Statistics meets Optimization: Fast randomized algorithms for large data sets

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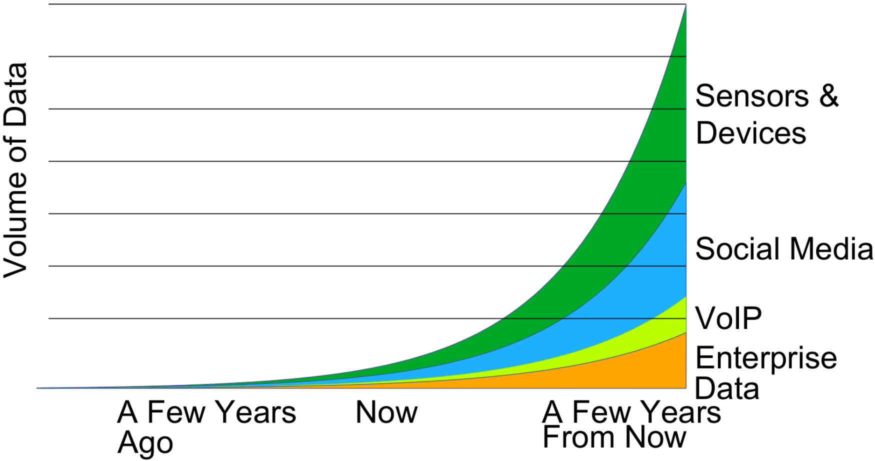
Joint work with: Mert Pilanci
UC Berkeley & Stanford University

What is the "big data" phenomenon?



- Every day: 2.5 billion gigabytes of data created
- Last two years: creation of 90% of the world's data (source: IBM)

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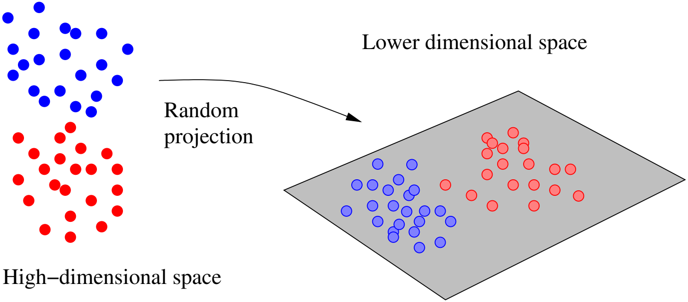
Randomized projection is a general purpose tool:

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



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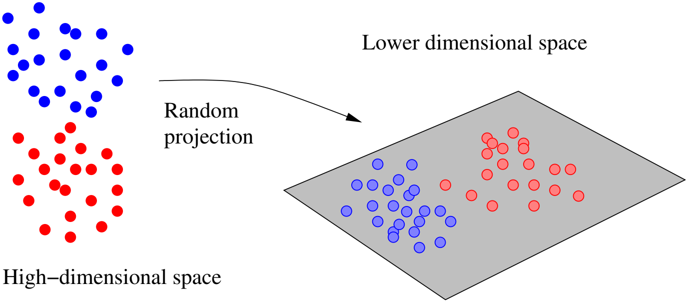

Widely studied and used:

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

Randomized sketching for optimization

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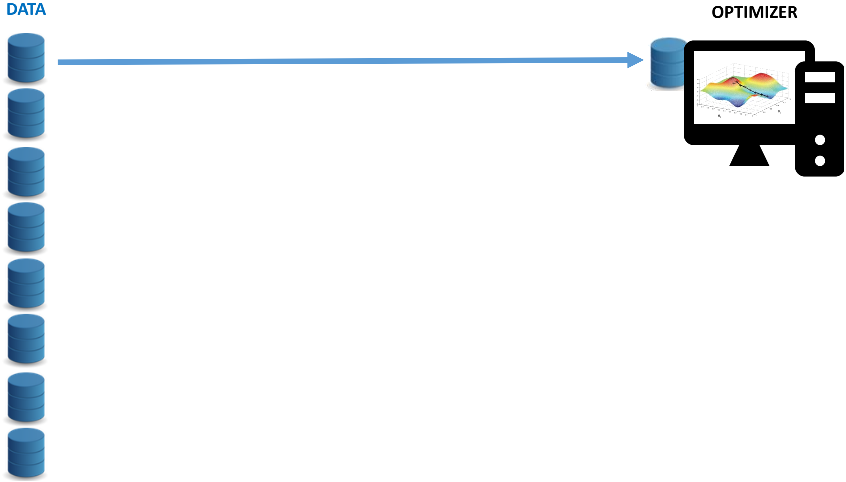

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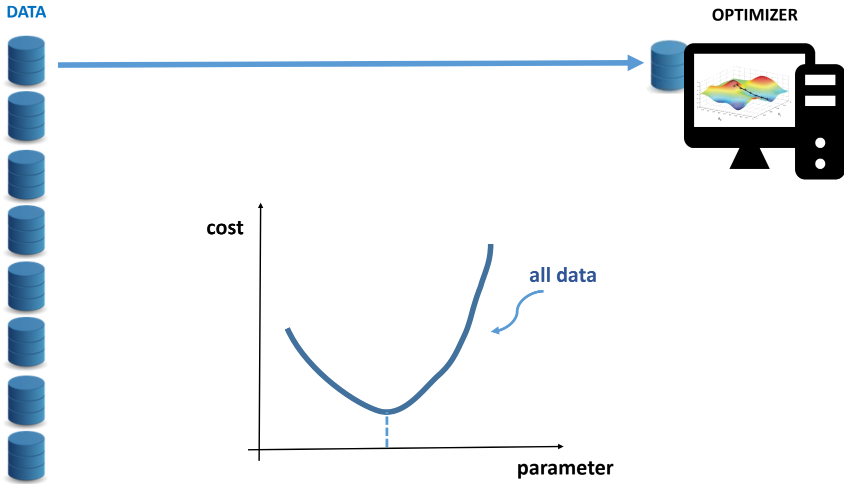

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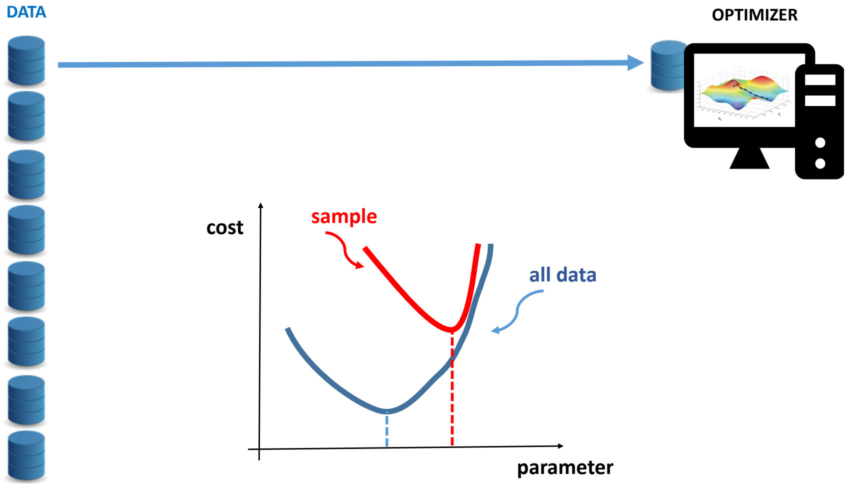

