Randomized iterative methods for linear systems

Robert Mansel Gower



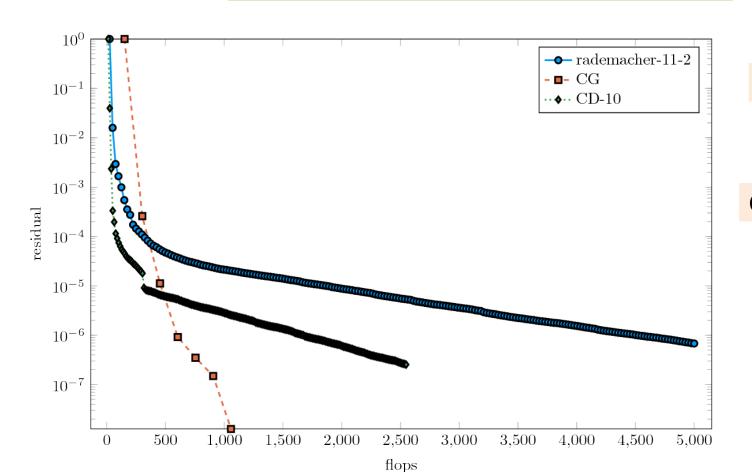




IMA Leslie Fox Prize Meeting, Strathclyde, June 2017

Motivation

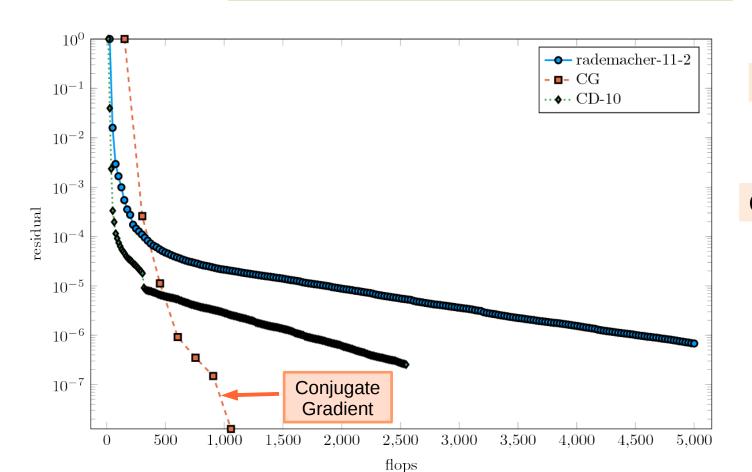
$$\min_{x} \frac{1}{2} ||Ax - y||_{2}^{2} + \frac{\lambda}{2} ||x||_{2}^{2}$$



Problem: a9a

 $A \in \mathbb{R}^{32,561 \times 123}$

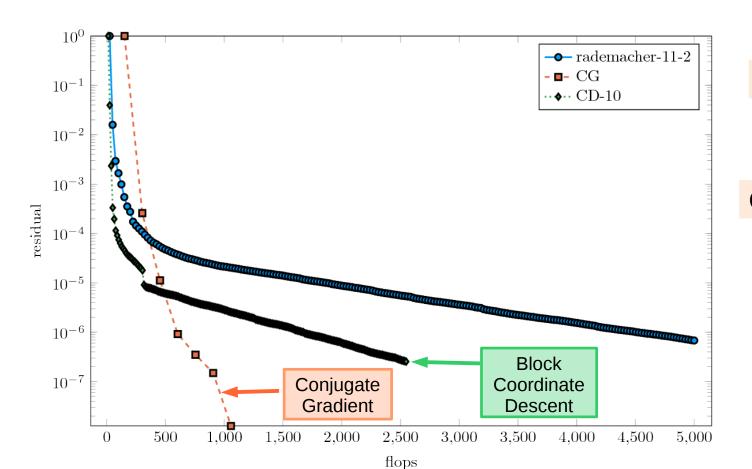
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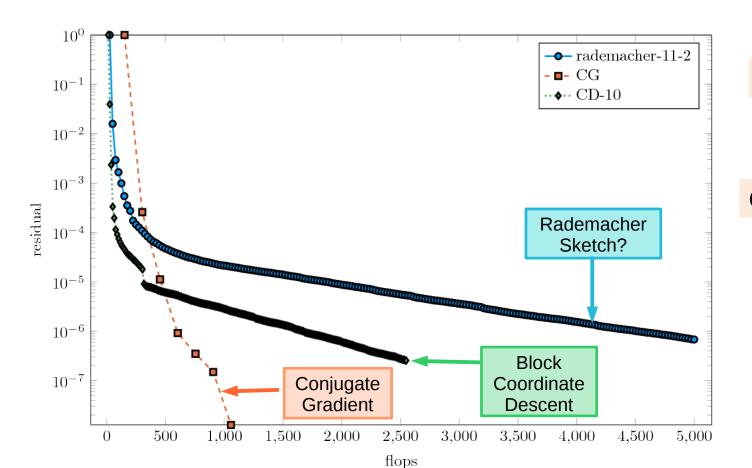
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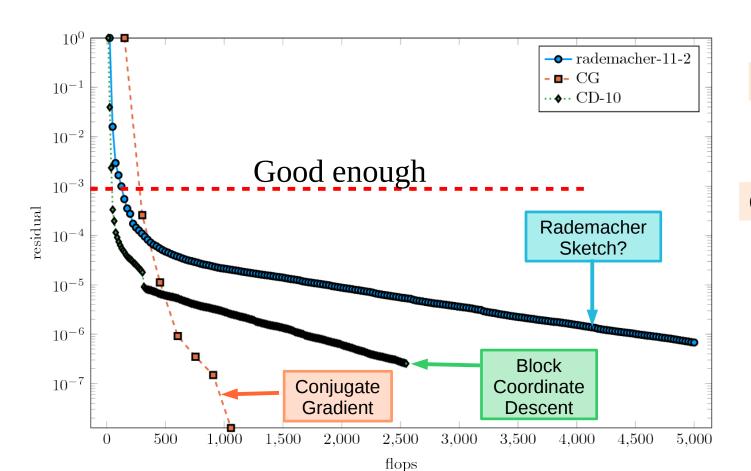
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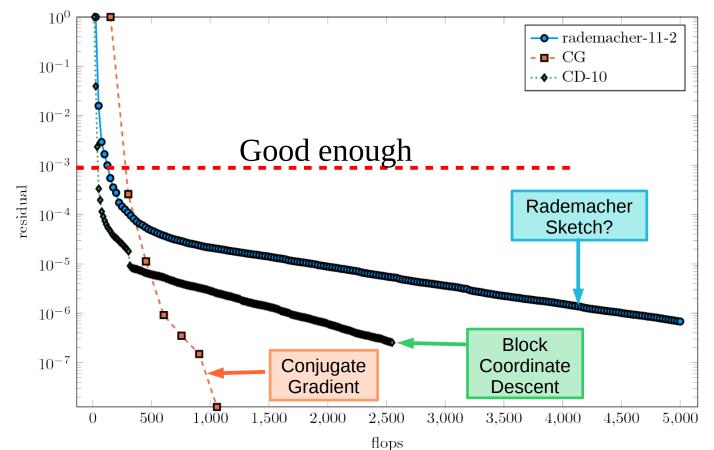
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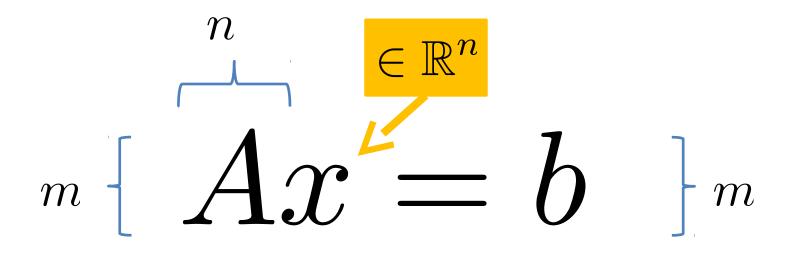
Origin: LIBSVM

