Randomized iterative methods for linear systems and inverting matrices

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Joint work with Peter Richtárik

University of Edinburgh

Cambridge, January 2016

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

RMG and Peter Richtárik
Stochastic Dual Ascent for Solving Linear Systems
Preprint arXiv:1512.06890, 2015

RMG and Peter Richtárik
Stochastic Iterative Matrix Inversion
In progress, 2016

Linear Systems

The Problem

$\in \mathbb{R}^n$

$$m\left\{\overbrace{A}^{n}\right. x = b \left.\right\} m$$

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

We can also think of this as *m* linear equations, where the i[th] equation looks as follows:

$$\sum_{j=1}^{n} A_{ij} x_j = b_i$$

$$A_{i:} x = b_i$$

The Problem

$$\langle x, y \rangle_B := x^T B y, \qquad \|x\|_B := \sqrt{\langle x, x \rangle_B}$$

B: Symmetric and positive definite

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

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

Standard Randomized Methods

The return of old methods

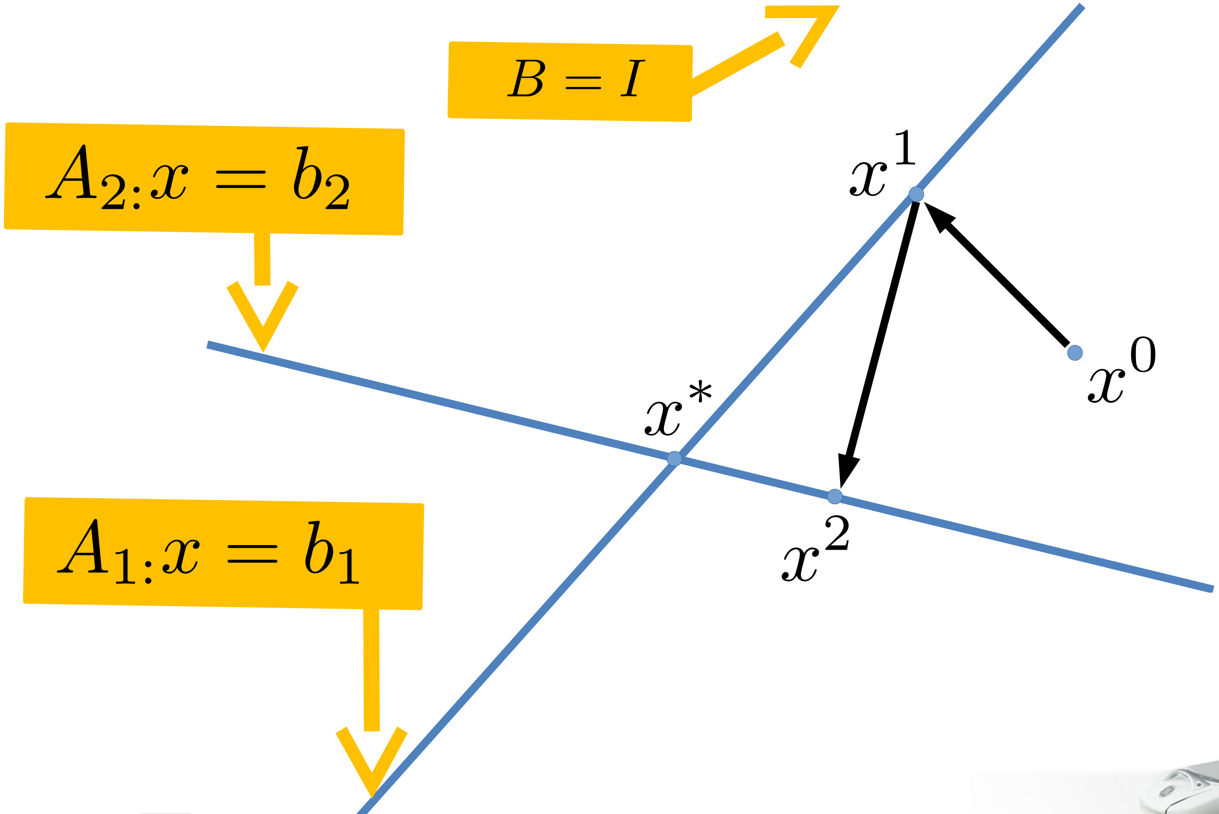
Old methods (Kaczmarz 1937, Guass-Seidel 1823) make a randomized return, why?

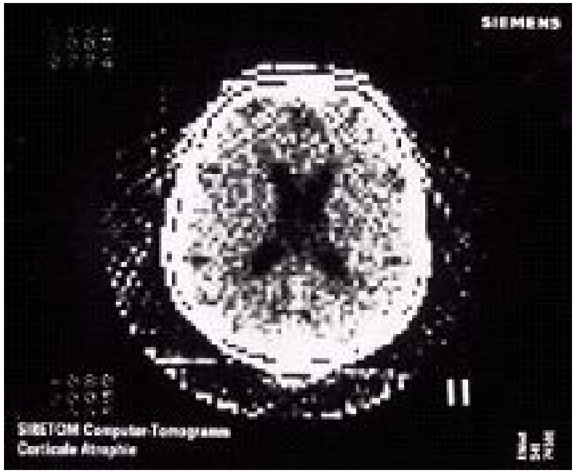
- Often suitable for Big Data problems (short recurrence, low iteration cost, low memory, block variants...etc)
- Easy to implement
- Easy to analyse, good complexity
- Often fits in parallel/distributed architecture