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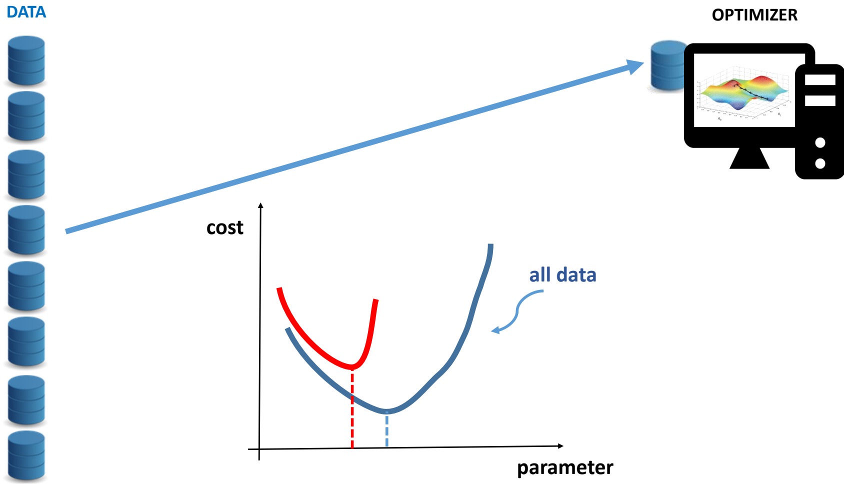

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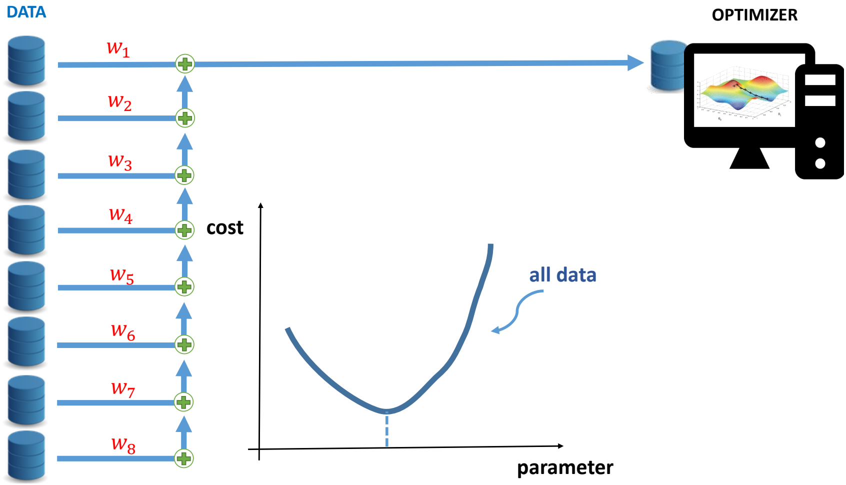

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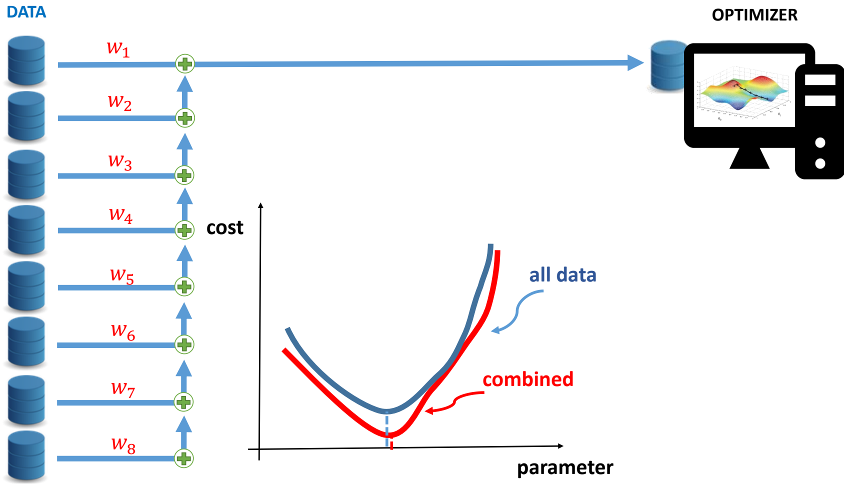

Randomized projection for constrained least-squares

- 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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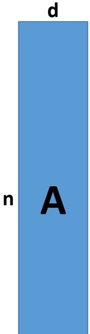

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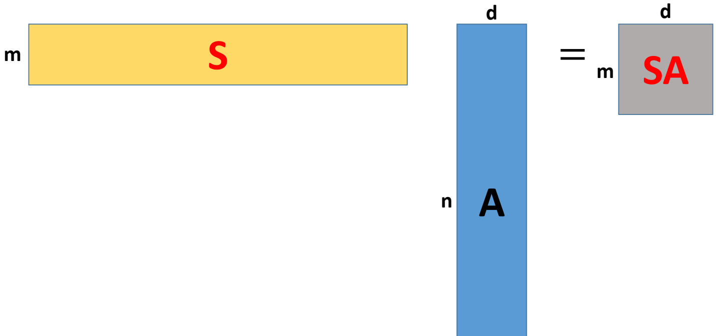
- Randomized approximation: (Sarlos, 2006)

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

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



A general approximation-theoretic bound

The randomized solution $\widehat{x} \in \mathcal{C}$ provides δ-accurate cost approximation if

$$f(Ax_{\text{LS}}) \;\le\; f(A\widehat{x}) \;\le\; (1+\delta)\, f(Ax_{\text{LS}}).$$

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Theorem (Pilanci & W, 2015)

For a broad class of random projection matrices, a sketch dimension

$$m \gtrsim \frac{\text{effrank}(A; \mathcal{C})}{\delta}$$

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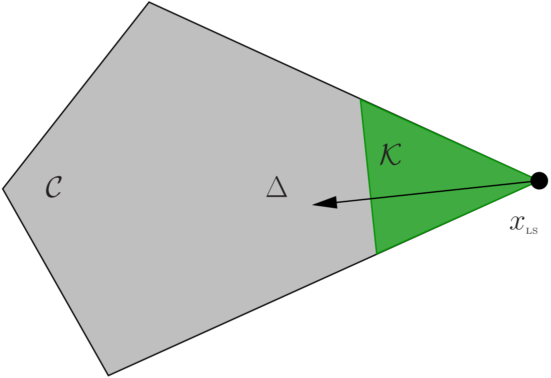
- past work on unconstrained case $\mathcal{C} = \mathbb{R}^d$: effective rank equivalent to rank(A) (Sarlos, 2006; Mahoney et al. 2011)
- effective rank can be much smaller than standard rank

