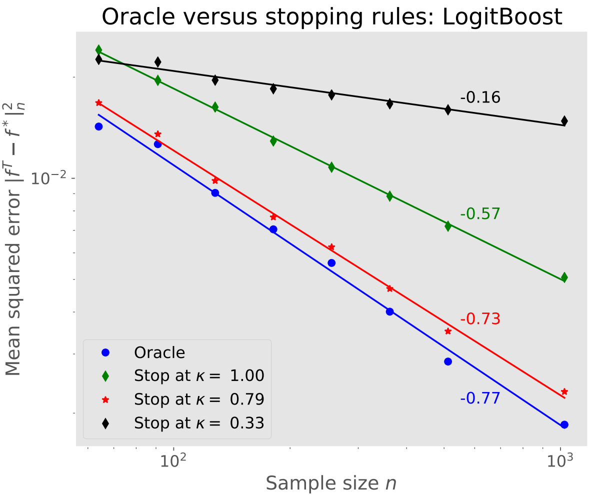
where $\{\widehat{\mu}_j\}_{j=1}^n$ are eigenvalues of kernel matrix, and $\sigma > 0$ is noise level.

LogitBoost: Error on linear scale



LogitBoost: Error on logarithmic scale



Optimal theoretical rate: $\left(\frac{\sigma^2}{n}\right)^{0.79}$

Summary

Many challenges lie at the interface of statistics and optimization:

- data sketches for randomized dimension reduction
- regularization via early stopping of iterative algorithms for optimization

<u>Some papers:</u>

Pilanci & W. (2016). Iterative Hessian sketch: Fast and accurate solution approximation for constrained least squares *J. Machine Learning Research.*

Pilanci & W. (2017). Newton sketch: A linear-time optimization algorithm with linear-quadratic convergence. *SIAM Journal on Optimization.*

Wei, Yang & W. (2017). Early stopping for kernel boosting algorithms. Arxiv pre-print.

Fast Johnson-Lindenstrauss sketch

Step 1: Choose some fixed orthonormal matrix $H \in \mathbb{R}^{n \times n}$.
Example: Hadamard matrices

$$H_2 = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix} \qquad H_{2^t} = \underbrace{H_2 \otimes H_2 \otimes \cdots \otimes H_2}_{\text{Kronecker product } t \text{ times}}$$

(E.g., Ailon & Liberty, 2010)

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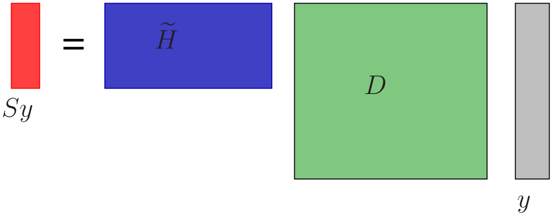


Step 2:

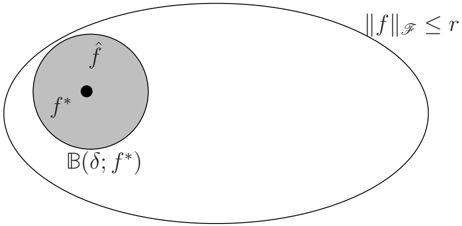
(A) Multiply data vector y with a diagonal matrix of random signs $\{-1, +1\}$

(B) Choose m rows of H to form sub-sampled matrix $\widetilde{H} \in \mathbb{R}^{m \times n}$

(C) Requires $\mathcal{O}(n \log m)$ time to compute sketched vector $Sy = \widetilde{H}\, D y$.

(E.g., Ailon & Liberty, 2010)

Tools for sharp analysis



Localized Gaussian complexity

How much can you align with i.i.d. noise sequence $\{w_i\}_{i=1}^n \sim N(0,1)$?

$$\mathscr{G}_n(\delta, r; \mathscr{F}) = \mathbb{E}_w \sup_{\substack{\|f\|_{\mathscr{F}} \leq r \\ \|f - f^*\| \leq \delta}} \left| \frac{1}{n} \sum_{i=1}^n w_i \big(f(x_i) - f^*(x_i) \big) \right|$$

(e.g., van de Geer, 2000; Bartlett et al., 2005; Koltchinski, 2006)