Linearly Convergent Randomized Iterative Methods for Computing the Pseudoinverse

Robert Mansel Gower

Joint work with Peter Richtarik

ÉCOLE NORMALE SUPÉRIEURE

INVENTEURS DU MONDE NUMÉRIQUE

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Sketch and project applications

Numerical Linear Algebra

- Linear systems
- Matrix inverse
- Pseudo inverse

Stochastic Optimization

- Stochastic Quasi-Newton methods
- Stochastic variance reduced gradients
- Stochastic Coordinate descent

Distributed Consensus

Three viewpoints of the Pseudoinverse
Three methods

Three Viewpoints

Given $A \in \mathbb{R}^{m \times n}$ compute an approx. $A^\dagger \in \mathbb{R}^{n \times m}$

$$A^\dagger \quad = \quad \arg \min_{X \in ^{n \times m}} ||X||_F^2$$

subject to

$(1)\; A^\top = A^\top A X$ or $(2)\; A^\top = X A A^\top$ or $(3)\; A X A = A$

Three Viewpoints

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Design three methods based on approximate stochastic projections

Three Viewpoints

Given $A \in \mathbb{R}^{m\times n}$ compute an approx. $A^\dagger \in \mathbb{R}^{n\times m}$

$$A^\dagger \quad = \quad \arg\min_{X\in^{n\times m}} ||X||_F^2$$

subject to

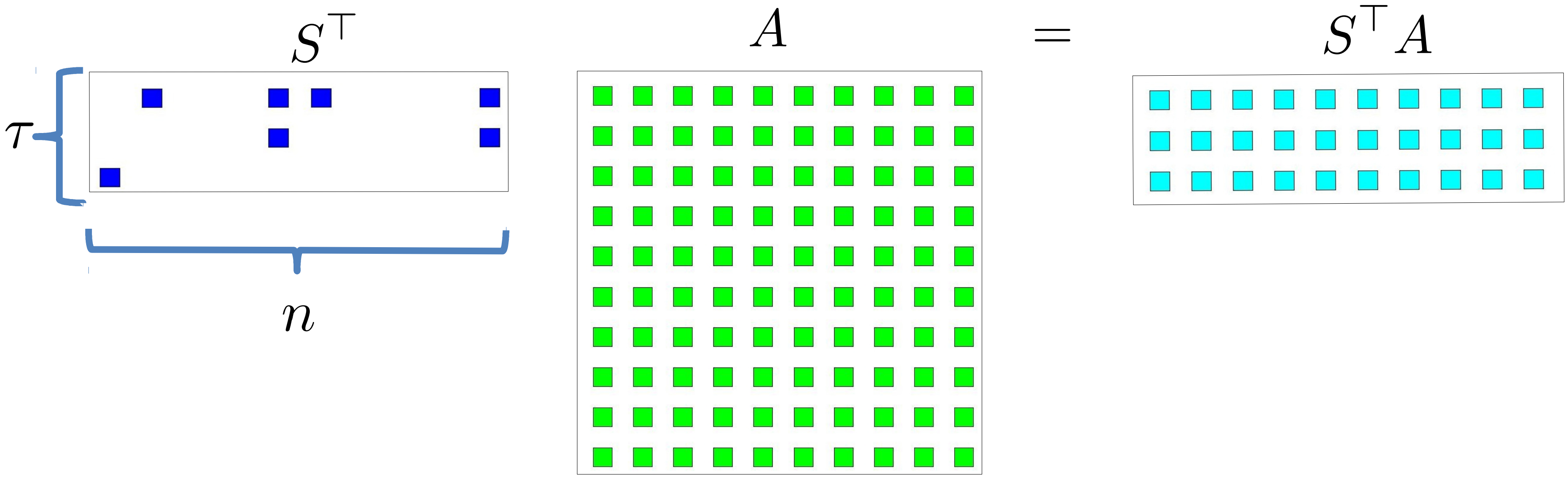
$(1)\ A^\top = A^\top A X$ or $(2)\ A^\top = XAA^\top$ or $(3)\ AXA = A$

Design three methods based on approximate stochastic projections

Use stochastic sketching to approximate the constraints

Sketching

Randomized Sketching



The Sketching Matrix

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

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

Method 1

Problem:

$$A^\dagger \quad = \quad \arg\min ||X||_F^2 \quad \text{subject to} \quad A^\top = A^\top A X$$