Randomized Kaczmarz

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

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





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

Framework for Randomized Methods

1. Relaxation Viewpoint "Sketch and Project"

$$\langle x, y \rangle_B := x^T B y, \qquad \|x\|_B := \sqrt{\langle x, x \rangle_B}$$

B: Symmetric and positive definite

$$x^{t+1} = \arg\min_{x \in \mathbb{R}^n} \|x - x^t\|_B^2$$

$$\text{subject to} \quad S^T A x = S^T b$$

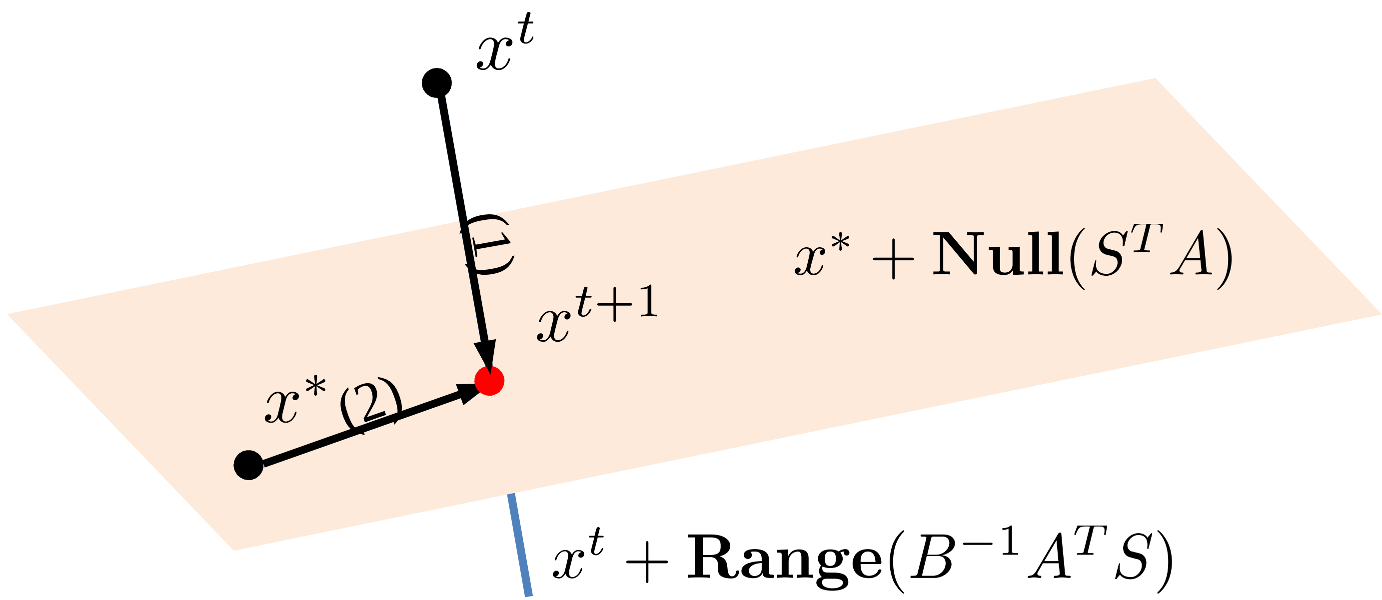
$$S^T \quad A \quad = \quad S^T A$$

S: random $m \times \tau$ matrix

2. Optimization Viewpoint
“Constrain and Approximate”

$$
\begin{aligned}
x^{t+1} \quad &= \quad \arg\min_{x \in \mathbb{R}^n} \|x - x^*\|_B^2 \\
\text{subject to} \quad & x = x^t + B^{-1}A^T S y \\
& y \quad \text{is free}
\end{aligned}
$$

3. Geometric Viewpoint "Random Intersect"



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

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

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

4. Algebraic Viewpoint
“Random Linear Solve”

$$x^{t+1} \quad = \quad \text{solution in } x \text{ of the linear system}$$

$$S^T A x = S^T b$$

$$x = x^t + B^{-1} A^T S y$$

Unknown: *x*

Unknown: *y*

5. Algebraic Viewpoint "Random Update"

$$x^{t+1} = x^t - \overbrace{B^{-1}A^T S\underbrace{(S^T A B^{-1} A^T S)^\dagger}_{\text{Small } \tau \times \tau \text{ matrix}} S^T (Ax^t - b)}^{\text{Random Update Vector}}$$

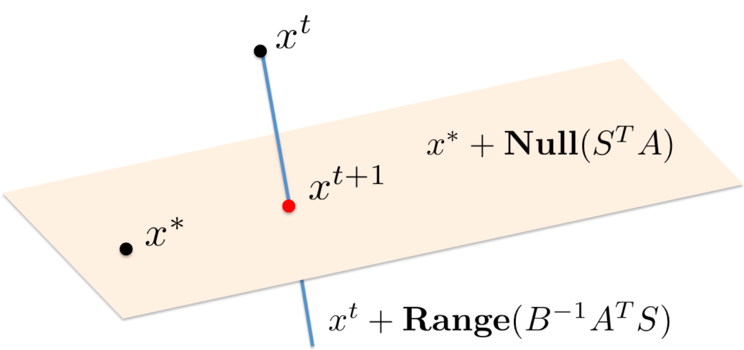
Moore-Penrose pseudo inverse

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

6. Analytic Viewpoint "Random Fixed Point"

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

$$x^{t+1} - x^* = \underbrace{(I - B^{-1} A^T H A)}_{\text{Random Iteration Matrix}}(x^t - x^*)$$