Favorable dependence on optimum x_{LS}

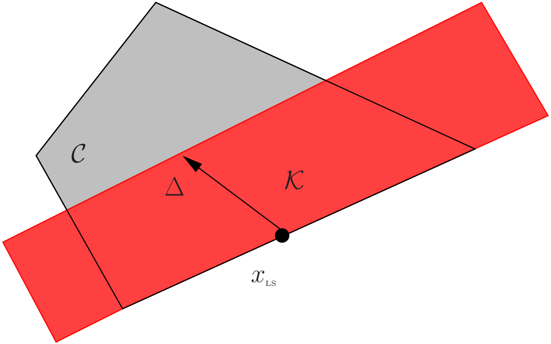


Tangent cone $\mathcal{K}$ at x_{LS}

Set of feasible directions at the optimum x_{LS}

$$\mathcal{K} = \left\{ \Delta \in \mathbb{R}^d \mid \Delta = t\,(x - x_{\text{LS}}) \quad \text{for some } x \in \mathcal{C}. \right\}.$$

Unfavorable dependence on optimum x_{LS}



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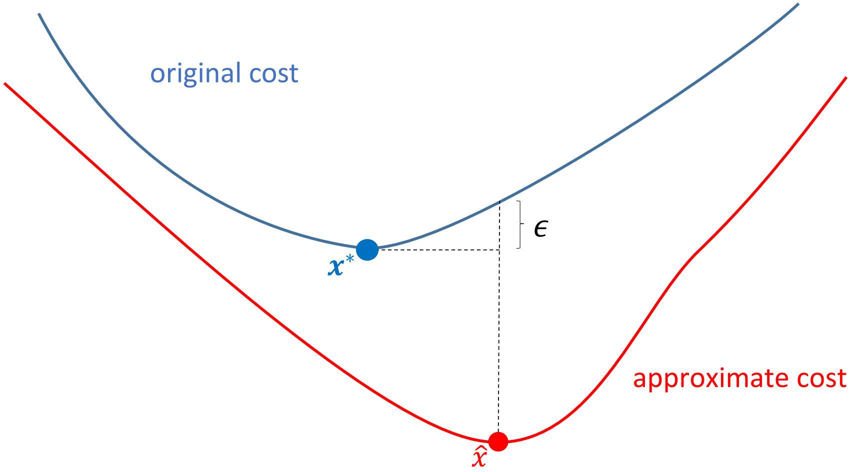
But what about solution approximation?

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



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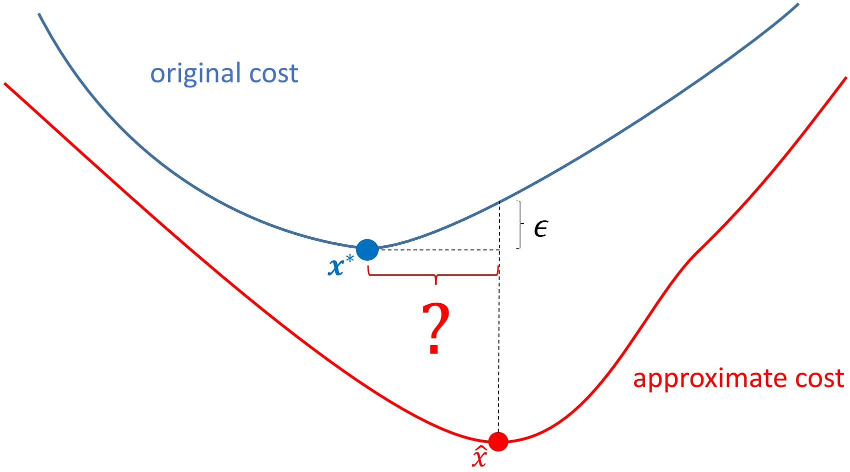

Failure of standard random projection

- Noisy observation model: $y = Ax^* + w$ where $w \sim N(0, \sigma^2 I_n)$.

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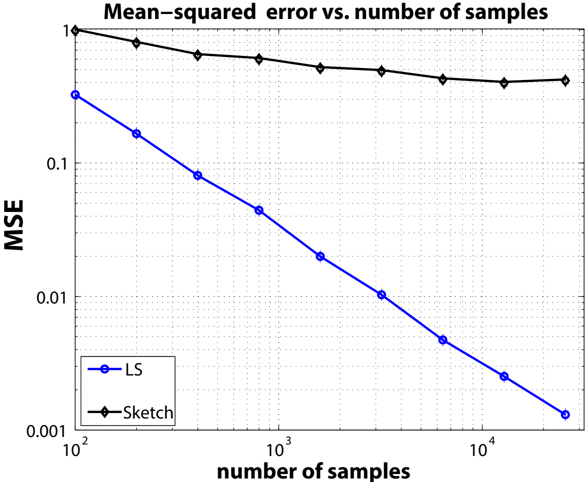
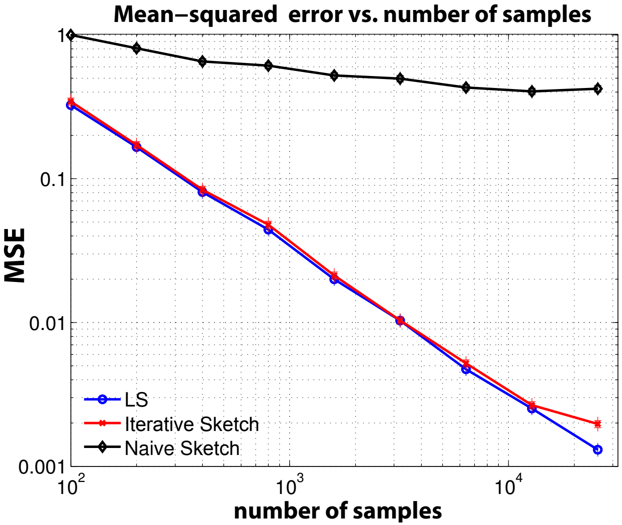


- Least-squares accuracy: $\mathbb{E}\|x_{\rm LS} - x^*\|_A^2 = \sigma^2 \frac{\text{rank}(A)}{n}$

