Lecture 14: Randomized Algorithms for Least Squares Problems

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Randomized Algorithms for Least Squares Problems

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Randomized Algorithms

Solve a deterministic problem by statistical sampling

- Monte Carlo Methods
  Von Neumann & Ulam, Los Alamos, 1946

  \[ \text{circle area} \approx 4 \frac{\text{#hits}}{\text{#darts}} \]

- Simulated Annealing: global optimization
This Talk: The Ideas behind Randomized Least Squares Solvers

- Deterministic Least Squares Solvers
- Kaczmarz: An Iterative Coordinate Descent Method
- Effect of Sampling on Statistical Model Uncertainty
- How to Do Randomized Sampling
- An Overview of Randomized Least Squares/Regression
- Randomized Row-wise Compression for Dense Matrices
- A Randomized Right Preconditioner for Sparse Matrices
- Probabilistic Bound for Deviation from Orthonormality
- A few Take Aways, and Bibliography
Deterministic Least Squares Solvers
Statistics: Linear Regression

Gaussian linear model

\[ b = Ax_0 + \epsilon, \quad \epsilon \sim \mathcal{N}(0, \sigma^2 I_m) \]

**Given:** Design matrix \( A \in \mathbb{R}^{m \times n} \)
Observation vector \( b \in \mathbb{R}^m \)

**Unknown:** Parameter vector \( x_0 \in \mathbb{R}^n \)
Noise vector: \( \epsilon \) has multivariate normal distribution

**Minimize** Residual Sum of Squares

\[ \text{RSS}(x) = (b - Ax)^T (b - Ax) \quad \{\text{superscript } T \text{ is transpose}\} \]

Minimizer \( x_* \) is maximum likelihood estimator of \( x_0 \)
This talk: Well-posed least squares problems

Given: \( A \in \mathbb{R}^{m \times n} \) with \( \text{rank}(A) = n \leq m \), \( b \in \mathbb{R}^m \)
{tall and skinny \( A \) with linearly independent columns}

Solve: \( \min_x \|Ax - b\|_2 \) \{two norm\}

Unique solution (in exact arithmetic): \( x_\ast = A^\dagger b \)

Moore-Penrose inverse: \( A^\dagger \equiv (A^T A)^{-1} A^T \)

Hat matrix: \( AA^\dagger = A(A^T A)^{-1} A^T \)
orthogonal projector onto range(\( A \))

Least squares residual: \( b - Ax_\ast = (I - AA^\dagger) b \)
orthogonal projection of \( b \) onto range(\( A \))\( ^\perp \)}
Least Squares Solvers for Dense Matrices

Idea: Basis transformation $A = QR$

- $Q$ has orthonormal columns: $Q^T Q = I_n$  
  \{Orthonormal basis for range($A$)\}
- $R$ is triangular nonsingular  
  \{Easy-to-compute relation between old and new bases\}
- Left inverse simplifies: $A^\dagger = (A^T A)^{-1} A^T = R^{-1} Q^T$

Direct method:

1. Thin QR factorization $A = QR$
2. Triangular system solve $R x_\ast = Q^T b$

Operation count: $O(mn^2)$ flops
Least Squares Solvers for Sparse Matrices

LSQR [Paige & Saunders 1982]

Krylov space method for solving system with \( \begin{pmatrix} I & A \\ A^T & 0 \end{pmatrix} \)

Matrix vector products with \( A \) and \( A^T \)

Conceptually:
Solution of \( A^T A x = A^T b \) with approximations at iteration \( k \)

\[ x_k \in \text{span} \left\{ A^T b, (A^T A) A^T b, \ldots, (A^T A)^k A^T b \right\} \]

Residuals decrease \( \{ \text{in exact arithmetic} \} \)

\[ \| b - A x_k \|_2 \leq \| b - A x_{k-1} \|_2 \]

Fast convergence if condition number \( \kappa(A) \equiv \| A \|_2 \| A^\dagger \|_2 \) small

\[ \| A(x_\ast - x_k) \|_2^2 \leq 2 \left( \frac{\kappa(A) - 1}{\kappa(A) + 1} \right)^k \| A(x_\ast - x_0) \|_2^2 \]
Summary: Deterministic Least Squares Solvers