$B^{-1} A^T H A$ projects orthogonally onto $\mathbf{Range}(B^{-1} A^T S)$
$I - B^{-1} A^T H A$ projects orthogonally onto $\mathbf{Null}(S^T A)$

Theory

Complexity / Convergence

Theorem [GR'15]

$$\mathbf{E}[x^{t+1} - x^*] = (I - B^{-1}A^T\mathbf{E}[H]A)\mathbf{E}[x^t - x^*]$$

$$x^0 = 0 \quad \text{and} \quad \mathbf{E}[H] \succ 0 \quad \Rightarrow$$

1 $$||\mathbf{E}[x^t - x^*]||_B \leq \rho^t ||x^0 - x^*||_B$$

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

$\lambda_{\min}^+(A) :=$ smallest nonzero eigenvalue

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

Proof of 1 for *A* full column rank

$$\mathbf{E}[x^{t+1} - x^*] = (I - B^{-1}A^T\mathbf{E}[H]A)\mathbf{E}[x^t - x^*]$$

Taking expectations conditioned on x^t, we get

$$\mathbf{E}[x^{t+1} - x^* \,|\, x^t] = (I - B^{-1}A^T\mathbf{E}[H]A)(x^t - x^*)$$

Taking expectation again gives

$$\begin{aligned}\mathbf{E}[x^{t+1} - x^*] &= \mathbf{E}[\mathbf{E}[x^{t+1} - x^* \,|\, x^t]] \\ &= \mathbf{E}[(I - B^{-1}A^T\mathbf{E}[H]A)(x^t - x^*)] \\ &= (I - B^{-1}A^T\mathbf{E}[H]A)\mathbf{E}[x^t - x^*]\end{aligned}$$

Applying norms to both sides we obtain

$$||\mathbf{E}[x^{t+1} - x^*]||_B \leq \underbrace{\boxed{||I - B^{-1}A^T\mathbf{E}[H]A||_B}}_{\rho} ||\mathbf{E}[x^t - x^*]||_B$$

Case study of $\mathbf{E}[H]$

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

Special Choice of Parameters

$$\mathbf{P}(S = e_i) = \frac{1}{m}$$

$$B = I$$

$$S = e^i$$

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

$$= \mathrm{diag}(||A_{i:}||_2^2)$$

No zero rows in A

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

Weak assumption

The rate: lower and upper bounds

Theorem [RG‘15]

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

$$\Downarrow$$

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

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

Insight: The lower bound on the rate is better for *A* low rank and when the dimension of the search space in the “constrain and approximate” viewpoint grows.

Special Case: Randomized Kaczmarz Method

Randomized Kaczmarz: derivation and rate

General Method

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

Special Choice of Parameters

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

$$B = I$$

$$S = e_i$$

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

Complexity Rate. All rows of A are nonzero $\Rightarrow \mathbf{E}[H]$ is nonsingular

$$p_i = \frac{\|A_{i:}\|^2}{\|A\|_F^2}$$

$$\mathbf{E}\left[\|x^t - x^*\|_2^2\right] \leq \left(1 - \frac{\lambda_{\min}(A^TA)}{\|A\|_F^2}\right)^t \|x^0 - x^*\|_2^2$$

Special Case: Randomized Coordinate Descent

Randomized Coordinate Descent: derivation and rate

General Method

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

Special Choice of Parameters

positve definite

$$B = A$$

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

$$S = e_i$$

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

Complexity Rate

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

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

Theory recovers known and new convergence results

Method	B	S	Convergence Rate ρ
Randomized CD Least square	$A^T A$	$P(S = e_i) = \frac{\|\|A_{:i}\|\|_2^2}{\|\|A\|\|_F^2}$	$1 - \frac{\lambda_{\min}(A^T A)}{\|\|A\|\|_F^2}^*$
Gaussian psd	A	$S \sim \mathcal{N}(0, I)$	$1 - \frac{2}{\pi}\frac{\lambda_{\min}(A^T A)}{\|\|A\|\|_F^2}$
Gaussian Kaczmarz	I	$S \sim \mathcal{N}(0, I)$	$1 - \frac{2}{\pi}\frac{\lambda_{\min}(A^T A)}{\|\|A\|\|_F^2}$

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

Convenient probability

Theorem [GR‘15]

$$\bar{S} := [S_1, \ldots, S_r] \quad \text{is nonsingular}$$

$$\mathbf{P}(S = S_i) = p_i = \frac{\mathbf{Tr}(S_i^T A B^{-1} A^T S_i)}{\mathbf{Tr}(\bar{S}^T A B^{-1} A^T \bar{S})}$$

$$\Downarrow$$

$$\rho = 1 - \frac{1}{\kappa^2(W^{1/2} A^T \bar{S})}$$

$$\kappa(W^{1/2} A^T \bar{S}) := ||(W^{1/2} A^T \bar{S})^{-1}||_2 ||W^{1/2} A^T \bar{S}||_F$$

Conclusion for linear systems

- **Unites** many randomized methods under a single framework
- **Improved convergence:** New lower bound, less assumptions, RK convergence without full rank assumption.
- **Design new methods:** S = Guassian, count-sketch, Walsh-Hadamard ...etc
- **Optimal Sampling:** We can choose a sampling that optimizes the convergence rate.

Inverting a Matrix

The Problem

$\in \mathbb{R}^{n\times n}$

Identity matrix

$$n\left\{\overbrace{A}^{n}\right. X = I$$

Assumption: The matrix *A* is nonsingular

Why iteratively invert a matrix?