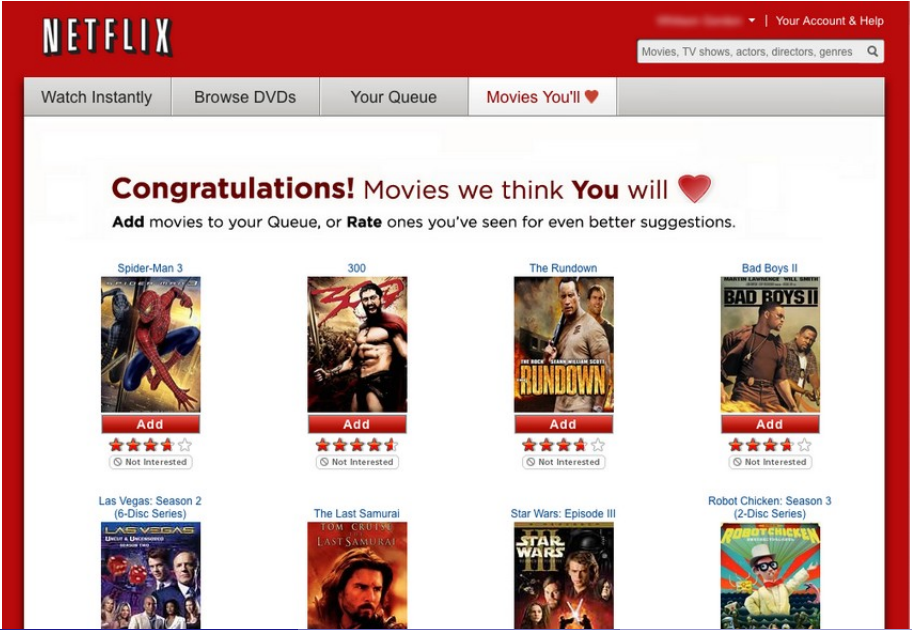
Overcoming this barrier?

Overcoming this barrier? Sequential scheme....



Iterative projection scheme yields accurate tracking of original least-squares solution.

Application to Netflix data



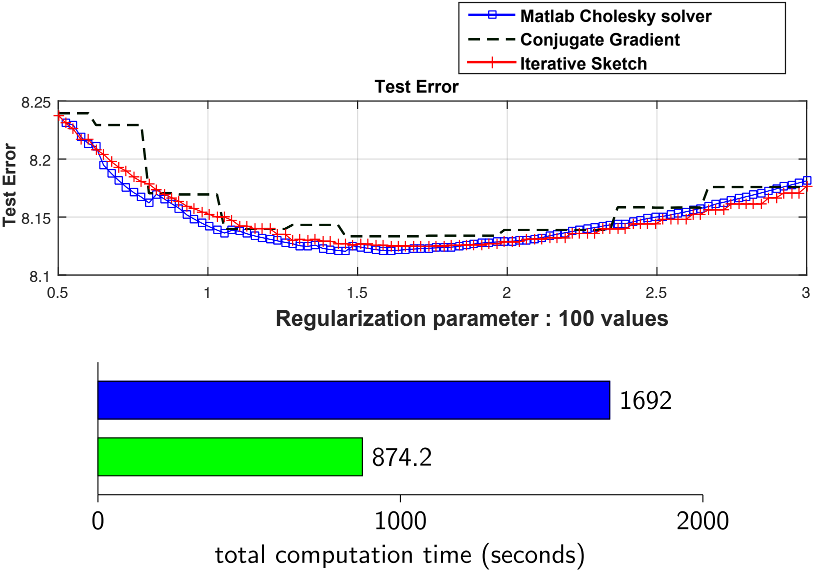
Netflix data set

- 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

$$\min_x \|Ax - y\|_2^2 + \lambda \|x\|_2^2$$

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

Fitting the full regularization path



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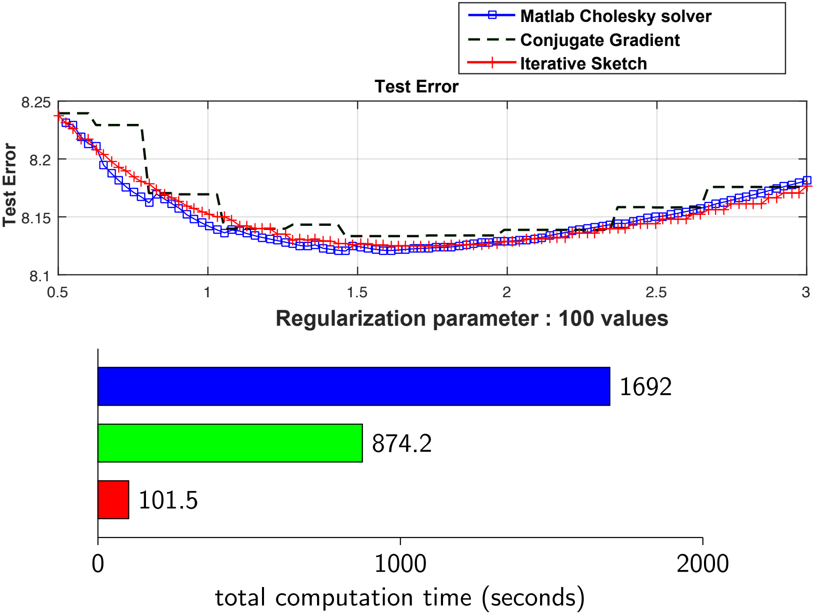
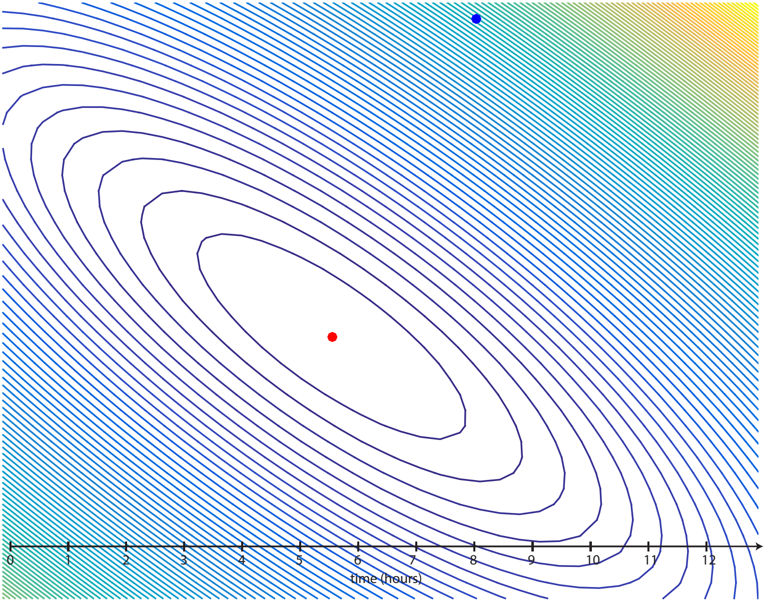


Gradient Descent



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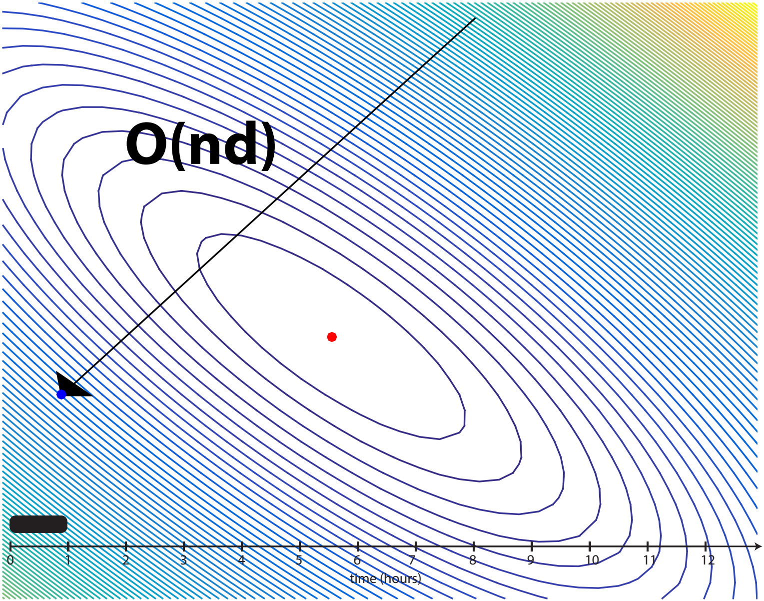