Sample $S \sim \mathcal{D}$

$$X_{t+1} \quad = \quad \arg\min_X ||X - X_t||_F^2 \quad \text{subject to} \quad S^\top A^\top = S^\top A^\top A X$$

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Or equivalently using duality

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Or equivalently using duality

$$X_{t+1} = \arg\min_{X,\Gamma} ||X - A^{\dagger}||_F^2 \quad \text{subject to} \quad X = X_t + A^{\top} A S \Gamma$$

Method 1

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$$X_{t+1} = X_t - A^\top A S \underbrace{(S^\top (A^\top A)^2 S)^\dagger}_{\tau \times \tau} S^\top A^\top (A X_t - I)$$

Method 1

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$$A^\dagger = \arg\min ||X||_F^2 \quad \text{subject to} \quad A^\top = A^\top A X$$

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

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Use powerful direct solver

$$X_{t+1} = X_t - A^\top A S \underbrace{(S^\top (A^\top A)^2 S)}_{\tau \times \tau}{}^\dagger S^\top A^\top (A X_t - I)$$

Linear Convergence

Theorem [GR'16]

$$\text{Let } H_S := S(S^\top (A^\top A)^2 S)^\dagger S^\top \succeq 0.$$

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If $X_0 \in \mathbf{Range}(A^\top A)$ and $\mathbf{E}[H_S] \succ 0$ then

$$\mathbf{E}[||X_t - A^\dagger||_F^2] \leq \rho^t ||X_0 - A^\dagger||_F^2$$

where

$$\rho := 1 - \lambda_{\min}^+(A^T A \mathbf{E}[H_S] A^\top A)$$

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where

Smallest nonzero eigenvalue

$$\rho := 1 - \lambda_{\min}^{+}(A^T A \mathbf{E}[H_S] A^\top A)$$

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

$$H := S(S^T(A^\top A)^2 S)^\dagger S^T$$

RMG, P. Richtarik (2016). **Stochastic Dual Ascent for Solving Linear Systems**, arXiv:1512.06890

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Special Choice of Parameters

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

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$$\mathbf{E}[H_S] \quad = \frac{1}{m}\sum_{i=1}^m \frac{e_i e_i^T}{||A^\top A_{:i}||_2^2}$$
$$= \mathrm{diag}(||A^\top A_{:i}||_2^2)$$

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No zero columns in A → $\mathbf{E}[H]$ is positive definite

RMG, P. Richtarik (2016). **Stochastic Dual Ascent for Solving Linear Systems**, arXiv:1512.06890

Interpretable Convergence

Theorem [GR'16] If $S = S_i$ with probability

$$p_i = \frac{\mathbf{Tr}(S_i^\top (A^\top A)^2 S_i)}{\mathbf{Tr}(\bar{S}^T (A^\top A)^2 \bar{S})}, \quad \text{for } i = 1, \ldots, r$$

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

$$\rho := 1 - \lambda_{\min}^{+}(A^T A \mathbf{E}[H_S] A^\top A) \leq 1 - \frac{1}{\kappa^2(A^T A \bar{S})}$$

$$\kappa^2(A^\top A \bar{S}) := \frac{\mathbf{Tr}\left(\bar{S}^\top (A^\top A)^2 \bar{S}\right)}{\lambda_{\min}(\bar{S}^\top (A^\top A)^2 \bar{S})}$$

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$\bar{S} = (A^\top A)^\dagger \approx X_t X_t^\top ?$

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Adaptive Sketching

$$\mathbf{E}[||X_t - A^\dagger||_F^2] \leq \left(1 - \boxed{\frac{\lambda_{\min}(\bar{S}^T(A^\top A)^2\bar{S})}{\mathbf{Tr}(\bar{S}^T(A^\top A)^2\bar{S})}}\right)^t ||X_0 - A^\dagger||_F^2$$

To minimize condition number:

$$\text{If } \bar{S} = A^\dagger A^{\top\dagger} \text{ then } \frac{\lambda_{\min}(\bar{S}^T(A^\top A)^2\bar{S})}{\mathbf{Tr}(\bar{S}^T(A^\top A)^2\bar{S})} = \frac{\lambda_{\min}(I)}{\mathbf{Tr}(I)} = \frac{1}{n}$$