- Needed to calculate a Schur complement or a projection operator
- Iterative methods are good when we can tolerate an error or have an initial guess $X^0 \approx A^{-1}$
- Staging for **randomized variable metric** methods and **randomized preconditioning**

Randomized Methods for Nonsymmetric Matrices

Equivalence to solving linear systems

$$\langle X, Y \rangle_{F(B)} = \mathbf{Tr}(X^T B Y B), \quad ||X||_{F(B)} = \sqrt{\langle X, X \rangle_{F(B)}}$$

B: Symmetric and positive definite

$$X^{t+1} = \arg \min_{X \in \mathbb{R}^{n \times n}} ||X - X^t||^2_{F(B)}$$
$$\text{subject to} \quad S^T A X = S^T$$

S: random $n \times \tau$ matrix

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

This method is equivalent to the sketch and project method for solving linear systems, but applied simultanously to the *n* equations defined by *AX* = *I*

Randomized Methods for Symmetric Matrices

$$A = A^T$$

Sketch and Project

$$X^{t+1} = \arg \min_{X \in \mathbb{R}^{n \times n}} ||X - X^t||^2_{F(B)}$$

$$\text{subject to} \quad S^T AX = S^T, \quad X = X^T$$

Connection to quasi-Newton Methods: This is a randomized block extension of the quasi-Newton updates. In the quasi-Newton setting

$$S = \delta \in \mathbb{R}^n \quad \text{and} \quad \gamma := A\delta$$

and A is an *unknown* operator. However, we can sample its action $A\delta$ *and*

$$S^T AX = S^T \Leftrightarrow X\gamma = \delta$$

is known as the *secant equation*

Goldfarb, D. (1970). **A Family of Variable-Metric Methods Derived by Variational Means**. Mathematics of Computation, 24(109), 23.

Constrain and Approximate

$$X^{t+1} = \arg \min_{X \in \mathbb{R}^{n \times n}} ||X - A^{-1}||^2_{F(B)}$$

$$\text{subject to} \quad X = X^t + YS^T AB^{-1} + B^{-1} A^T S Y^T$$

$$Y \in \mathbb{R}^{n \times \tau} \text{ is free}$$

Duality: This is dual problem of the sketch and project viewpoint, new insight into quasi-Newton methods.

New viewpoint for BFGS

Sketch and project

$$X^{t+1} = \arg \min_{X \in \mathbb{R}^{n \times n}} ||X - X^t||^2_{F(A)}$$

$$\text{subject to} \quad X\gamma = \delta, \quad X = X^T$$

Constrain and approximate

$$X^{t+1} = \arg \min_{X \in \mathbb{R}^{n \times n}} ||AX - I||^2_F$$

$$\text{subject to} \quad X = X^t + y\delta^T + \delta y^T$$

$$y \in \mathbb{R}^n \text{ is free}$$

Duality: The BFGS minimizes a residual restricted to an affine space of symmetric matrices

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

Random Update

$$X^{t+1} = X^t - (X^t A - I) H A B^{-1} \\ + B^{-1} A H (A X^t - I) \left(A H A B^{-1} - I \right)$$

Low rank 3 X τ update

Random Fixed Point

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

Complexity / Convergence

Theorem [GR'16]

$$||A||_B = ||B^{1/2}AB^{1/2}||_2$$

1. $$||\mathbf{E}[X^t - A^{-1}]||_B \leq \rho^t \, ||X^0 - A^{-1}||_B$$

2. $$\mathbf{E}[H] \succ 0 \quad \Rightarrow \quad 0 \leq \rho < 1$$

$$\Downarrow$$

$$\mathbf{E}[||X^t - A^{-1}||_{F(B)}^2] \leq \rho^t \, ||X^0 - A^{-1}||_{F(B)}^2$$

Special Case: Randomized Block BFGS

Randomized BFGS

$$X^{t+1} = \arg\min_{X \in \mathbb{R}^{n\times n}} ||X - X^t||_{F(A)}^2$$
$$\text{subject to} \quad S^T A X = S^T, \quad X = X^T$$

Special Choice of Parameters

positve definite $\Rightarrow B = A$

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

$$X^{t+1} = H + (I - HA)X^t(I - AH)$$

Complexity Rate. A is positive definite $\Rightarrow \mathbf{E}[H]$ is nonsingular

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

$$\mathbf{E}[||AX^t - I||_F^2] \leq \left(1 - \frac{\lambda_{\min}(A)}{\mathbf{Tr}(A)}\right)^t ||AX^0 - I||_F^2$$

Randomized Block BFGS

$$X^{t+1} = \arg \min_{X \in \mathbb{R}^{n \times n}} ||X - X^t||^2_{F(A)}$$

$$\text{subject to} \quad S^T A X = S^T, \quad X = X^T$$

Special Choice of Parameters

positve definite

$$B = A$$

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

$$S = S_i$$

$$X^{t+1} = H + (I - HA)X^t(I - AH)$$

Complexity Rate If A is positive definite $\rightarrow$ $\mathbf{E}[H]$ is nonsingular

Idea: To minimize condition number, choose S so that $\bar{S}$ is an approximate inverse of $A^{1/2}$

$$p_i = \frac{\mathbf{Tr}(S_i^T A S_i)}{\mathbf{Tr}(\bar{S}^T A \bar{S})}$$

$$\mathbf{E}[||AX^t - I||_F^2] \leq \left(1 - \frac{1}{\boxed{\kappa^2(A^{1/2}\bar{S})}}\right) ||AX^0 - I||_F^2$$