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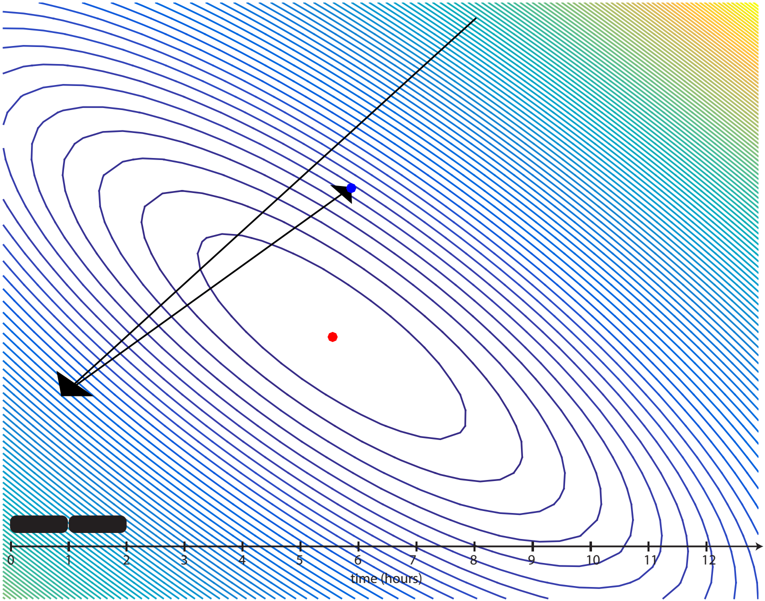

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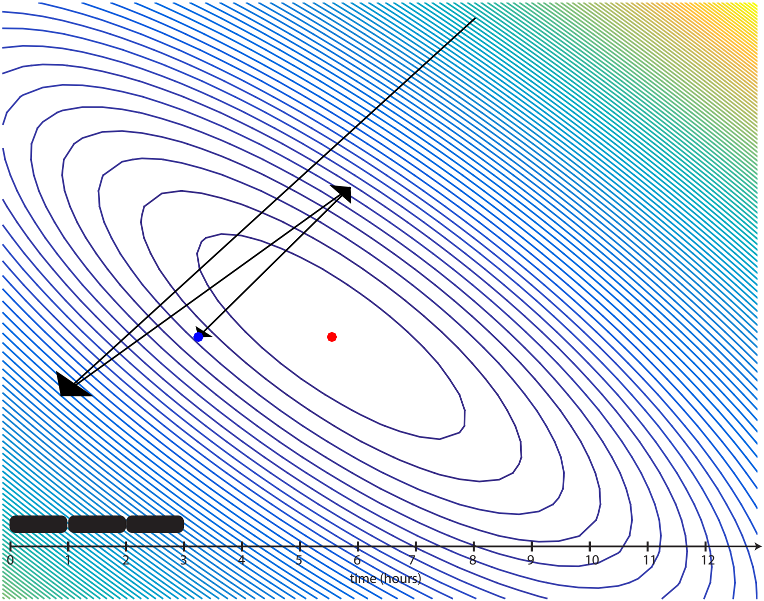

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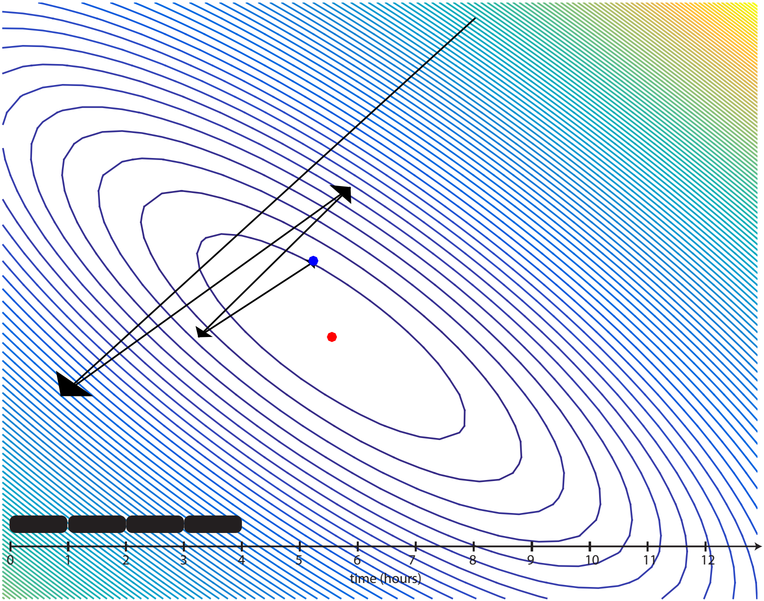

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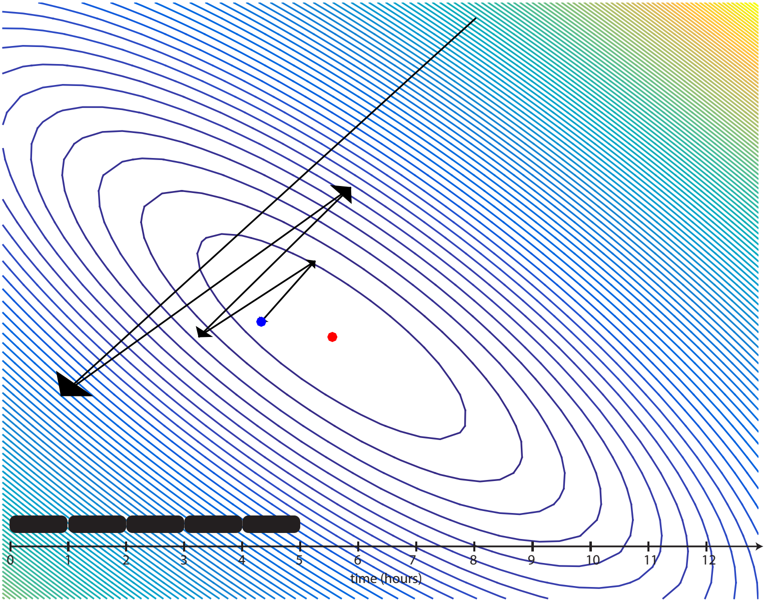