GitHub: BigRidge



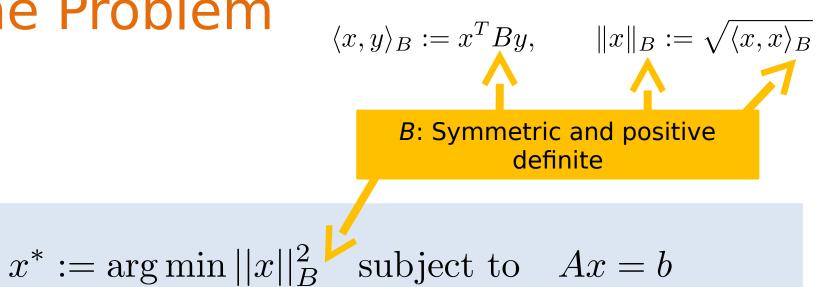
Cheikh S. Toure

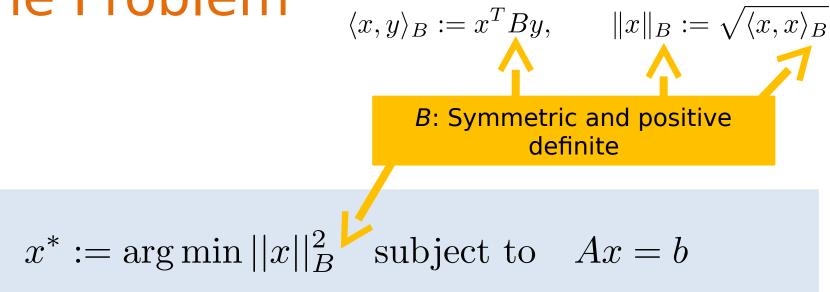
Linear Systems



Assumption: The system is consistent (i.e., has a solution)

$$x^* := \arg\min ||x||_B^2$$
 subject to $Ax = b$





As there are possibly multiple solutions, we compute the solution with the least B-norm.

Randomized Methods

The return of old methods

Old methods (Kaczmarz 1937, Gauss-Seidel 1823) make a randomized return, why?



Suitable for large scale problems: short recurrence, low iteration cost and low memory

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Easy to implement

Easy to analyse, good complexity

Often fits in parallel/distributed architecture

Stochasticity inherent in problem

Old Methods



$$x^{t+1} = \arg\min ||x - x^t||_2^2$$
 subject to $A_{i:}x = b_i$

$$A_{2:}x = b_2$$

$$x^*$$

$$x^0$$



$$x^{t+1} = \arg\min ||x - x^t||_2^2$$
 subject to $A_i : x = b_i$

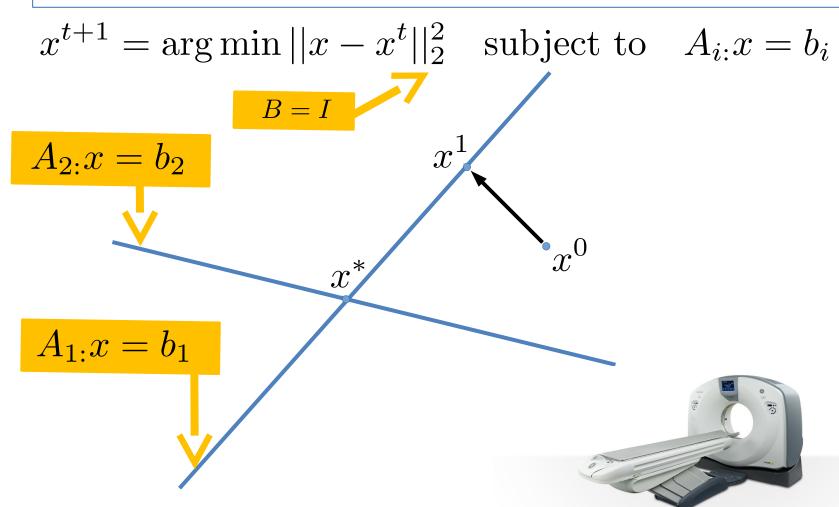
$$A_2 : x = b_2$$

$$x^*$$

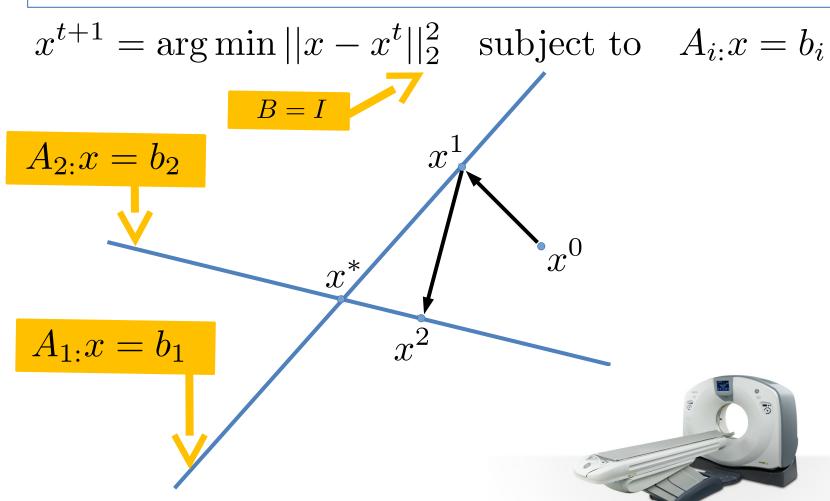
$$x^0$$

$$A_1 : x = b_1$$



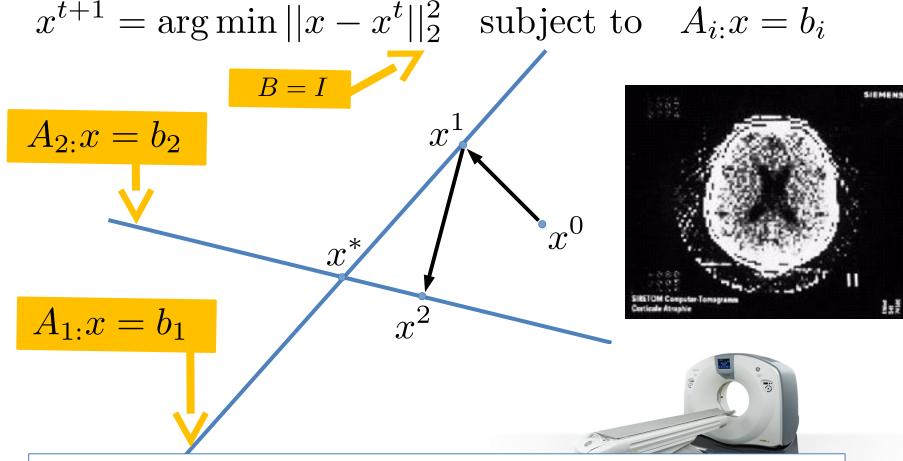








Karczmarz, M. S. (1937). **Angenäherte Auflösung von Systemen linearer Gleichungen**. *Bulletin International de l'Académie Polonaise Des Sciences et Des Lettres*, 35, 355–357.