BFGS with Randomized Self-Conditioning (RASC)

$$\mathbf{E}[||AX^t - I||_F] \leq \left(1 - \frac{1}{\boxed{\kappa^2(A^{1/2}\bar{S})}}\right)^t ||AX^0 - I||_F$$

$$X_k \to A^{-1} \qquad\qquad X_k^{1/2} \to A^{-1/2}$$

$$\text{Maintain and update } L_k = X_k^{1/2}*$$

Self conditioning sampling:

$\texttt{RASC\_cols:}$ $\quad S = L_k I_{:C}, \quad C \subset \{1, \ldots, n\}$ random set

$\texttt{RASC\_guass:}$ $\quad S \sim \mathcal{N}(0, X_k)$

*Gratton, S., Sartenaer, A., & Ilunga, J. T. (2011). **On a Class of Limited Memory Preconditioners for Large-Scale Nonlinear Least-Squares Problems**. SIAM Journal on Optimization, 21(3), 912–935.

Experiments

Current state of the art

Symmetric Newton-Schulz

$$X^{t+1} = 2X^t - X^t A X^t$$

Self-conditioning Minimal Residual (MR)

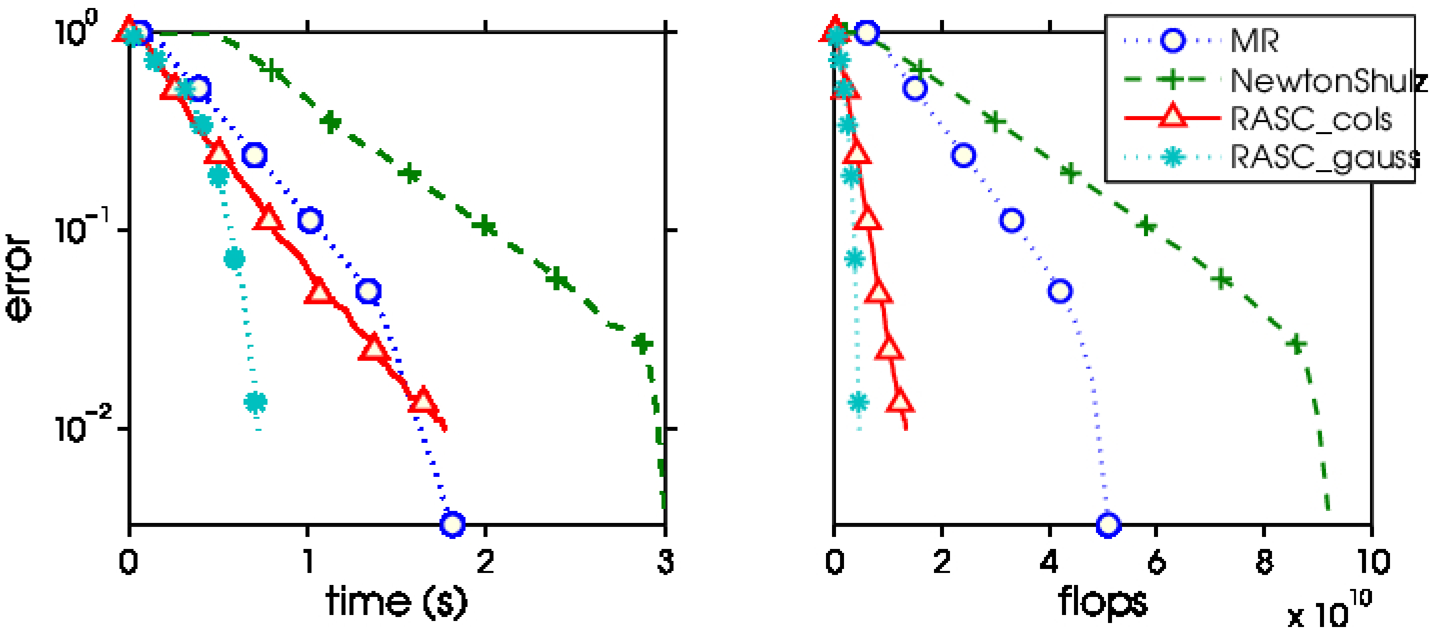
$$\min_{\alpha} ||AX - I||_F^2 \quad \text{subject to} \quad X = X^t + \alpha X^t R^t$$

$$\Rightarrow X^{t+1} = X^t - \frac{\mathbf{Tr}((R^t)^T A X^t R^t)}{\mathbf{Tr}(AX^t R^t)^T A X^t R^t} X^t R^t$$