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$$S = I_C X_t X_t^\top, \quad C \subset \{1, \dots, n\}$$

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$$X_k \to A^\dagger \quad \Longrightarrow \quad X_t X_t^\top \to A^\dagger A^{\dagger\top}$$

Didn't work well in practice

$$S = I_C X_t X_t^\top \qquad C \subset \{1, \ldots, n\}$$

Choosing the Sketching

Sample $S \sim \mathcal{D}$

$$X_{t+1} = \arg\min_{X} ||X - X_t||_F^2 \quad \text{subject to} \quad S^\top A^\top = S^\top A^\top A X$$

Adaptive method

`SATAX-ada` $\quad \mathbf{Prob}[S = X_t I_C] = 1/\binom{|C|}{n}, \quad C \subset \{1, \ldots, n\}$

Uniform coordinates

`SATAX-uni` $\quad \mathbf{Prob}[S = I_C] = 1/\binom{|C|}{n}, \quad C \subset \{1, \ldots, n\}$

Numerics

Benchmark

Symmetric Newton-Schulz

$$X_{t+1} = 2X_t - X_t A X_t$$

$$X_0 = \frac{1}{2}\frac{A^\top}{||A||_F^2} \Rightarrow ||I - X_0 A|| < 1$$

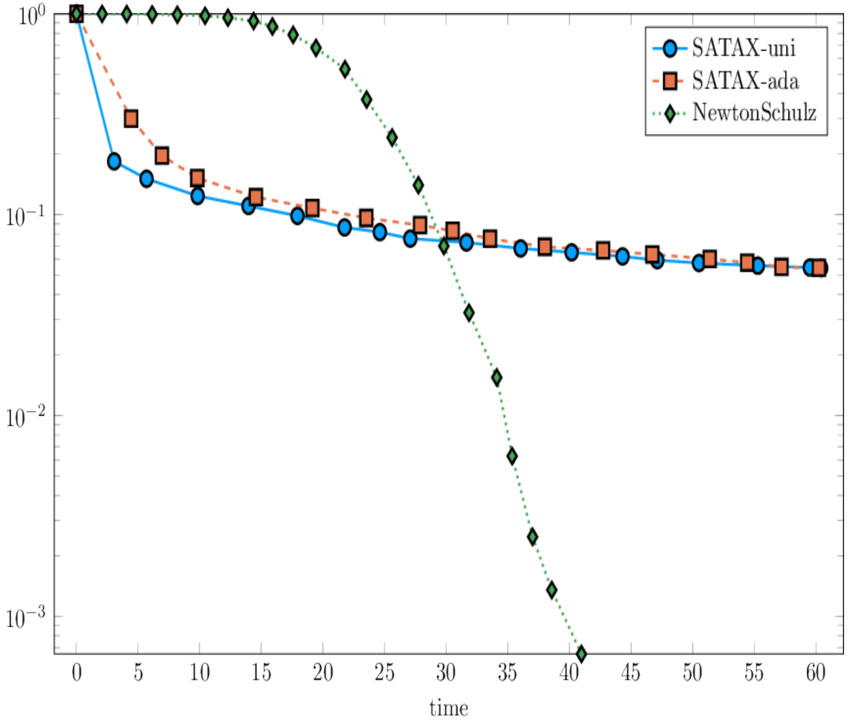
Guarantees convergence

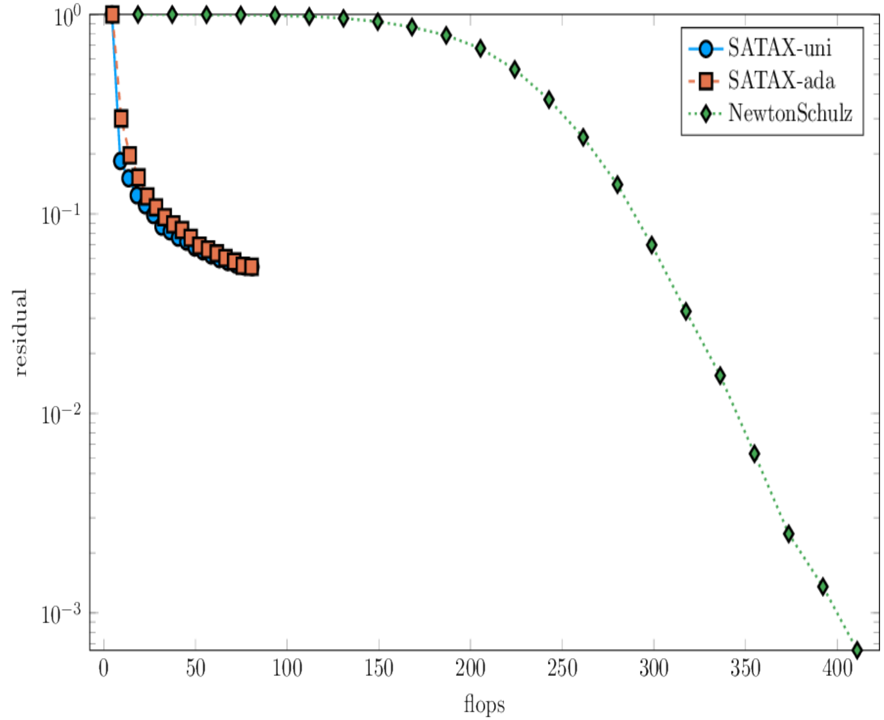
Residual

$$r_t = ||A - AX_tA||_F$$

Sparse Matrices from Engineering

UF collection



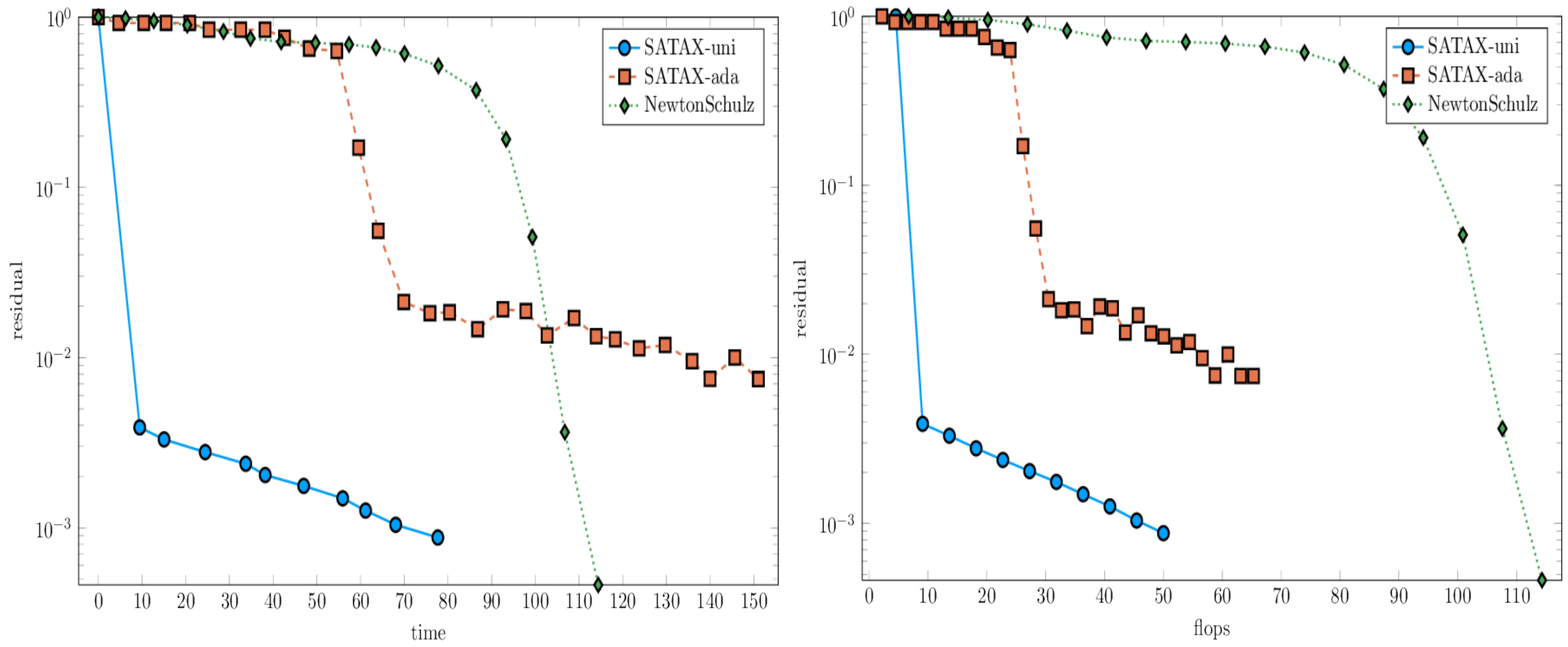


$$\tau = \lfloor \sqrt{m} \rfloor = 48$$

LPnetlib/lp ken 07 (m; n) = (2, 426; 3, 602).