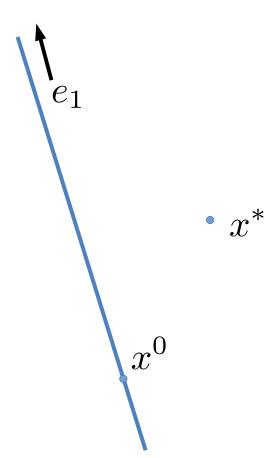




G.N. Hounsfield. Computerized transverse axial scanning (tomography): Part I. description of the system. British Journal Radiology. 1973



$$x^{t+1} = \arg\min ||x - x^*||_A^2$$
 subject to $x = x^t + \alpha e_i$

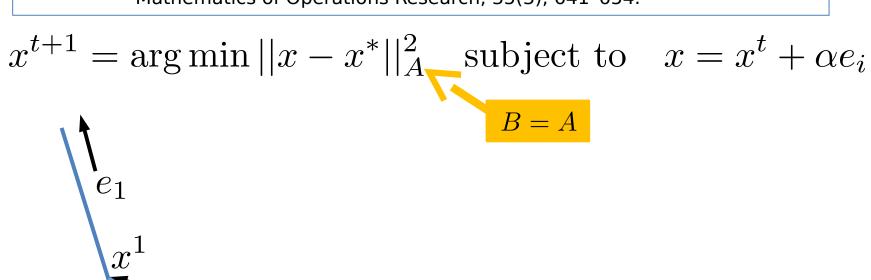




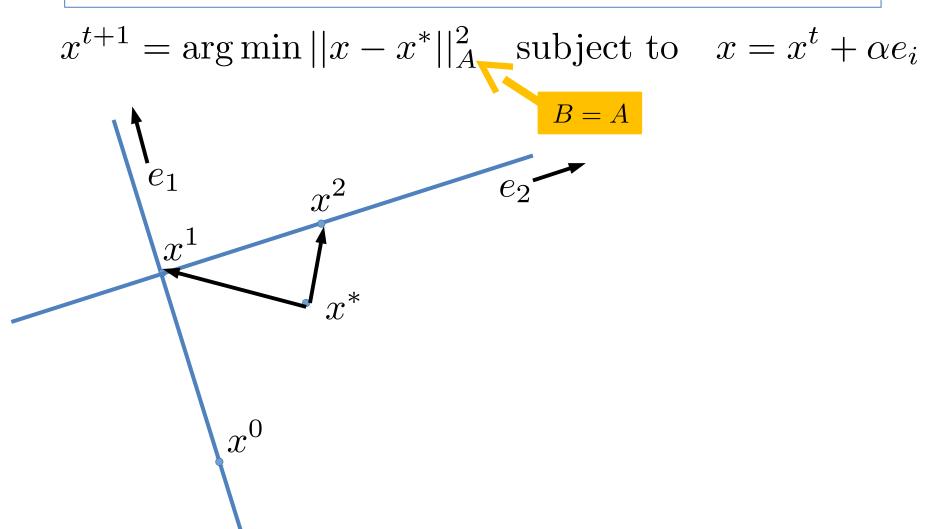
$$x^{t+1} = \arg\min||x - x^*||_A^2 \text{ subject to } x = x^t + \alpha e_i$$