where $R^t := I - AX^t$

Synthetic Problems

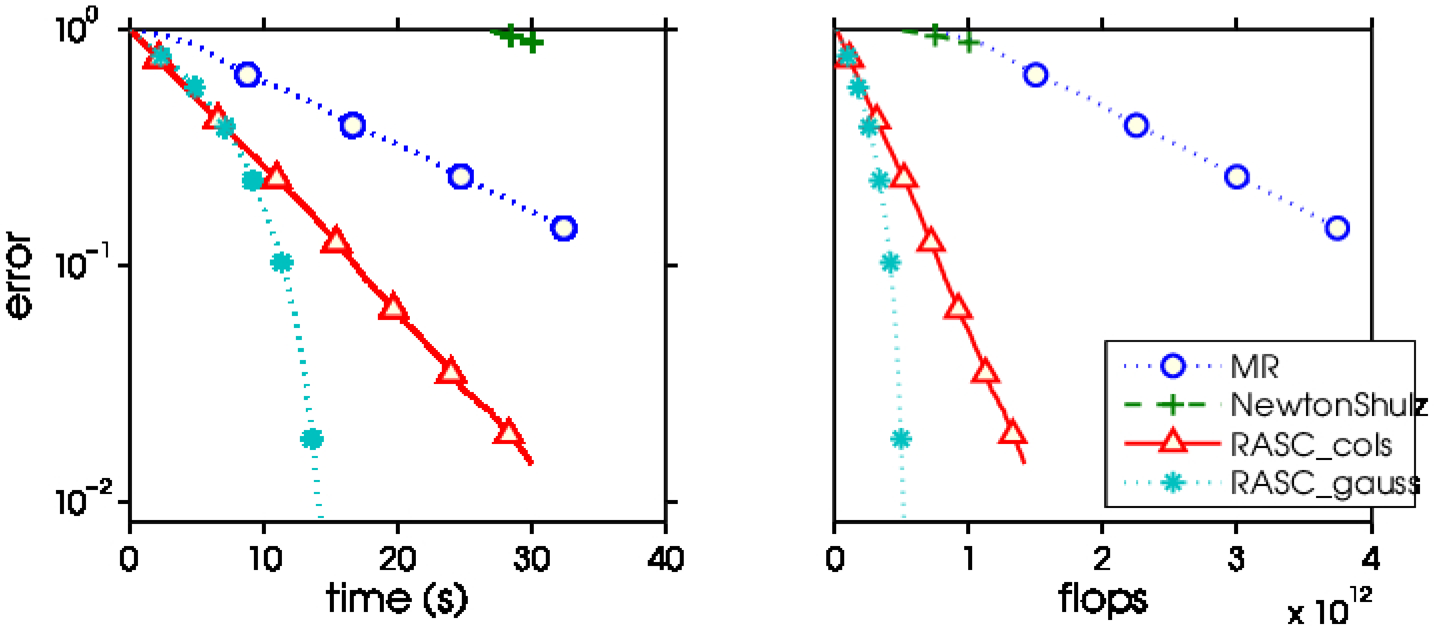
Synthetic data



($randn$, n = 1000)

Synthetic Problems

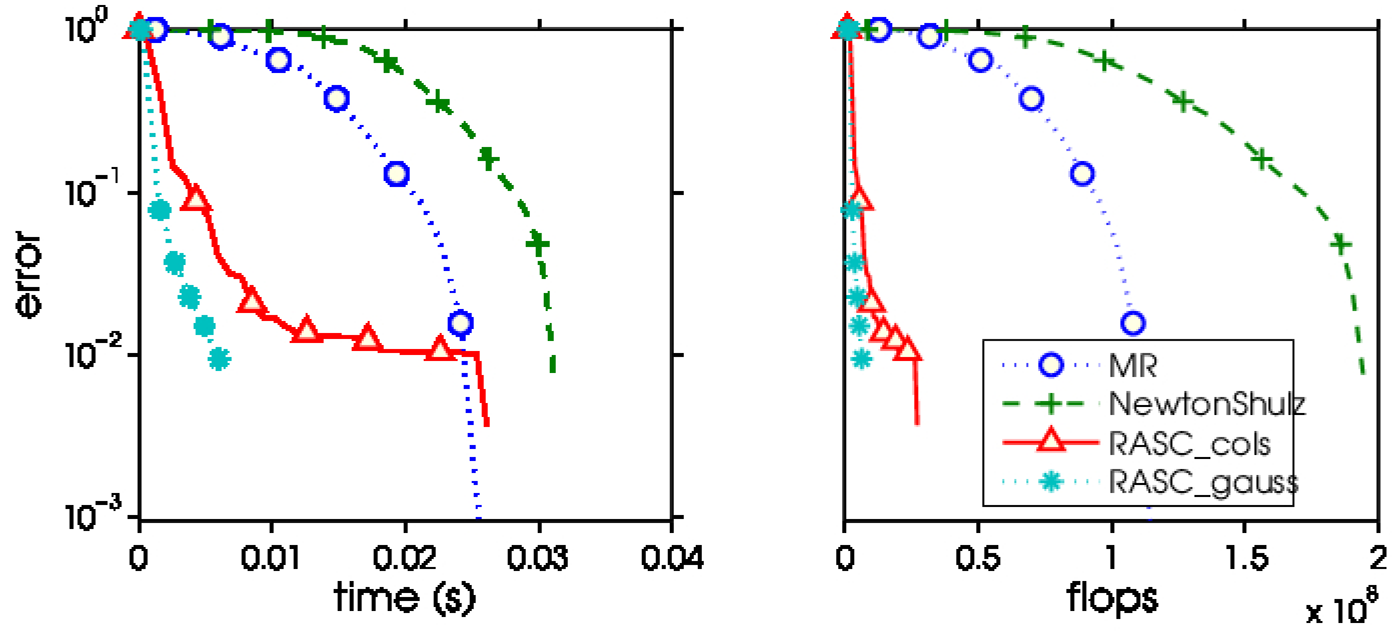
Synthetic data



(*randn*, n = 5000)