Given: $A \in \mathbb{R}^{m \times n}$ with $\text{rank}(A) = n$

Want: Unique solution $x_*$ of $\min_x \|Ax - b\|_2$

- Dense matrix $A$
  
  $A = QR$ requires $O(mn^2)$ flops
  
  Too expensive when $A$ is large or sparse
  
  QR produces fill-in

- Sparse matrix $A$
  
  Matrix vector products with $A$ and $A^T$
  
  Convergence of LSQR depends on $\kappa(A)$
  
  Need convergence acceleration (preconditioner) with low cost per iteration
Kaczmarz: An Iterative Coordinate Descent Method
Idea Behind Kaczmarz Methods

Each iteration projects on a particular equation

\[
A = \begin{pmatrix}
a_1^T \\
\vdots \\
a_m^T \\
\end{pmatrix} \in \mathbb{R}^{m \times n} \quad b = \begin{pmatrix}
b_1 \\
\vdots \\
b_m \\
\end{pmatrix} \in \mathbb{R}^m
\]

Given iterate \(x^{(k-1)}\), compute next iterate \(x^{(k)} = x^{(k-1)} + z\) so that \(x^{(k)}\) solves equation \(i\)

\[
z = e_i^T \left( b - Ax^{(k-1)} \right) \frac{a_i}{a_i^T a_i} = \frac{b_i - a_i^T x^{(k-1)}}{\|a_i\|_2^2} a_i
\]

Then \(a_i^T x^{(k)} = b_i\)
Kaczmarz Methods for Linear Systems

Input: \( A \in \mathbb{R}^{m \times n} \) with \( \text{rank}(A) = n \), \( b \in \mathbb{R}^m \), \( x^{(0)} \in \mathbb{R}^n \)
Output: Approximate solution to \( Ax_\star = b \)

for \( k = 1, 2, \ldots \) do

Choose equation \( i \)

\( x^{(k)} = x^{(k-1)} + \frac{b_i - a_i^T x^{(k-1)}}{\|a_i\|_2^2} a_i \)

end for

How to choose equation \( i \)?

- **Deterministic** [Kaczmarz 1937]
  
  Cycle through the equations: \( i = k \mod m + 1 \)

- **Randomized: Uniform Sampling** [Natterer 1986]
  
  Sample \( i \) from \( \{1, \ldots, m\} \) with probability \( 1/m \), independently and with replacement
Randomized Kaczmarz with Non-Uniform Sampling

Let $A \in \mathbb{R}^{m \times n}$ with $\text{rank}(A) = n$

Scaled condition number: $\kappa_{F,2}(A) = \|A\|_F \|A^\dagger\|_2$

Sample rows with large norms

Sample $i$ from $\{1, \ldots, m\}$ with probability $\|a_i\|^2_2/\|A\|_F^2$

independently and with replacement

Convergence in expectation

- Linear systems $Ax_* = b$ [Strohmer, Vershynin 2009]

$$\mathbb{E} \left[ \|x^{(k)} - x_*\|^2_2 \right] \leq \left( 1 - \frac{1}{(\kappa_{F,2}(A))^2} \right)^k \|x^{(0)} - x_*\|^2_2$$

- Least squares $\min_x \|Ax - b\|_2$ [Needell 2010]

$$\mathbb{E} \left[ \|x^{(k)} - x_*\|^2_2 \right] \leq \left( 1 - \frac{1}{(\kappa_{F,2}(A))^2} \right)^k \|x^{(0)} - x_*\|^2_2 + (\kappa_{F,2}(A))^2 \|b - Ax_*\|^2_\infty$$
Connections, and Related Work: A Very Small Selection

- **Sampling rows according to row norms:** Diagonal scaling for optimal condition numbers [Van der Sluis 1969]
- **Kaczmarz with relaxation factors for least squares** [Hanke, Niethammer 1990, 1995]
- **Greedy Kaczmarz-Motzkin algorithms** [Haddock, Ma 2021]
- **Randomized Gauss-Seidel for least squares** [Niu, Zheng, 2021]
- **Direct projection methods for linear systems** [Benzi, Meyer 1995]
- **Kaczmarz for detection of corrupted matrix elements** [Haddock, Needell 2019]
- **Application to medical imaging, computer tomography** [Natterer 2001]
Effect of Sampling on Statistical Model Uncertainty
Example: Effect of Sampling on Model Uncertainty