$$e_1$$

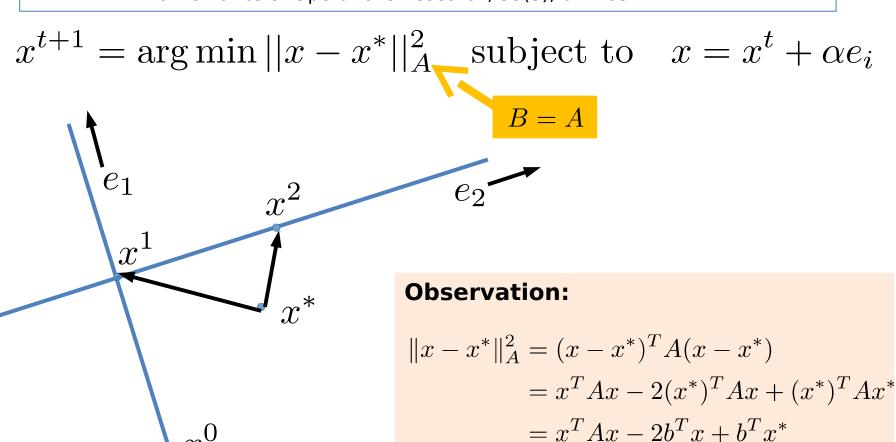




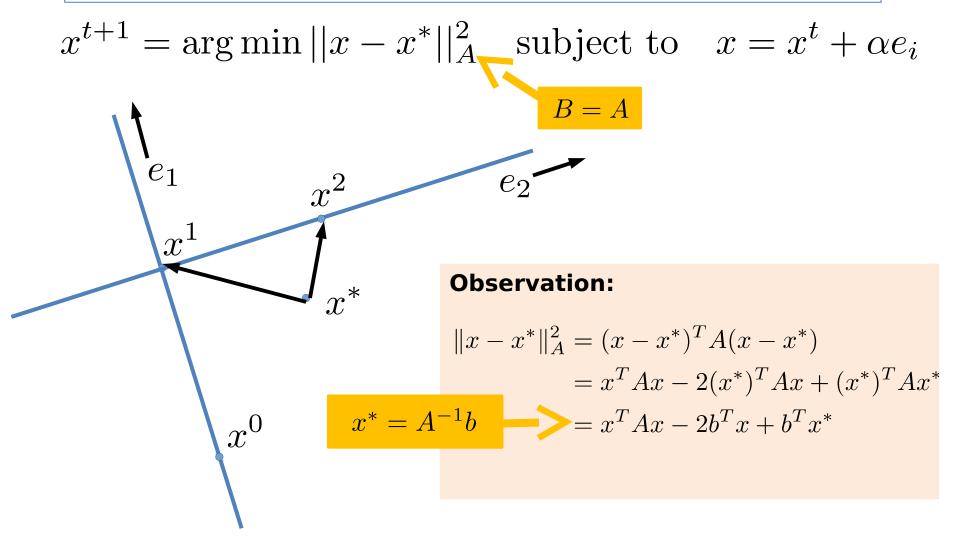




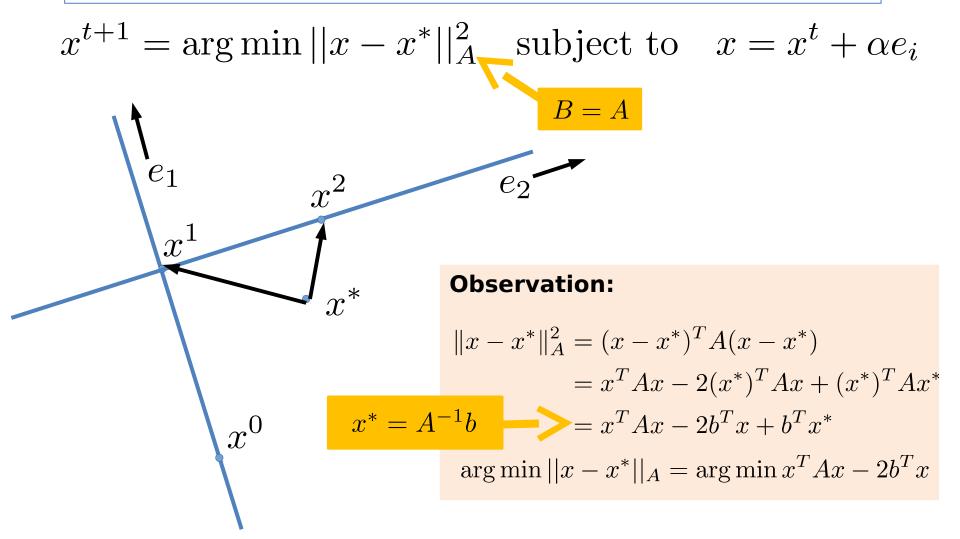




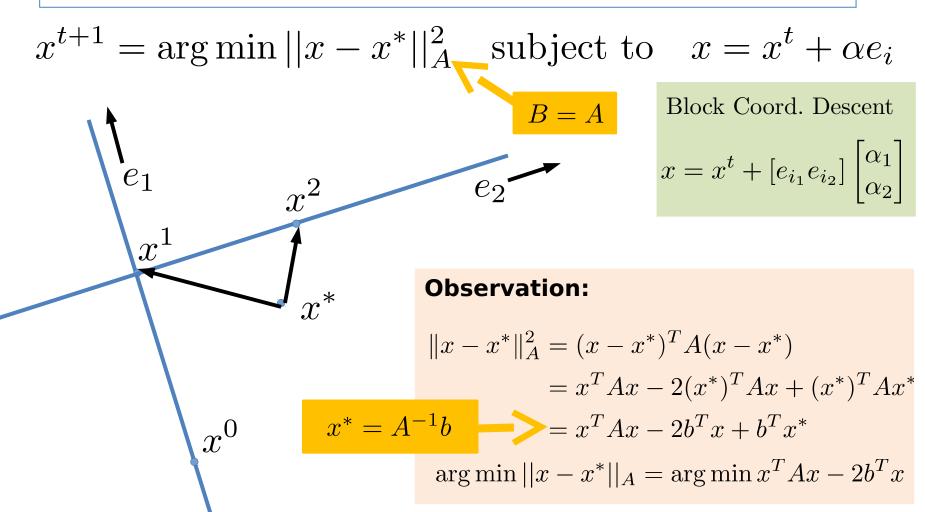






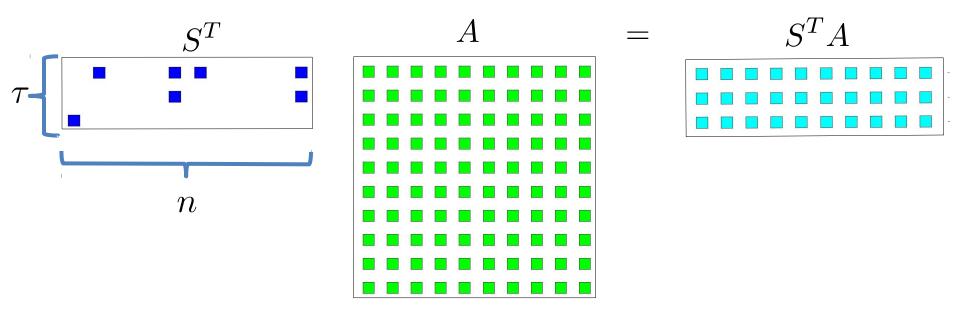






Modern Sketching

Randomized Sketching



The Sketching Matrix

 $S \sim \mathcal{D}$ a distribution over matrices $S \in \mathbb{R}^{m \times \tau}$ and $\tau \ll m, n$



W. B. Johnson and J. Lindenstrauss (1984). Contemporary Mathematics, 26, Extensions of Lipschitz mappings into a Hilbert space.



David P. Woodruff (2014), Foundations and Trends® in Theoretical Computer, **Sketching as a Tool for Numerical Linear Algebra.**

Sketching and Projecting

1. Relaxation Viewpoint "Sketch and Project"

Sample
$$S \sim \mathcal{D}$$

$$x^{t+1} = \arg\min_{x \in \mathbb{R}^n} ||x - x^t||_B^2$$
 subject to $S^T A x = S^T b$

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$$\tau \left\{ \begin{array}{c|c} S^T \\ A \end{array} \right. = \left. \begin{array}{c} S^T A \end{array} \right.$$

2. Optimization Viewpoint "Constrain and Approximate"

Sample
$$S \sim \mathcal{D}$$

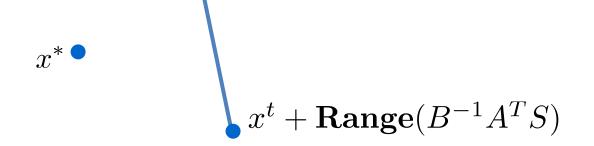
$$x^{t+1} = \arg\min_{x \in \mathbb{R}^n} ||x - x^*||_B^2$$
 subject to $x = x^t + B^{-1}A^TSy$ y is free

$$x^t + \mathbf{Range}(B^{-1}A^TS)$$

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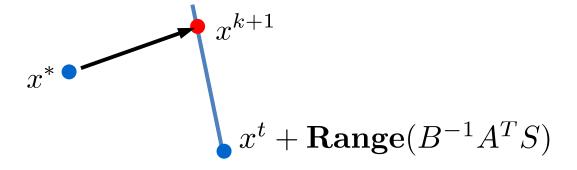
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 \bullet x^t