Sparse Matrices from Engineering

UF collection

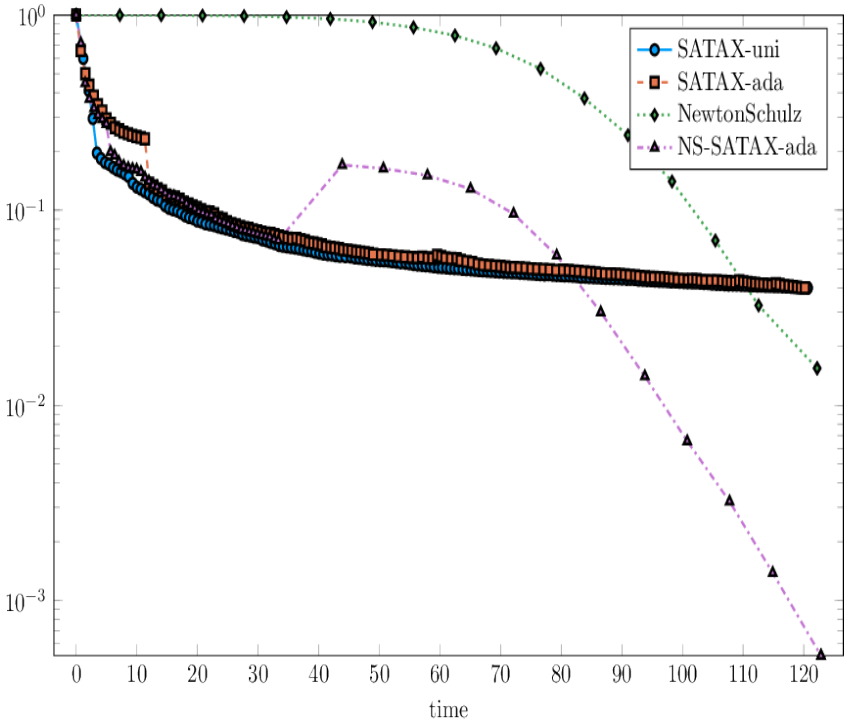


$$\tau = \lfloor \sqrt{m} \rfloor = 39$$

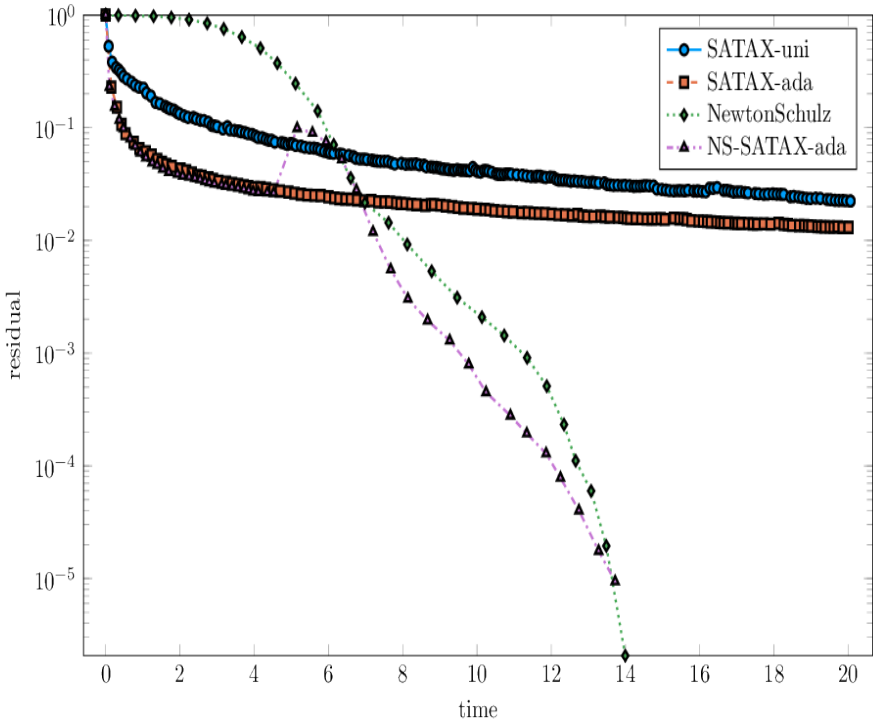
Meszaros/primagaz (m; n) = (1, 554; 10, 836)