Gaussian linear model

\[ b = A \mathbf{x}_0 + \epsilon \quad A = \begin{pmatrix} 1 & 0 \\ 0 & 1 \\ 1 & 0 \\ 0 & 0 \end{pmatrix} \quad \epsilon \sim \mathcal{N}(0, \sigma^2 I_4) \]

Least squares problem \( \min_x \|Ax - b\|_2 \) has solution

\[ x^* = A^\dagger b \quad A^\dagger = (A^T A)^{-1} A^T = \begin{pmatrix} \frac{1}{2} & 0 & \frac{1}{2} & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix} \]

Solution is unbiased estimator

\[ \mathbb{E}_\epsilon [x^*] = A^\dagger \mathbb{E}_\epsilon [b] = A^\dagger A \mathbf{x}_0 = \mathbf{x}_0 \]

with nonsingular variance \( \text{Var}_\epsilon [x^*] = \sigma^2 (A^T A)^{-1} = \sigma^2 \begin{pmatrix} \frac{1}{2} & 0 \\ 0 & 1 \end{pmatrix} \)
Example: Sampling Preserves Rank

Fixed sampling matrix $S$ with $\text{rank}(SA) = \text{rank}(A)$.

$$\min_x \|S(Ax - b)\|_2$$ has unique solution $	ilde{x} = (SA)^\dagger Sb$

- Sampled matrix has full column-rank

$$SA = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & 1 \\ 1 & 0 \\ 0 & 0 \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} = (SA)^\dagger$$

- Unbiased estimator $\mathbb{E}_\varepsilon[\tilde{x}] = (SA)^\dagger S \mathbb{E}_\varepsilon[b] = x_0$

- Increase in variance

$$\mathbb{V} \text{ar}_\varepsilon[\tilde{x}] = \sigma^2 \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \approx \sigma^2 \begin{pmatrix} \frac{1}{2} & 0 \\ 0 & 1 \end{pmatrix} = \mathbb{V} \text{ar}_\varepsilon[x_*]$$
Example: Sampling Fails to Preserve Rank

Fixed sampling matrix $S$ with \( \text{rank}(SA) < \text{rank}(A) \)
\[
\min_x \|S(Ax - b)\|_2 \text{ has minimal-norm solution } \tilde{x} = (SA)^\dagger Sb
\]

- Sampled matrix is rank-deficient

\[
SA = \begin{pmatrix}
1 & 0 & 0 & 0 \\
0 & 0 & 0 & 1 \\
0 & 0 & 0 & 1 \\
1 & 0 & 0 & 0
\end{pmatrix}
= \begin{pmatrix}
1 & 0 \\
0 & 1 \\
1 & 0 \\
0 & 0
\end{pmatrix}
= (SA)^\dagger
\]

- Biased estimator \( \mathbb{E}_\epsilon[\tilde{x}] = (SA)^\dagger(SA)x_0 = \begin{pmatrix}
1 & 0 \\
0 & 0
\end{pmatrix}x_0 \neq x_0 \)

- Singular variance

\[
\mathbb{V}
\text{ar}_\epsilon[\tilde{x}] = \sigma^2 \begin{pmatrix}
1 & 0 \\
0 & 0
\end{pmatrix} \neq \sigma^2 \begin{pmatrix}
\frac{1}{2} & 0 \\
0 & 1
\end{pmatrix} = \mathbb{V}
\text{ar}_\epsilon[x_*]
\]
Summary: Effect of Sampling on Model Uncertainty

\[ \min_x \|S(Ax - b)\|_2 \] has minimal-norm solution \( \tilde{x} = (SA)^\dagger (Sb) \) with expectation \( \mathbb{E}_\epsilon [\tilde{x}] = (SA)^\dagger (SA)x_0 \)

- If \( S \) preserves rank: \( \text{rank}(SA) = \text{rank}(A) \)
  - \( (SA)^\dagger \) is left inverse: \( (SA)^\dagger (SA) = I \)
  - \( \tilde{x} \) is unbiased estimator: \( \mathbb{E}_\epsilon [\tilde{x}] = x_0 \)