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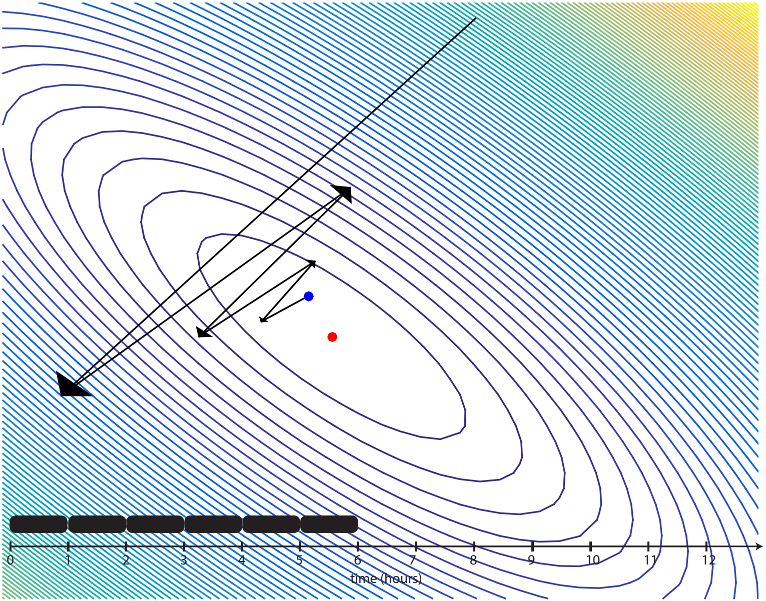
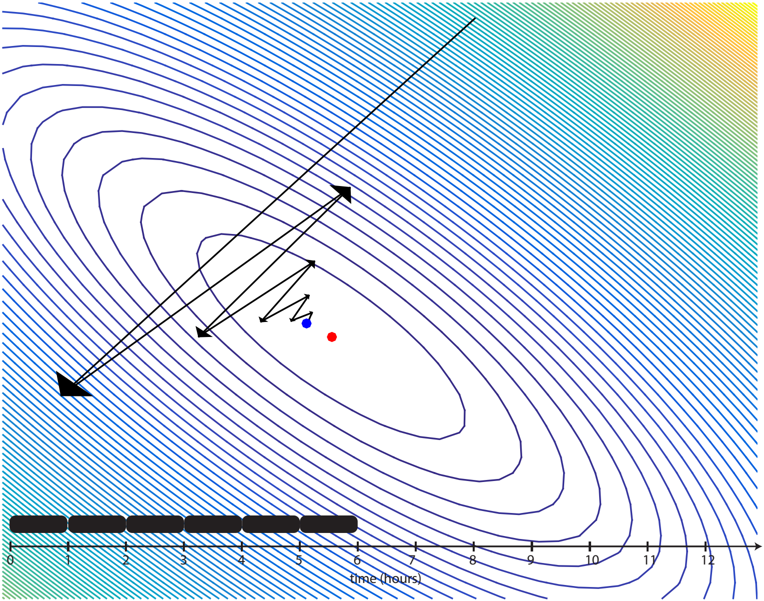
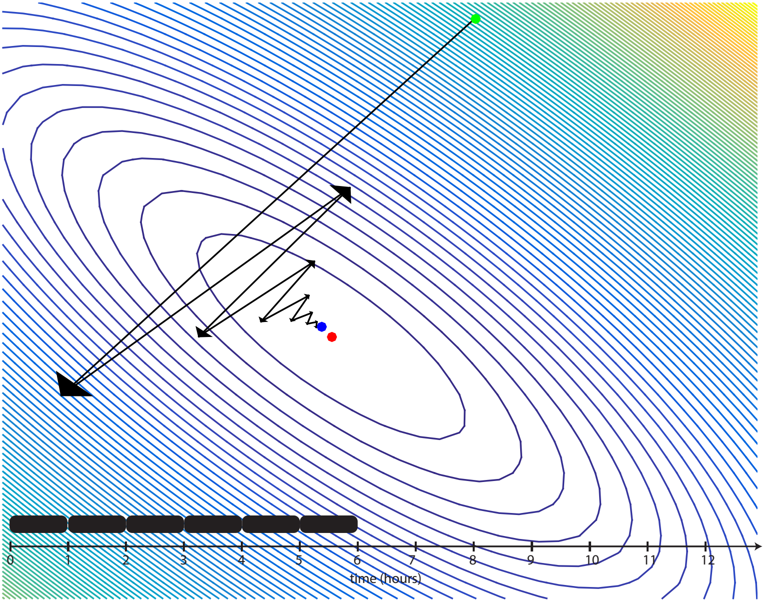


Gradient Descent vs



Gradient Descent vs Newton's Method



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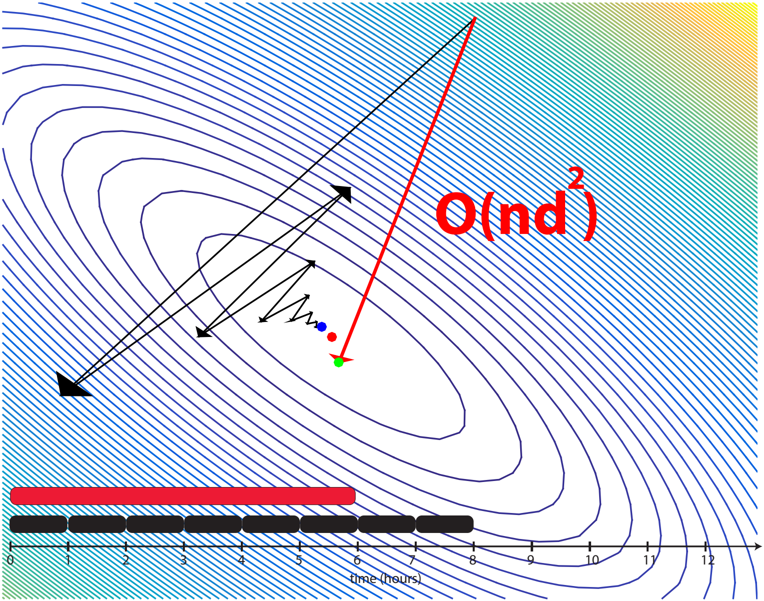

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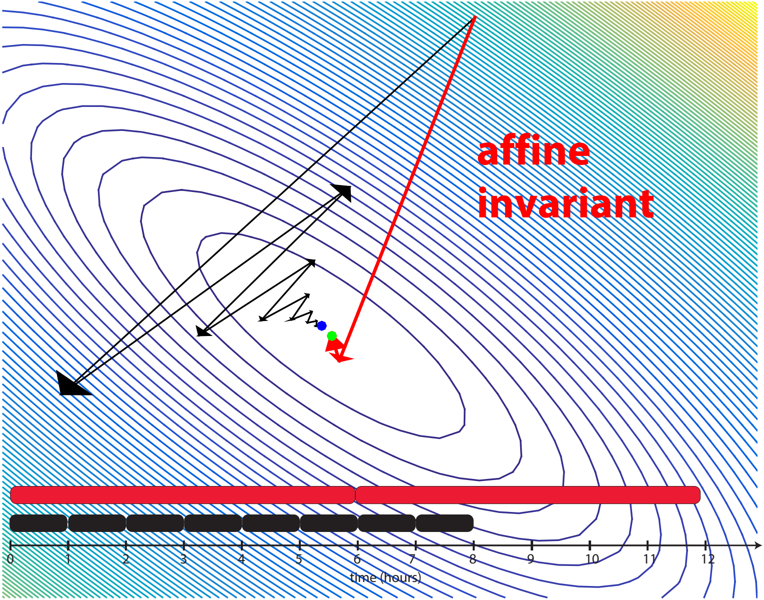