Sparse Matrices from Engineering

UF collection



lp ken 07 (m; n) = (2, 426; 3, 602).



Maragal_3 (m; n) = (1,690; 860).

Symmetric Rank deficient Matrices $A = A^T$

The Symmetric Method

Problem:

$$\begin{aligned} A^{\dagger} \quad &= \quad \arg\min ||X||_F^2 \\ &\quad\ \text{subject to} \quad A = AXA \end{aligned}$$

The Symmetric Method

Problem:

$$A^\dagger \quad = \quad \arg\min ||X||_F^2 \quad \text{subject to} \quad A = AXA$$

Sample $S \sim \mathcal{D}$

$$X_{t+1} \quad = \quad \arg\min_{X} ||X - X_t||_F^2 \quad \text{subject to} \quad S^\top A S = S^\top A X A S$$

Or equivalently using duality

$$X_{t+1} \quad = \quad \arg\min_{X,\Gamma} ||X - A^\dagger||_F^2 \quad \text{subject to} \quad X = X_t + AS\Gamma S^\top A$$

The Symmetric Method

Problem:

$$A^\dagger = \arg\min ||X||_F^2 \quad \text{subject to} \quad A = AXA$$

Sample $S \sim \mathcal{D}$

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$$X_{t+1} = \arg\min_{X,\Gamma} ||X - A^\dagger||_F^2 \quad \text{subject to} \quad X = X_t + AS\Gamma S^\top A$$

$$X_{t+1} = X_t + AS(\underbrace{S^\top A^2 S}_{\tau \times \tau})^\dagger S^\top (A - AX_tA)S(S^\top A^2 S)^\dagger S^\top A$$

Symmetric iterates

Choosing the Sketching

Sample $S \sim \mathcal{D}$

$$\begin{aligned} X_{t+1} \quad &= \quad \arg\min_{X} ||X - X_t||_F^2 \\ &\quad \text{subject to} \quad S^\top A S = S^\top A X A S \end{aligned}$$

Adaptive method

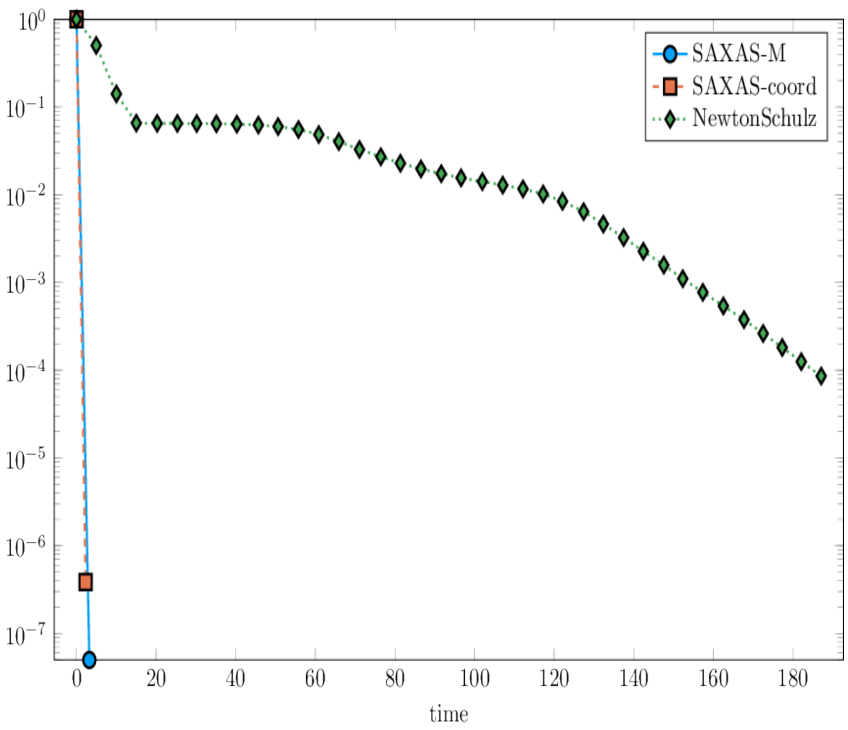
`SAXAS-ada` $\quad S = X_t I_C, \quad C \subset \{1, \ldots, n\}$