- If \( S \) loses rank: \( \text{rank}(SA) < \text{rank}(A) \)
  - No left inverse: \( (SA)^\dagger (SA) \neq I \)
  - \( \tilde{x} \) is biased estimator: \( \mathbb{E}_\epsilon [\tilde{x}] \neq x_0 \)
  - Variance \( \text{Var}_\epsilon [\tilde{x}] \) is singular

This was a best case analysis: A fixed sampling matrix \( S \).
We did not incorporate the uncertainty due to randomization.
How to do Randomized Sampling
Sample $t$ from $\{1, \ldots, m\}$ with probability $p_t$

- **Uniform sampling:** $p_i = 1/m$, $1 \leq i \leq m$
  
  $\nu = \text{rand} \quad \{\text{uniform [0,1] random variable}\}$
  
  $t = \lfloor 1 + m\nu \rfloor$

- **Non-uniform sampling:**
  
  $\nu = \text{rand}$, $t = 1$, $F = p_1$
  while $\nu > F$
  
  $t = t + 1$, $F = F + p_t$

  Inversion by sequential search: $F(i) \equiv \sum_{j=1}^{i} p_j$ so that $p_i = F(i) - F(i - 1)$
  
  $t$ defined by $F(t - 1) < \nu \leq F(t)$

**Matlab:** randi, datasample

**R:** sample
Different Sampling Methods

Want: Sampling matrix $S$ with $\mathbb{E}[S^T S] = I_m$

1. **Uniform sampling with replacement**
   
   Sample $k_t$ from $\{1, \ldots, m\}$ with probability $\frac{1}{m}$, $1 \leq t \leq c$
   
   $$S = \sqrt{\frac{m}{c}} (e_{k_1} \ldots e_{k_c})^T$$

2. **Uniform sampling without replacement**
   
   Let $k_1, \ldots, k_m$ be a permutation of $1, \ldots, m$
   
   $$S = \sqrt{\frac{m}{c}} (e_{k_1} \ldots e_{k_c})^T$$

3. **Bernoulli sampling**
   
   $$S(t,:) = \sqrt{\frac{m}{c}} \begin{cases} 
   e_t^T & \text{with probability } \frac{c}{m} \\
   0_{1 \times m} & \text{with probability } 1 - \frac{c}{m}
   \end{cases} \quad 1 \leq t \leq m$$

   Alternative simulation:
   
   Sample $\tilde{c}$ from $\{1, \ldots, m\}$ with $\mathbb{P}[\tilde{c} = k] = \binom{m}{k} \left(\frac{c}{m}\right)^k \left(1 - \frac{c}{m}\right)^{m-k}$
   
   Sample $k_1, \ldots, k_{\tilde{c}}$ without replacement
Comparison of Different Sampling Methods

Sampling rows from matrices with orthonormal columns
$10^4 \times 5$ matrices $Q$ with $Q^T Q = I$

Plots for $5 \leq c \leq 10^4$

1. Percentage of numerically rank-deficient $SQ$ \[ \{ \kappa(SQ) \geq 10^{16} \} \]
2. Condition number of full column-rank $SQ$
\[ \kappa(SQ) = \|SQ\|_2 \|(SQ)^\dagger\|_2 \]
Comparison of Sampling Methods

Sampling with replacement

Sampling without replacement

Bernoulli sampling
Summary:
Comparison of Different Sampling Methods

Three different sampling methods:
- Uniform sampling with replacement
- Uniform sampling without replacement
- Bernoulli sampling

Conclusion:
*Little difference* among sampling methods for small amounts of sampling

From now on:
Use sampling *with* replacement
An Overview of Randomized Least Squares/Regression
Randomized Least Squares/Regression

(Solvers mostly not ready for production yet)

\[
\min_{x \in \mathbb{R}^n} \|Ax - b\|_2 \text{ for } A \in \mathbb{R}^{m \times n} \text{ with } m \geq n
\]

Direct methods require \(O(mn^2)\) flops

Classification [Thanei, Heinze, Meinshausen 2017]

- **Row-wise** compression: \(\min_{x \in \mathbb{R}^n} \|S(Ax - b)\|_2\)
  \(S \in \mathbb{R}^{c \times m}\) with \(c \leq m\)
  Solver requires \(O(cn^2)\) flops after compression