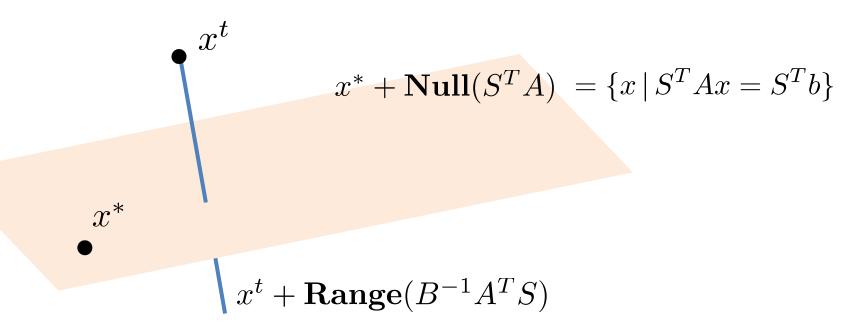
 x^*

 x^*

 \bullet x^t

$$x^* + \mathbf{Null}(S^T A) = \{x \mid S^T A x = S^T b\}$$

 x^*



$$x^{t}$$

$$x^{*} + \mathbf{Null}(S^{T}A) = \{x \mid S^{T}Ax = S^{T}b\}$$

$$x^{t+1}$$

$$x^{t} + \mathbf{Range}(B^{-1}A^{T}S)$$

$$\{x^{t+1}\} = (x^* + \mathbf{Null}(S^T A)) \cap (x^t + \mathbf{Range}(B^{-1}A^T S))$$

$$x^{t}$$

$$x^{*} + \mathbf{Null}(S^{T}A) = \{x \mid S^{T}Ax = S^{T}b\}$$

$$x^{t+1}$$

$$\mathbf{Null}(S^{T}A) \oplus \mathbf{Range}(B^{-1}A^{T}S) = \mathbb{R}^{n}$$

$$x^{t} + \mathbf{Range}(B^{-1}A^{T}S)$$

$$\{x^{t+1}\} = (x^* + \mathbf{Null}(S^T A)) \cap (x^t + \mathbf{Range}(B^{-1}A^T S))$$

ndom Intersect"
$$x^{t}$$

$$x^{*} + \mathbf{Null}(S^{T}A) = \{x \mid S^{T}Ax = S^{T}b\}$$

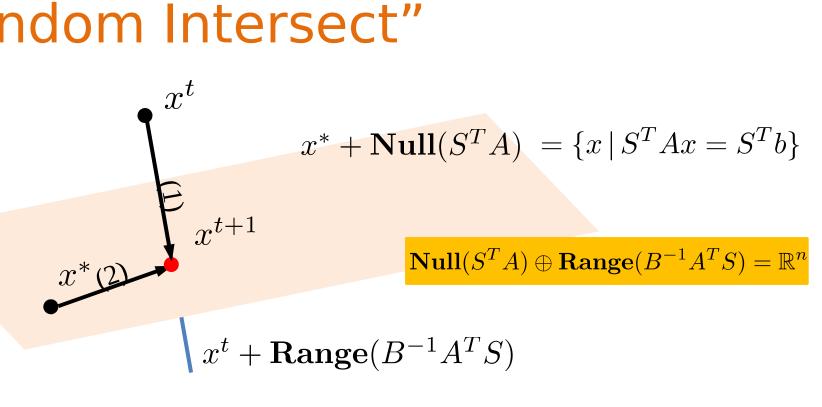
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$$\mathbf{Null}(S^{T}A) \oplus \mathbf{Range}(B^{-1}A^{T}S) = \mathbb{R}^{n}$$

$$x^{t} + \mathbf{Range}(B^{-1}A^{T}S)$$

(1)
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 subject to $S^T A x = S^T b$

$$\{x^{t+1}\} = (x^* + \mathbf{Null}(S^T A)) \cap (x^t + \mathbf{Range}(B^{-1}A^T S))$$



- (1) $x^{t+1} = \arg\min||x x^t||_B^2$ subject to $S^T A x = S^T b$
- (2) $x^{t+1} = \arg\min ||x x^*||_B^2$ subject to $x = x^t + B^{-1}A^TSy$

$$\{x^{t+1}\} = (x^* + \mathbf{Null}(S^T A)) \cap (x^t + \mathbf{Range}(B^{-1}A^T S))$$

4. Algebraic Viewpoint "Random Update"

Random Update Vector

$$x^{t+1} = x^t - B^{-1}A^T S (S^T A B^{-1} A^T S)^{\dagger} S^T (A x^t - b)$$

4. Algebraic Viewpoint "Random Update"

Random Update Vector

$$x^{t+1} = x^t - B^{-1}A^T S(S^T A B^{-1} A^T S)^{\dagger} S^T (A x^t - b)$$

Moore-Penrose pseudo inverse

Fact: Every (not necessarily square) real matrix M has a real pseudo-inverse M^{\dagger} .

4. Algebraic Viewpoint "Random Update"

Random Update Vector

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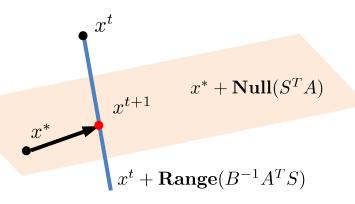
Small $\tau \times \tau$ matrix

Moore-Penrose pseudo inverse

Fact: Every (not necessarily square) real matrix M has a real pseudo-inverse M^{\dagger} .

5. Analytic Viewpoint "Random Fixed Point"

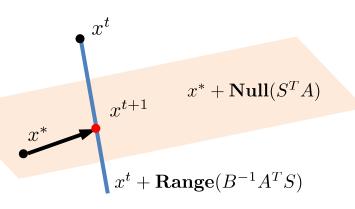
$$x^{t+1} - x^* = (I - B^{-1}A^T H A)(x^t - x^*)$$



5. Analytic Viewpoint "Random Fixed Point"

$$H := S(S^T A B^{-1} A^T S)^{\dagger} S^T \in \mathbb{R}^{m \times m}$$

$$x^{t+1} - x^* = (I - B^{-1}A^THA)(x^t - x^*)$$



5. Analytic Viewpoint "Random Fixed Point"

$$x^{t+1} - x^* = (I - B^{-1}A^THA)(x^t - x^*)$$

$$x^{t}$$
Random Iteration
Matrix
$$x^{t} + \text{Null}(S^TA)$$

$$x^{t} + \text{Range}(B^{-1}A^TS)$$

$$I - B^{-1}A^THA \text{ projects orthogonally onto } \text{Range}(B^{-1}A^TS)$$

$$I - B^{-1}A^THA \text{ projects orthogonally onto } \text{Null}(S^TA)$$



Complexity / Convergence

Theorem [GR'15]

If
$$x^0 \in \mathbf{Range}(A^T)$$
 and $\mathbf{E}[H] \succ 0$ then

$$\mathbf{E}[||x^t - x^*||_B^2] \le \rho^t ||x^0 - x^*||_B^2$$

where

$$\rho := 1 - \lambda_{\min}^{+}(B^{-1/2}A^{T}\mathbf{E}[H]AB^{-1/2})$$

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where

Smallest nonzero eigenvalue

$$\rho := 1 - \lambda_{\min}^{+}(B^{-1/2}A^{T}\mathbf{E}[H]AB^{-1/2})$$

$$H := S(S^T A B^{-1} A^T S)^{\dagger} S^T$$

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$$B = I$$

$$P(S = e_i) = \frac{1}{m} \longrightarrow S = e^i$$

$$H := S(S^T A B^{-1} A^T S)^{\dagger} S^T$$

$$B = I$$

$$S = e^{i}$$

$$\mathbf{E}[H] = \frac{1}{m} \sum_{i=1}^{m} \frac{e_i e_i^T}{||A_{i:}||_2^2}$$
$$= \operatorname{diag}(||A_{i:}||_2^2)$$