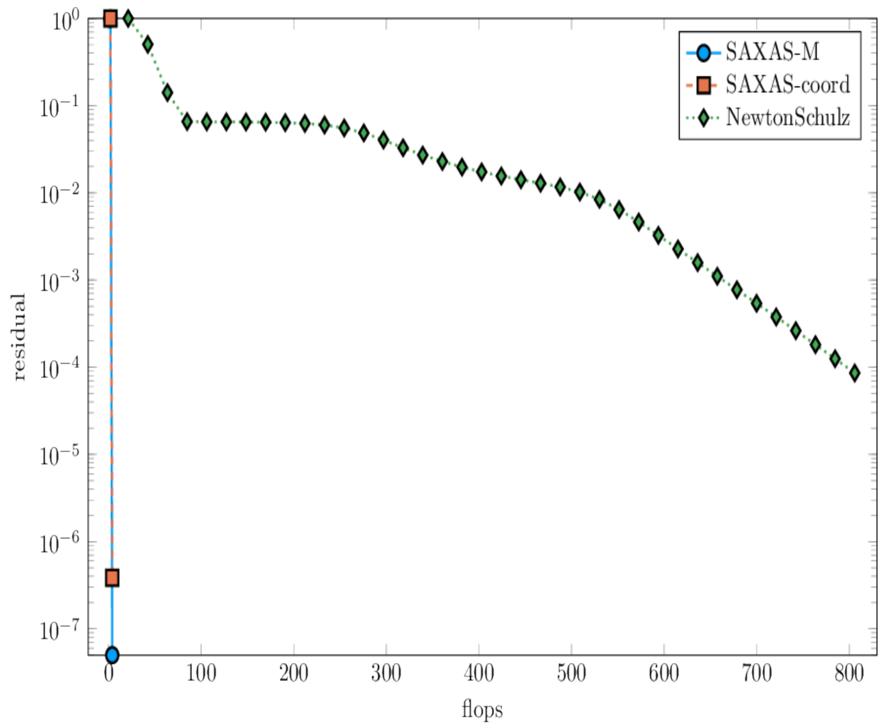
Uniform coordinates

`SAXAS-uni` $\quad S = I_C, \quad C \subset \{1, \ldots, n\}$

Hessian of linear least squares

LIBSVM data

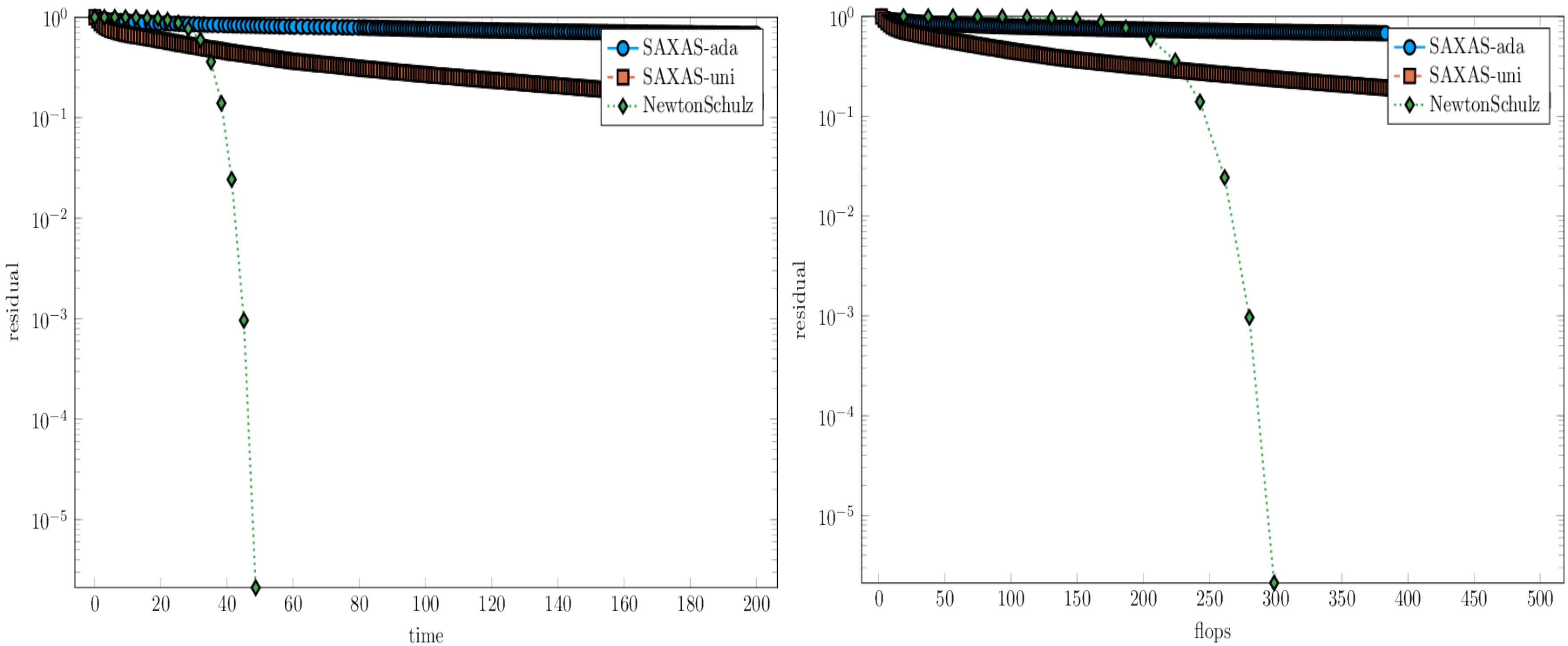




$$\tau = \lfloor \sqrt{m} \rfloor = 70$$

(gisette, n = 5,000)

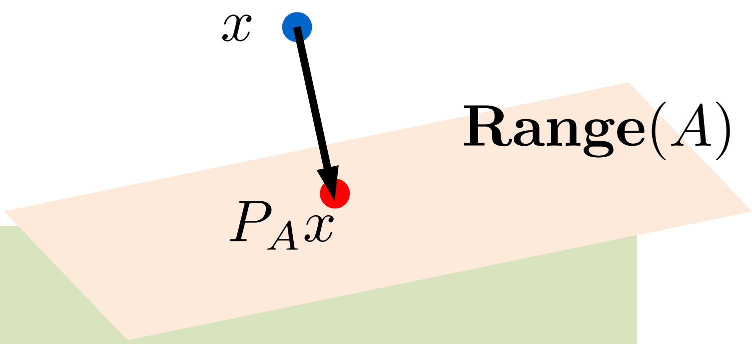
Low rank approx of Gaussian



$$\tau = \lfloor \sqrt{m} \rfloor = 70$$

(best rank 1000 approx to the matrix $G+G^T$
where G is a $5000X5000$ Gaussian matrix)

Related Problems



Range Space Projection

$$\begin{aligned} P_A \quad = \quad & \arg\min_P ||P||_F^2 \\ & \text{subject to} \quad PA = A, \quad P = P^\top, \quad P \succ 0 \end{aligned}$$

Sketch and Project

$$\begin{aligned} P_{t+1} \quad = \quad & \arg\min_P ||P - P_t||_F^2 \\ & \text{subject to} \quad PAS = AS, \quad P = P^\top, \quad P \succ 0 \end{aligned}$$

$$\mathbf{E}[||P_t - P_A||_F^2] \leq \left(1 - \frac{\lambda_{\min}(\bar{S}^T A^2 \bar{S})}{\mathbf{Tr}(\bar{S}^T A^2 \bar{S})}\right)^t ||P_0 - P_A||_F^2$$

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

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

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Randomized quasi-Newton updates are linearly convergent matrix inversion algorithms
Preprint arXiv:1602.01768, 2016

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Linearly Convergent Randomized Iterative Methods for Computing the Pseudoinverse
Preprint arXiv:1612.06255, 2016