- **Column-wise** compression: \(\min_{y \in \mathbb{R}^c} \|ASy - b\|_2\)
  \(S \in \mathbb{R}^{n \times c}\) with \(c \leq n\)
  Solver requires \(O(mc^2)\) flops after compression

**Special case**: \(S \in \mathbb{R}^{n \times n}\) nonsingular
  Right preconditioning to accelerate iterative methods
Existing Work

Row-wise compression

Bartels, Hennig (2016); Becker, Jawas, Patrick, Ramamurthy (2017)
Boutsidis, Drineas (2009); Dhillon, Lu, Foster, Ungar (2013)
Drineas, Mahoney, Muthukrishnan (2006)
Drineas, Mahoney, Muthukrishnan, Sarlós (2011)
Ipsen, Wentworth (2014)
McWilliams, Krummenacher, Lučič, Buhmann (2014)
Meng, Saunders, Mahoney (2014); Wang, Zhu, Ma (2018)

Column-wise compression

Kabán (2014); Mallard, Munos (2009)
Meng, Saunders, Mahoney (2014)
Thanei, Heinze, Meinshausen (2017)

Right preconditioning

Avron, Maymounkov, Toledo (2010)
Ipsen, Wentworth (2014); Rokhlin, Tygert (2008)

Statistical properties

Ahfock, Astle, Richardson (2017); Chi, Ipsen (2020)
Lopes, Wang, Mahoney (2018); Ma, Mahoney, Yu (2014, 2015)
Raskutti, Mahoney (2016); Thanei, Heinze, Meinshausen (2017)
Randomized Row-Wise Compression for Dense Matrices
Uniform Sampling with Replacement

[Drineas, Kannan & Mahoney 2006]

\( S \in \mathbb{R}^{c \times m} \) samples \( c \) rows from identity \( I_m = \begin{pmatrix} e_1^T \\ \vdots \\ e_m^T \end{pmatrix} \)

for \( t = 1 : c \) do
  Sample \( k_t \) from \( \{1, \ldots, m\} \) with probability \( 1/m \) independently and with replacement
end for

Sampling matrix \( S = \sqrt{\frac{m}{c}} \begin{pmatrix} e_{k_1}^T \\ \vdots \\ e_{k_c}^T \end{pmatrix} \)

- Expected value \( \mathbb{E} [S^T S] = I_m \)
- \( S \) can sample a row more than once
Example: Uniform Sampling with Replacement

Sample 2 out of 4 rows: $m = 4$, $c = 2$, $\sqrt{\frac{m}{c}} = \sqrt{2}$

$$A = \begin{pmatrix} 1 & 0 \\ 0 & 1 \\ 1 & 0 \\ 0 & 0 \end{pmatrix}, \quad S^{(ij)} = \sqrt{2} \begin{pmatrix} e_i^T \\ e_j^T \end{pmatrix}, \quad 1 \leq i, j \leq 4$$

Examples of sampled matrices

$$S^{(11)} A = \sqrt{2} \begin{pmatrix} 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & 1 \\ 1 & 0 \\ 0 & 0 \end{pmatrix} = \sqrt{2} \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}$$

$$S^{(42)} A = \sqrt{2} \begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 1 & 0 & 0 \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & 1 \\ 1 & 0 \\ 0 & 0 \end{pmatrix} = \sqrt{2} \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}$$

Sampling matrices are unbiased estimators of identity

$$\mathbb{E}[S^T S] = \sum_{i=1}^{4} \sum_{j=1}^{4} \frac{1}{16} \left(S^{(ij)}\right)^T S^{(ij)} = I_4$$
Row Sampling Algorithm for $\min_{x \in \mathbb{R}^n} \|Ax - b\|_2$

Special case of [Drineas, Mahoney, Muthukrishnan, Sarlós, 2011]

Input: $A \in \mathbb{R}^{m \times n}$ with $\text{rank}(A) = n$, $b \in \mathbb{R}^m$

$c \geq 1$ \{sampling amount\}

$S = 0_{c \times m}$ \{initialize sampling matrix\}

for $t = 1 : c$ do

Sample $k_t$ from $\{1, \ldots, m\}$ with probability $1/m$

independently and with replacement

$S(t,:) = \sqrt{\frac{m}{c}} e_{k_t}^T$ \{row $t$ of sampling matrix\}

end for

Output: Minimal norm solution $\tilde{x}$ of $\min_x \|S(Ax - b)\|_2$
Error due to Randomization