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$$H := S(S^T A B^{-1} A^T S)^{\dagger} S^T$$

Special Choice of Parameters

$$B = I$$

$$S = e^{i}$$

$$\mathbf{E}[H] = \frac{1}{m} \sum_{i=1}^{m} \frac{e_i e_i^T}{||A_{i:}||_2^2}$$
$$= \operatorname{diag}(||A_{i:}||_2^2)$$

No zero rows in A



 $\mathbf{E}[H]$ is positive definite

Theorem [RG'15]

$$\mathbf{E}[H] \succ 0$$



$$0 \le 1 - \frac{\mathbf{E}[\mathbf{Rank}(S^T A)]}{\mathbf{Rank}(A)} \le \rho \le 1$$

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Insight: The method is a contraction (without any assumptions on S whatsoever). That is, things can not get worse.

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Insight: lower rank of A and great rank of S^TA gives better lower bound. In other words, when the dimension of the search space in the "constrain and approximate" viewpoint grows.

Special Case: Randomized Kaczmarz Method



T. Strohmer and R. J. Vershynin, (2009). **A Randomized Kaczmarz Algorithm with Exponential Convergence** Journal of Fourier Analysis and Applications, 15:262

General Method

$$x^{t+1} = x^t - B^{-1}A^TS (S^TAB^{-1}A^TS)^{\dagger} S^T(Ax^t - b)$$

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$$x^{t+1} = x^t - B^{-1}A^TS (S^TAB^{-1}A^TS)^{\dagger} S^T(Ax^t - b)$$

$$B = I$$

$$\mathbf{P}(S = e_i) = p_i$$

$$S = e_i$$

General Method

$$x^{t+1} = x^t - B^{-1}A^TS (S^TAB^{-1}A^TS)^{\dagger} S^T(Ax^t - b)$$

$$B = I$$

$$S = e_i$$

$$x^{t+1} = x^t - \frac{A_{i:}x^t - b_i}{\|A_{i:}\|_2^2} (A_{i:})^T$$

General Method

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General Method

$$x^{t+1} = x^t - B^{-1}A^TS \left[(S^T A B^{-1} A^T S)^{\dagger} \right] S^T (A x^t - b)$$

$$B = I$$

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Randomized Kaczmarz: derivation and rate

General Method

$$x^{t+1} = x^t - B^{-1}A^TS (S^TAB^{-1}A^TS)^{\dagger} S^T(Ax^t - b)$$

Special Choice of Parameters

$$B = I S = e_i$$

$$x^{t+1} = x^t - \frac{A_{i:}x^t - b_i}{\|A_{i:}\|_2^2} (A_{i:})^T$$

Complexity Rate. All rows of A are nonzero \Rightarrow **E**[H] is nonsingular

$$p_i = \frac{\|A_{i:}\|^2}{\|A\|_F^2} \qquad \mathbf{E} ||x^t - x^*||_2^2 \le \left(1 - \frac{\lambda_{\min}^+(A^T A)}{\|A\|_F^2}\right)^t ||x^0 - x^*||_2^2$$

Special Case: Randomized Coordinate Descent



Leventhal, D., & Lewis, A. S. (2010). Randomized Methods for Linear Constraints: Convergence Rates and Conditioning. Mathematics of Operations Research, 35(3), 641–654.

General Method

$$x^{t+1} = x^t - B^{-1}A^TS (S^TAB^{-1}A^TS)^{\dagger} S^T(Ax^t - b)$$

$$B = A$$

$$\mathbf{P}(S = e_i) = p_i$$

$$S = e_i$$

General Method

$$x^{t+1} = x^t - B^{-1}A^TS (S^TAB^{-1}A^TS)^{\dagger} S^T(Ax^t - b)$$

positive definite
$$B = A$$

$$P(S = e_i) = p_i$$
 $S = e_i$

General Method

$$x^{t+1} = x^t - B^{-1}A^TS (S^TAB^{-1}A^TS)^{\dagger} S^T(Ax^t - b)$$

positive definite
$$B = A$$

$$\mathbf{P}(S = e_i) = p_i$$

$$S = e_i$$

$$x^{t+1} = x^t - \frac{(A_{i:})^T x^t - b_i}{A_{ii}} e^i$$

General Method

$$x^{t+1} = x^t - B^{-1}A^TS (S^TAB^{-1}A^TS)^{\dagger} S^T(Ax^t - b)$$

positive definite
$$B = A$$

$$\mathbf{P}(S = e_i) = p_i$$

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General Method

$$x^{t+1} = x^t - B^{-1}A^TS \left[(S^T A B^{-1} A^T S)^{\dagger} \right] S^T (A x^t - b)$$

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Special Choice of Parameters

positive definite
$$B = A$$

$$S = e_i$$

$$x^{t+1} = x^t - \underbrace{(A_{i:})^T x^t - b_i}_{A_{ii}} e^i$$

Complexity Rate

$$A \succ 0 \Rightarrow \mathbf{E}[H] = \operatorname{diag}(A_{11}, \dots, A_{nn}) \succ 0$$

$$p_i = \frac{A_{ii}}{\mathbf{Tr}(A)}$$

$$\mathbf{E}\left[\|x^t - x^*\|_A^2\right] \le \left(1 - \frac{\lambda_{\min}(A)}{\mathbf{Tr}(A)}\right)^t \|x^0 - x^*\|_A^2$$

Theory recovers known and new convergence results

Method

Convergence Rate ρ

Randomized CD Least square

$$A^T A$$

$$A^T A$$
 $P(S = e_i) = \frac{||A_{:i}||_2^2}{||A||_F^2}$

$$1 - \frac{\lambda_{\min}(A^T A)}{||A||_F^2}^*$$

Gaussian psd

$$S \sim \mathcal{N}(0, I)$$

$$1 - \frac{2}{\pi} \frac{\lambda_{\min}(A^T A)}{||A||_F^2}$$

Gaussian Kaczmarz

$$S \sim \mathcal{N}(0, I)$$

$$1 - \frac{2}{\pi} \frac{\lambda_{\min}(A^T A)}{||A||_F^2}$$



Designing New Methods

Optimal choice

$$\max_{B,\mathcal{D}} \rho = \lambda_{\min}^+(B^{-1/2}A^T \mathbf{E}_{S \sim \mathcal{D}}[H]AB^{-1/2})$$