Ridge Regression Hessian

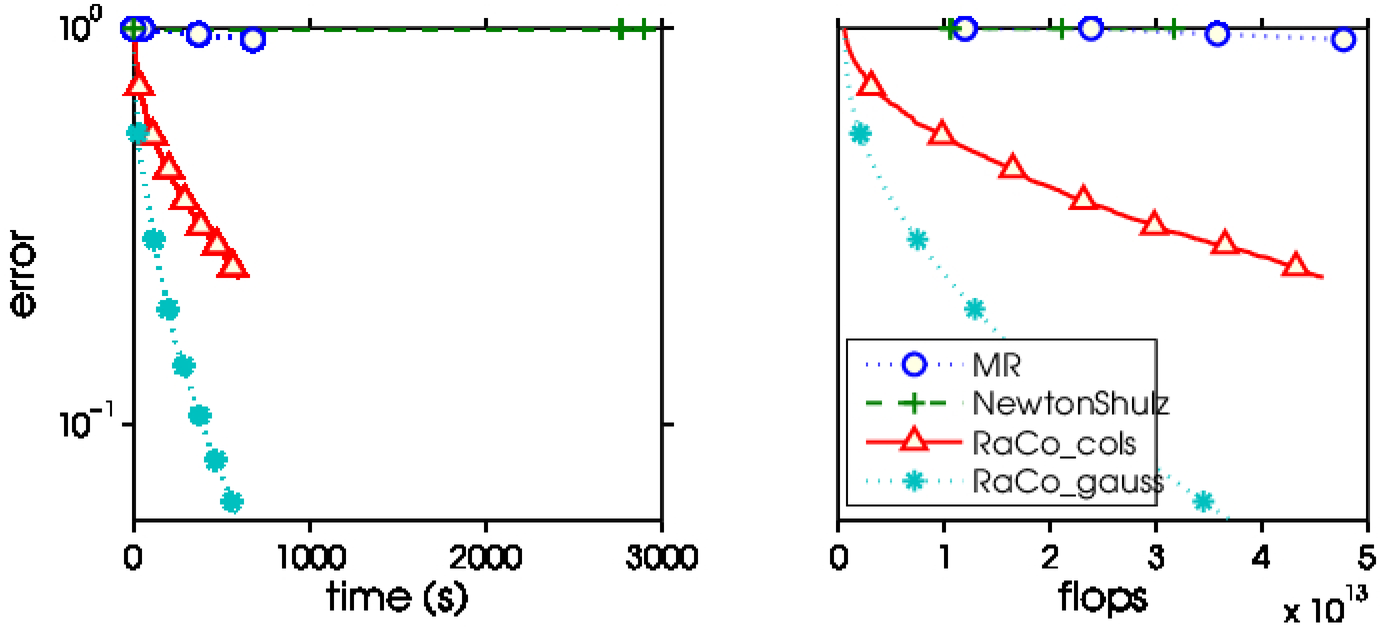
LIBSVM data



(aloi, n = 128)

Ridge Regression Hessian

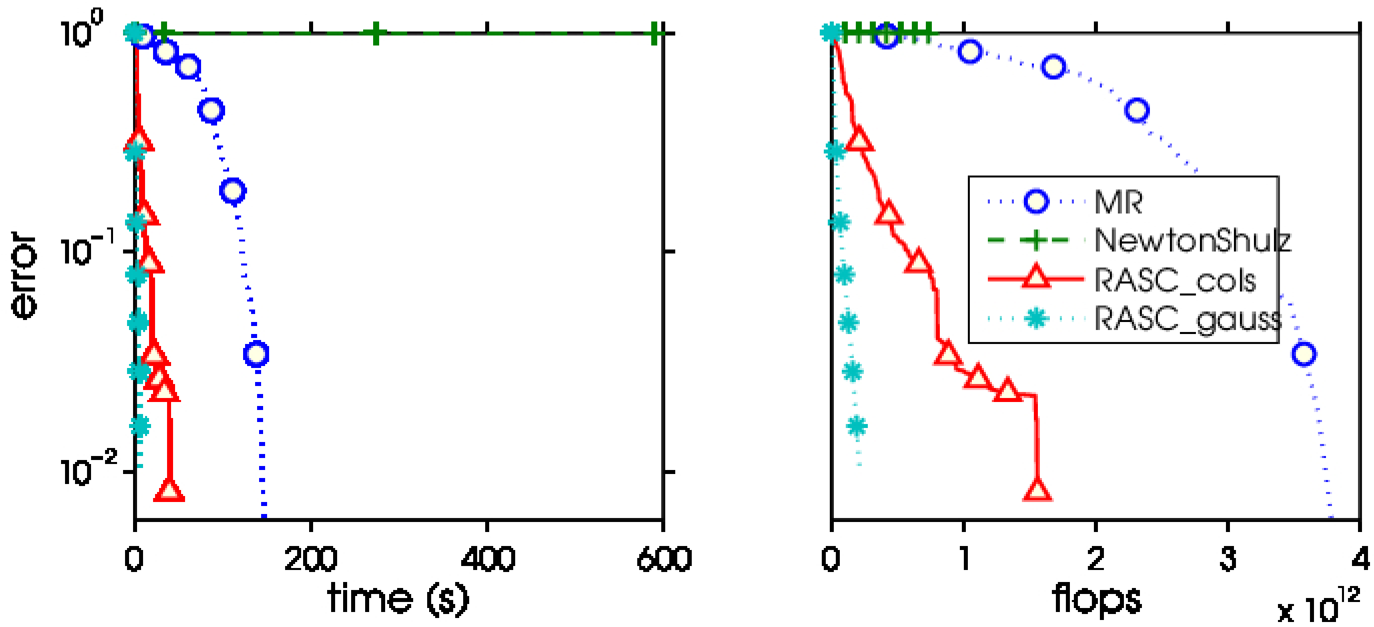
LIBSVM data



(aloi, n = 20,958)