Derivation in two steps

1. Structural bound:
   Treat sampling matrix $SA$ as fixed perturbation
   Carry deterministic analysis as far as possible

2. Probabilistic bound:
   Treat sampled matrix $SA$ as random matrix
   Use matrix concentration inequalities
**Structural Bound: Absolute Error**

- Exact solution \( x_* = A^\dagger b \)
- Randomized solution \( \tilde{x} = (SA)^\dagger Sb \)
  
  Assume: \( \text{rank}(SA) = \text{rank}(A) \)

- Change of basis: \( A = QR \)

- Geometric interpretation of error

\[
\tilde{x} - x_* = (SA)^\dagger Sb - A^\dagger b = A^\dagger Q(SQ)^\dagger S (b - Ax_*)
\]

\( Q(SQ)^\dagger S \) is oblique projector onto range\((A)\)

\( b - Ax_* \) is exact least squares residual

- If \( \|S(b - Ax_*)\|_2 \leq (1 + \epsilon)\|b - Ax_*\|_2 \) then

\[
\|\tilde{x} - x_*\|_2 \leq (1 + \epsilon)\|A^\dagger\|_2\|(SQ)^\dagger\|_2\|b - Ax_*\|_2
\]
Structural Bound: Relative Error

[Drineas, Mahoney, Muthukrishnan, Sarlós, 2011]

If \( \text{rank}(SA) = n \) and \( \| S(b - Ax_*) \|_2 \leq (1 + \epsilon) \| b - Ax_* \|_2 \) then

\[
\frac{\| \tilde{x} - x_* \|_2}{\| x_* \|_2} \leq (1 + \epsilon) \| (SQ)^\dagger \|_2 \kappa(A) \frac{\| b - Ax_* \|_2}{\| A \|_2 \| x_* \|_2}
\]

\( \kappa(A) = \| A \|_2 \| A^\dagger \|_2 \) condition of \( A \) w.r.t. left inversion

- Relative error depends only on \( \kappa(A) \) but not \( \kappa(A)^2 \)
- Sensitivity to multiplicative perturbations from randomization is lower than sensitivity to deterministic additive perturbations
- Probabilistic bound for \( \| (SQ)^\dagger \|_2 \)

Has to take care of \( \text{rank}(SA) = n \), and quantify \( \epsilon \)
Towards a Probabilistic Bound

Given $A \in \mathbb{R}^{m \times n}$ with $\text{rank}(A) = n$

$$\frac{\|\tilde{x} - x_*\|_2}{\|x_*\|_2} \leq (1 + \epsilon) \|(SQ)\|_2 \kappa(A) \frac{\|b - Ax_*\|_2}{\|A\|_2\|x_*\|_2}$$

- For the analysis (but not computed): $A = QR$
  where $Q \in \mathbb{R}^{m \times n}$ with $Q^T Q = I$

- Idea: $SA = (SQ) R$
  Sampling rows from $A$ amounts to sampling rows from $Q$

- Simplify the analysis to $SQ$:
  Sampling rows from matrices $Q$ with orthonormal columns

Before doing the analysis:
Look at a randomized solver for sparse matrices, which faces the same situation
A Randomized Right Preconditioner for Sparse Matrices
Right Preconditioning LSQR

Convergence acceleration for LSQR applied to \( \min_x \|Ax - b\|_2 \)

Right preconditioning = change of variables

\[
\min_y \|AP^{-1}(Px) - b\|_2
\]

1. \( \min_y \|AP^{-1}y - b\|_2 \) \( \{ \text{Solve preconditioned problem} \} \)
2. Solve \( PX^* = y \) \( \{ \text{Retrieve solution to original problem} \} \)

Requirements for preconditioner \( P \)

Fast convergence: \( \kappa(AP^{-1}) \approx 1 \)
Linear systems with \( P \) are cheap to solve
The Ideal Right Preconditioner

- QR factorization $A = QR$, $Q^TQ = I_n$, $R$ is \triangle

- Use $R$ as preconditioner

- Preconditioned matrix $AR^{-1} = Q$
  - Orthonormal columns
  - Perfect condition number $\kappa(Q) = 1$