Optimal choice

$$\max_{B,\mathcal{D}} \rho = \lambda_{\min}^+(B^{-1/2}A^T \mathbf{E}_{S \sim \mathcal{D}}[H]AB^{-1/2})$$

$$A \succ 0$$

$$\mathbf{Rank}(A) = n$$
 any A

B

$$A^T A$$

Optimal choice

$$\max_{B,\mathcal{D}} \rho = \lambda_{\min}^+(B^{-1/2}A^T \mathbf{E}_{S \sim \mathcal{D}}[H]AB^{-1/2})$$

$$A \succ 0$$

$$\mathbf{Rank}(A) = n$$
 any A

$$A^T A$$

Optimal S

$$\mathbf{Range}(S) = \mathbf{Range}(A^{-T}B^{1/2})$$

Optimal choice

$$\max_{B,\mathcal{D}} \rho = \lambda_{\min}^+(B^{-1/2}A^T \mathbf{E}_{S \sim \mathcal{D}}[H]AB^{-1/2})$$

$$A \succ 0$$

$$\mathbf{Rank}(A) = n$$
 any A

 $A^T A$

Optimal S

$$\mathbf{Range}(S) = \mathbf{Range}(A^{-T}B^{1/2})$$

S with fixed range

$$\mathbf{Prob}[S = S_i] = p_i,$$

for
$$i = 1, \ldots, r$$

Optimal choice

$$\max_{B,\mathcal{D}} \rho = \lambda_{\min}^+(B^{-1/2}A^T \mathbf{E}_{S \sim \mathcal{D}}[H]AB^{-1/2})$$

$$A \succ 0$$

$$\mathbf{Rank}(A) = n$$
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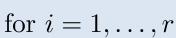
Optimal S

$$\mathbf{Range}(S) = \mathbf{Range}(A^{-T}B^{1/2})$$

S with fixed range

Optimal
$$p_i$$
's

$$\mathbf{Prob}[S=S_i]=p_i,$$





Optimal choice

$$\max_{B,\mathcal{D}} \rho = \lambda_{\min}^+(B^{-1/2}A^T \mathbf{E}_{S \sim \mathcal{D}}[H]AB^{-1/2})$$

$$A \succ 0$$

 $\mathbf{Rank}(A) = n$ any A

 $A^T A$

Optimal S

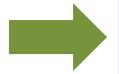
$$\mathbf{Range}(S) = \mathbf{Range}(A^{-T}B^{1/2})$$

S with fixed range

$$\mathbf{Prob}[S=S_i]=p_i,$$

for $i = 1, \ldots, r$

Optimal p_i 's



max $t, p \in \Delta_r$

sub. to
$$\sum_{i=1}^{r} p_i V_i (V_i^T V_i)^{-1} V_i^T \succ t \cdot I$$

Difficult SDP

$$V_i = B^{1/2} A^T S_i, \quad i = 1, \dots, r$$

Practical New Methods

One Shot Sketches

$$x_s^* = \arg_x \min ||S^T A x - S^T b||_2$$

where
$$||x^* - x_s^*||_2 \le (1 + \epsilon)||x^*||$$



Practical New Methods

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S

Computing S^TA

Gaussian Matrix

 $O(mn\tau)$

Subsampled Hadamard-Welsh

 $O(mn\log(\tau))$

Countmin Sketch

O(nnz(A))



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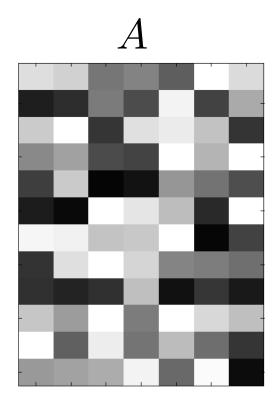
O(nnz(A))

Rademacher Sketch

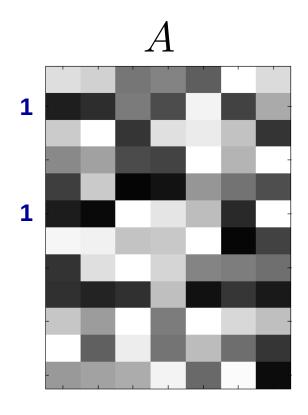
O(nnz(A))



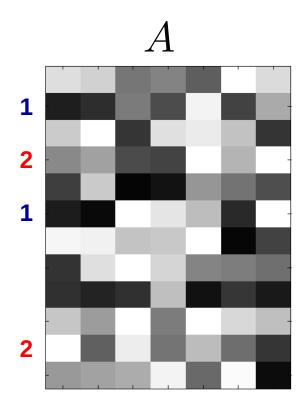
N. Ailon and B. Chazelle (2006). **Approximate nearest neighbors and the fast Johnson-Lindenstrauss transform.** Mathematics of Operations Research, 35(3), 641–654.



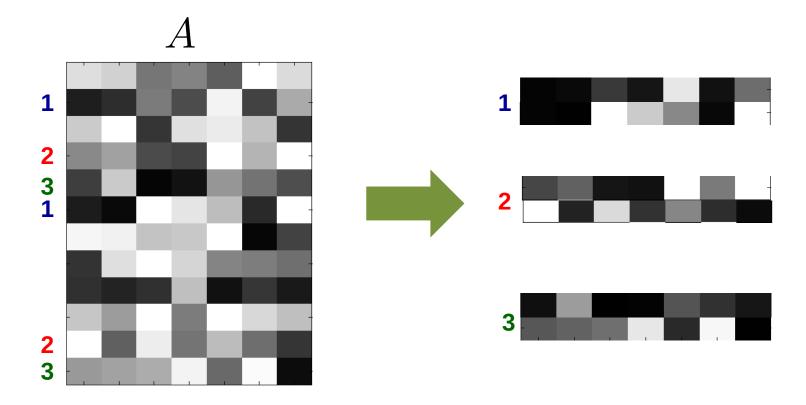
sketch size $\tau = 3$ density = 2



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sketch size \tau = 3
density = 2
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sketch size \tau = 3
density = 2
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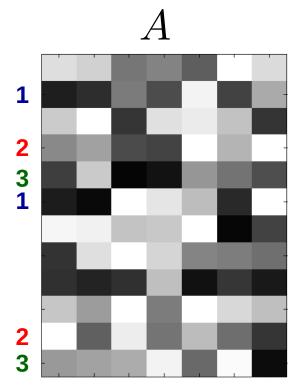