Sparse Matrices from Engineering

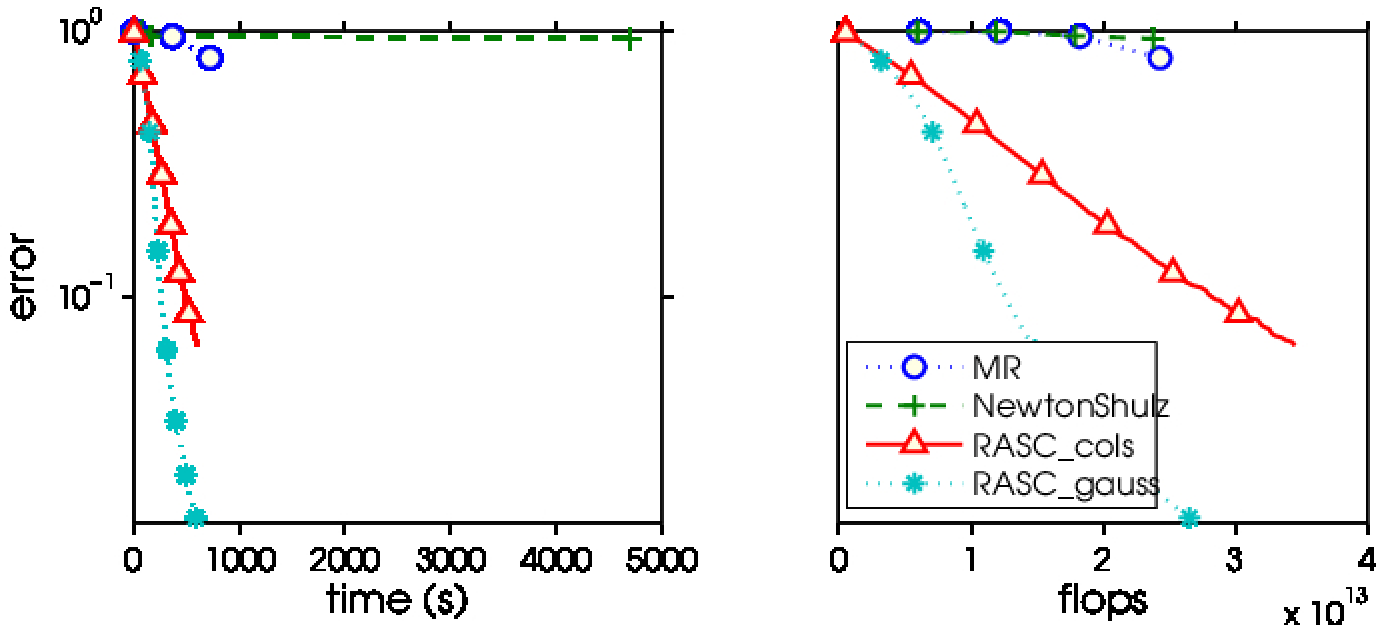
UF collection



(Nasa-nasa, n = 4,705)

Sparse Matrices from Engineering

UF collection



(ND-nd6k, n = 18,000)

Consequences and Future Work

Smooth minimization

$$\min_{x \in \mathbf{R}^n} f(x)$$

$$f \in C^2(\mathbf{R}^n)$$

$$\left(\frac{d}{dy} \nabla f(x + Sy) \right) |_{y=0} = \nabla^2 f(x) S$$

Cheap to calculate, costs
τ X function evaluations

Variable metric methods

$$
\begin{aligned}
&\textbf{Initialize } X^0 \in \mathbf{R}^{n\times n}\\
&\textbf{For } t = 0, 1, \ldots,\\
&1. \quad x^{t+1} = x^t + \alpha_t X^t \nabla f(x^t)\\
&2. \quad S = \mathrm{compute\_sample\_matrix}(X^t)\\
&3. \quad Y = \nabla^2 f(x^t) S\\
&4. \quad X^{t+1} = \arg\min_X ||X - X^t||^2_{\nabla^2 f(x^t)}\\
&\qquad\qquad \text{s.t.} \quad Y^T X = S^T,\ X = X^T
\end{aligned}
$$

Update metric with
RASC update

Preconditioning Sketched Newton

Sketch and project Newton system
$\nabla^2 f(x^t)x^t = -\nabla f(x^t)$

Initialize $X^0 \in \mathbf{R}^{n\times n}$

For $t = 0, 1, \ldots,$

1. $S = \text{compute\_sample\_matrix}(X^t)$
2. $Y = \nabla^2 f(x^t) S$
3. $x^{t+1} = \arg\min_x \|x - x^t\|^2_{\nabla^2 f(x^t)}$ s.t. $Y^T x = -S^T \nabla f(x^t)$
4. $X^{t+1} = \arg\min_X \|X - X^t\|^2_{\nabla^2 f(x^t)}$ s.t. $Y^T X = S^T,\ X = X^T$

Update metric with RASC update

Conclusion for Inverting Matrices

- **New randomized methods** capable of inverting large-scale matrices
- **Convergence rates** which can form the basis of convergence of preconditioning or variable metric methods.
- **Dual viewpoints** of classic quasi-Newton methods
- **Can be extended** to calculating pseudo-inverse

Thank you,
Questions?