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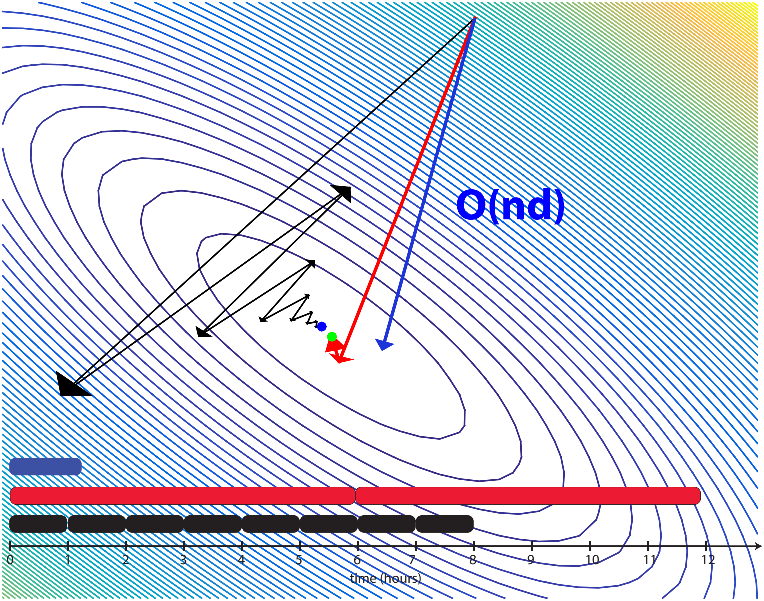

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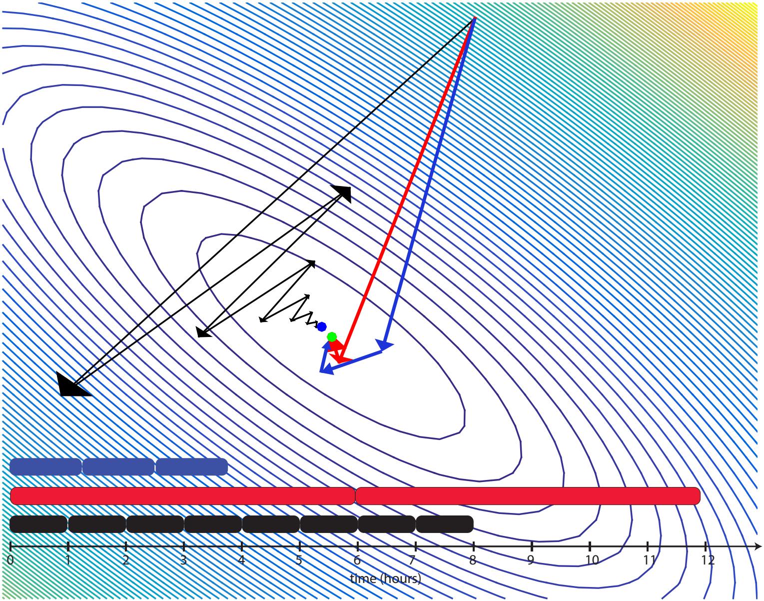

Exact and approximate forms of Newton's method

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:

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

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Approximate Newton steps:

- various types of quasi-Newton updates: Nocedal & Wright book: Chap. 6
- BFGS method; SR1 method etc.
- stochastic gradient + stochastic quasi-Newton (e.g., Byrd, Hansen, Nocedal & Singer 2014)

Iterative sketching for general convex functions

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

$$c_2 \log(1/\epsilon)$$

where (c_0, c_1, c_2) are universal (problem-independent) constants.

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

Algorithm	Computational cost
Gradient Descent	$\mathcal{O}(\kappa\, n\, d\, \log(1/\epsilon))$
Acc. gradient Descent	$\mathcal{O}(\sqrt{\kappa}\, nd \log(1/\epsilon))$
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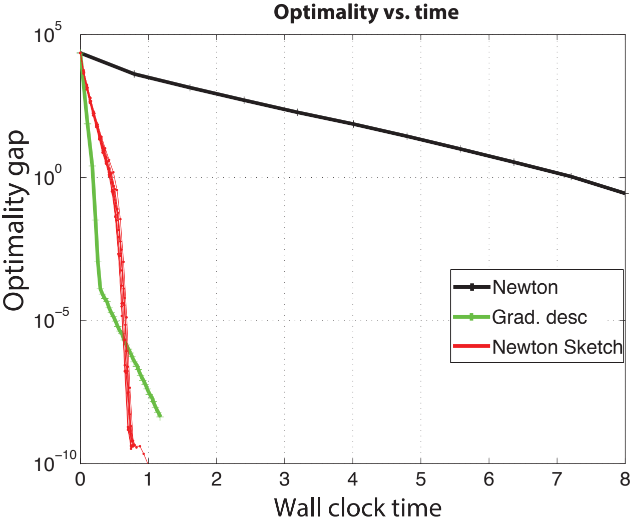
Note: Dependence on condition number κ unavoidable among 1st-order methods (Nesterov, 2004)

Logistic regression: uncorrelated features



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

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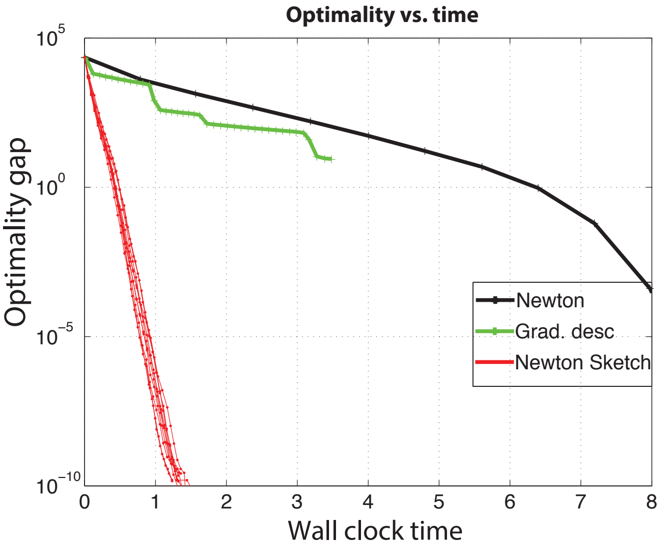

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Consequences for linear programming

- LP in standard form:

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- interior point methods for LP solving: based on unconstrained sequence

$$x_\mu := \arg\min_{x \in \mathbb{R}^d} \Big\{ \mu c^T x - \sum_{i=1}^n \log(b_i - a_i^T x) \Big\}.$$

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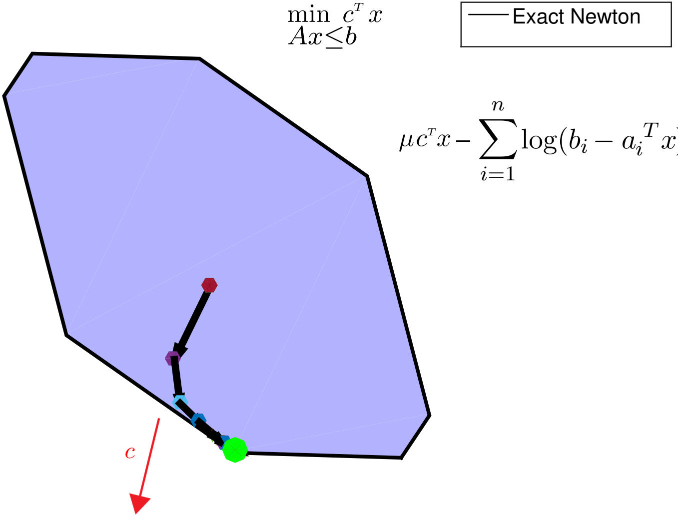
- as parameter $\mu \to +\infty$, the path x_μ approaches an optimal solution x^* from the interior

Standard central path

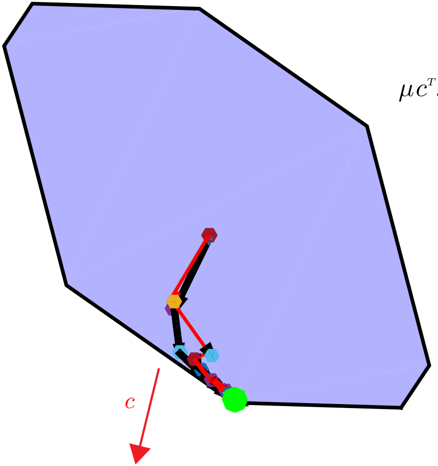
$$\min \; c^T x \quad Ax \leq b$$

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



Newton sketch follows central path

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



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

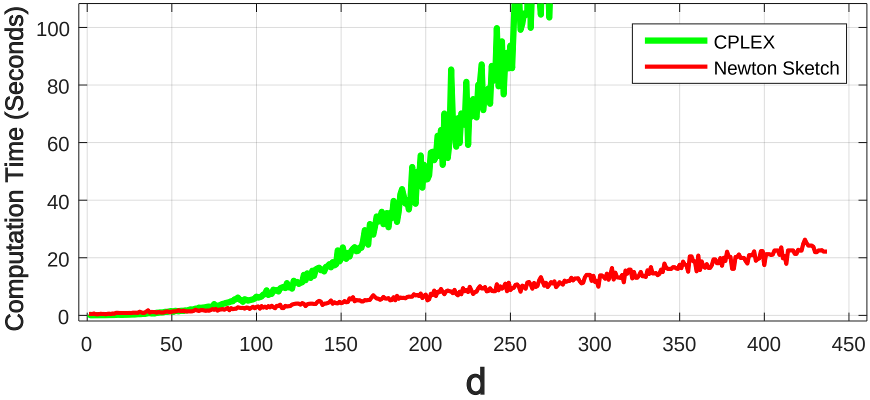
Linear Programs

Consequence: An LP with n constraints and d variables can be solved in $\approx O(nd)$ time when $n \gg d$.

Performance compared to CPLEX

Random ensembles of linear programs

Sample size $n = 10,000$
Dimensions $d = 1, 2, ..., 500$



CODE: `eecs.berkeley.edu/~mert/LP.zip`

Summary

- high-dimensional data: challenges and opportunities
- optimization at large scales:
  - Need fast methods...
  - But approximate answers are OK
  - randomized algorithms (with strong control) are useful
- this talk:
  - the power of random projection
  - information-theoretic analysis reveals deficiency of classical sketch
  - Newton sketch: a fast and randomized Newton-type method

Summary

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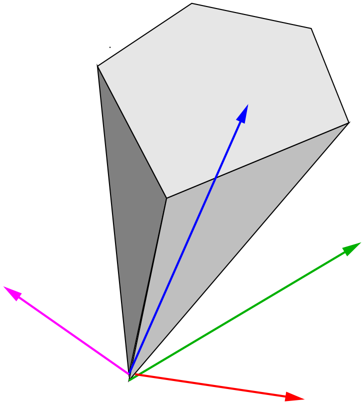
Papers/pre-prints:

- Pilanci & W. (2015): Randomized sketches of convex programs with sharp guarantees, *IEEE Transactions on Information Theory*
- Pilanci & W. (2016a): Iterative Hessian Sketch: Fast and accurate solution approximation for constrained least-squares, *Journal of Machine Learning Research*
- Pilanci & W. (2016b): Newton Sketch: A linear-time optimization algorithm with linear-quadratic convergence. To appear in *SIAM Journal of Optimization.*

Gaussian width of transformed tangent cone



Gaussian width of set
$A\mathcal{K} \cap \mathcal{S}^{n-1} = \{A\Delta \mid \Delta \in \mathcal{K}, \|A\Delta\|_2 = 1\}$

$$\mathcal{W}(A\mathcal{K}) := \mathbb{E}\Big[\sup_{z \in A\mathcal{K} \cap \mathcal{S}^{n-1}} \langle g, z\rangle\Big]$$

where $g \sim N(0, I_{n \times n})$.

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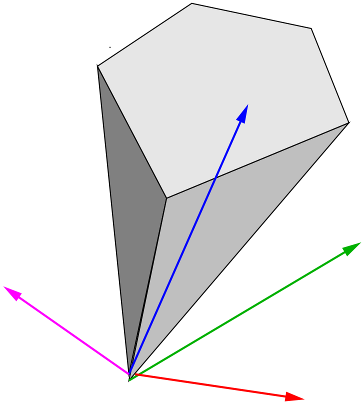

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Gaussian widths used in many areas:

- Banach space theory: Pisier, 1986, Gordon 1988
- Empirical process theory: Ledoux & Talagrand, 1991, Bartlett et al., 2002
- Geometric analysis, compressed sensing: Mendelson, Pajor & Tomczak-Jaegermann, 2007

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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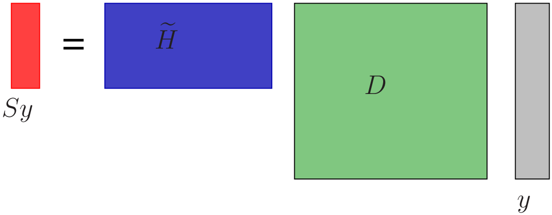

Step 2:

(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 $Sy = \widetilde{H}\, Dy$.

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