sketch size $\tau = 3$ density = 2

Flip the sign with 50% probability

sum

+ sum

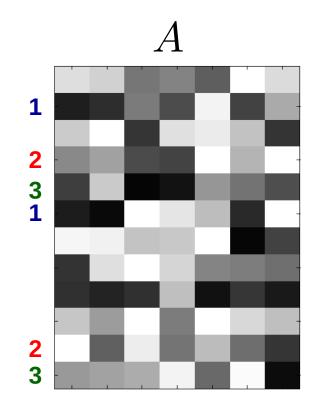




sketch size
$$\tau = 3$$

density = 2

Flip the sign with 50% probability











sketch size $\tau = 3$ density = 2

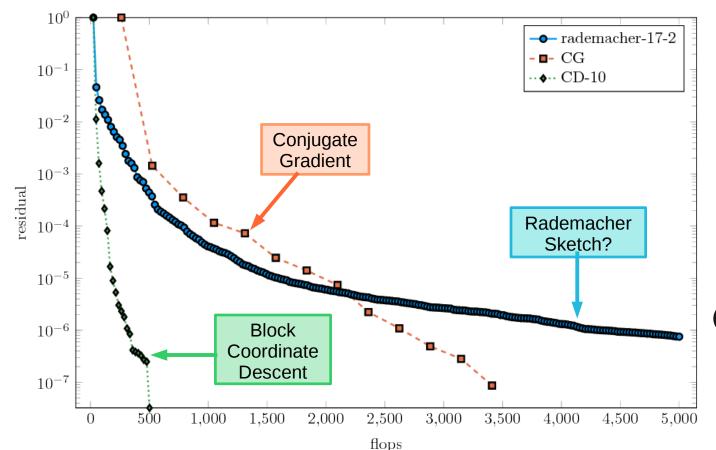
$$S^T A =$$



Experiments

Large scale Ridge Regression

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



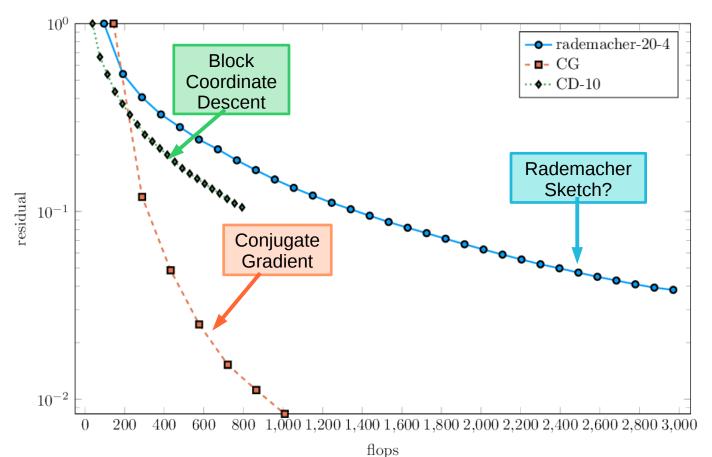
Problem: w8a

 $A \in \mathbb{R}^{49749 \times 300}$

Origin: LIBSVM

Large scale Ridge Regression

$$\min_{x} \frac{1}{2} ||Ax - y||_2^2 + \frac{\lambda}{2} ||x||_2^2$$



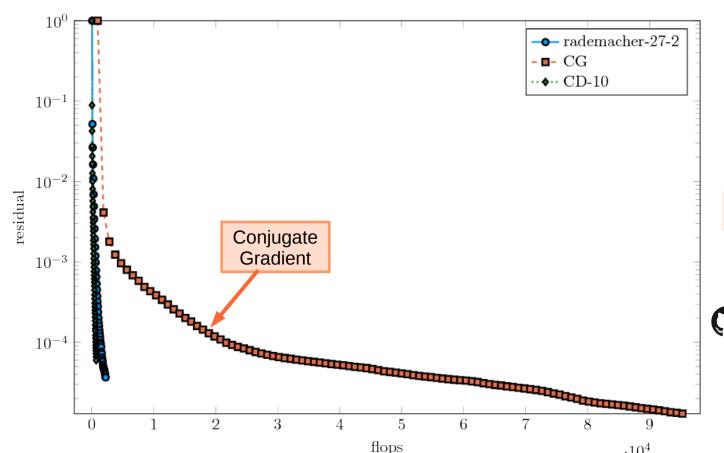
Problem: rcv1

 $A \in \mathbb{R}^{20\,242\times47\,236}$

Origin: LIBSVM

Large scale Ridge Regression

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



Problem: mnist

 $A \in \mathbb{R}^{60\,000 \times 780}$

Origin: LIBSVM

Conclusions

Unites many randomized methods under a single framework

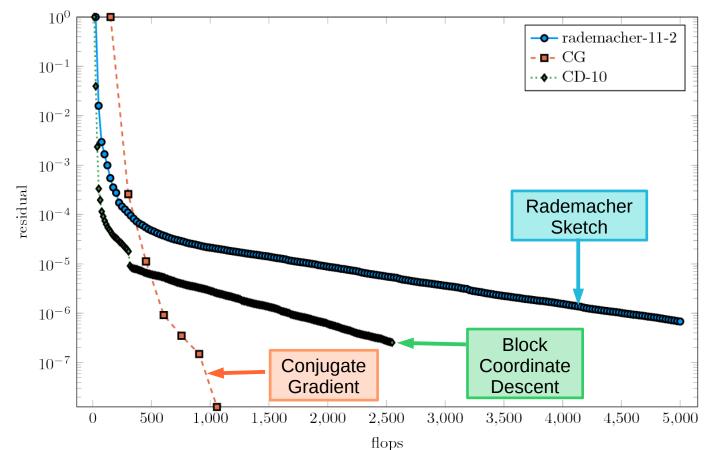
Improved convergence New lower bounds, less assumptions, tightest results.

Design new methods S = Guassian, count-sketch, Walsh-Hadamard ...etc

Optimal Sampling We can choose a sampling that optimizes the convergence rate.

Large scale Ridge Regression

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



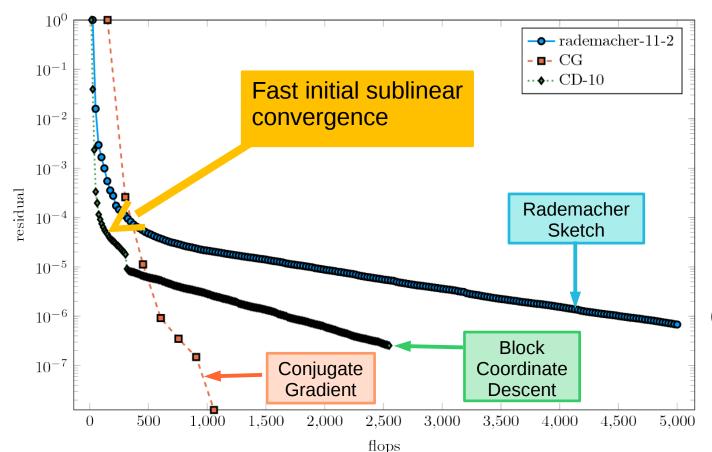
Problem: a9a

 $A \in \mathbb{R}^{32,561 \times 123}$

Origin: LIBSVM

Large scale Ridge Regression

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



Problem: a9a

 $A \in \mathbb{R}^{32,561 \times 123}$

Origin: LIBSVM



RMG and Peter Richtárik

Randomized Iterative Methods for
Linear Systems. SIAM. J. Matrix Anal. &
Appl., 36(4), 1660–1690, 2015. Most
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RMG and Peter Richtárik

Stochastic Dual Ascent for Solving
Linear Systems

Preprint arXiv:1512.06890, 2015



RMG and Peter Richtárik

Randomized quasi-Newton updates are linearly convergent matrix inversion algorithms

Preprint arXiv:1602.01768, 2016

Thank you, Questions?