- LSQR solves pre-conditioned system in 1 iteration

But:

This is what we are trying to avoid in the first place
Construction of preconditioner is way too expensive
A Randomized Preconditioner

Idea: QR factorization from a few rows of $m \times n$ matrix $A$

1. Sample $c \geq n$ rows of $A$: $SA$

2. QR factorization of sampled matrix

$$SA = Q_s R_s \quad Q_s^T Q_s = I_n, \ R_s \text{ is } \triangle$$

3. Randomized preconditioner $R_s^{-1}$

Operation count: $\mathcal{O}(cn^2)$ \{independent of large dimension $m$\}
QR Factorization from a Few Rows

\[ A = QR \]

\[ SA = Q_s R_s \]
Input: $m \times n$ matrix with $\text{rank}(A) = n$, $m \times 1$ vector $b$
Sampling amount $c \geq n$
Output: Solution $x_*$ to $\min_x \|Ax - b\|_2$

\{Construct preconditioner\}
Sample $c$ rows of $A \rightarrow SA$ \{fewer rows\}
QR factorization $SA = Q_s R_s$

\{Solve preconditioned problem\}
Solve $\min_y \|AR_s^{-1} y - b\|_2$ with LSQR
Solve $R_s x_* = y$ \{$\triangle$ system\}

We hope:

$AR_s^{-1}$ has almost orthonormal columns
Condition number almost perfect: $\kappa(AR_s^{-1}) \approx 1$
Two QR factorizations

- **Computed factorization of sampled matrix:** $SA = Q_s R_s$
- **Conceptual factorization of full matrix:** $A = QR$

Idea

1. **Sampling rows of $A$** $\triangleq$ **Sampling rows of $Q$**

   $$\text{rank}(SA) = \text{rank}(SQ)$$

2. **Condition number of preconditioned matrix (2-norm)**

   $$\kappa(AR_s^{-1}) = \kappa(SQ)$$

Simpler problem

**Sample from matrices with orthonormal columns**
Sampling from Matrices with Orthonormal Columns
What To Expect

Given: $Q \in \mathbb{R}^{8 \times 2}$ with $Q^T Q = I$

Want: Sampled matrix $SQ$ with $\text{rank}(SQ) = 2$

Which one is easier?

$Q = \begin{pmatrix}
1 & 0 \\
0 & 1 \\
0 & 0 \\
0 & 0 \\
0 & 0 \\
0 & 0 \\
0 & 0 \\
0 & 0
\end{pmatrix}$

versus

$Q = \frac{1}{\sqrt{8}} \begin{pmatrix}
1 & 1 \\
1 & 1 \\
1 & 1 \\
1 & -1 \\
1 & -1 \\
1 & -1 \\
1 & -1
\end{pmatrix}$
Sampling from Matrices with Orthonormal Columns

What To Expect

Given: \( Q \in \mathbb{R}^{8 \times 2} \) with \( Q^T Q = I \)
Want: Sampled matrix \( SQ \) with \( \text{rank}(SQ) = 2 \)
Which one is easier?

\[
Q = \begin{pmatrix}
1 & 0 \\
0 & 1 \\
0 & 0 \\
0 & 0 \\
0 & 0 \\
0 & 0 \\
0 & 0 \\
0 & 0 \\
\end{pmatrix}
\quad \text{versus} \quad
Q = \frac{1}{\sqrt{8}} \begin{pmatrix}
1 & 1 \\
1 & 1 \\
1 & 1 \\
1 & 1 \\
1 & -1 \\
1 & -1 \\
1 & 1 \\
1 & -1 \\
\end{pmatrix}
\]

Row norms (squared)
\[
\| e_1^T Q \|_2^2 = \| e_2^T Q \|_2^2 = 1 \\
\| e_j^T Q \|_2^2 = 0 \quad \text{for } j \geq 3 \\
\| e_j^T Q \|_2^2 = \frac{2}{8} = \frac{1}{4} \quad \text{for all } j
\]
Sampling from Matrices with Orthonormal Columns

\[ Q \in \mathbb{R}^{8 \times 2} \text{ with } Q^T Q = I \]

\[
Q = \begin{pmatrix}
1 & 0 \\
0 & 1 \\
0 & 0 \\
0 & 0 \\
0 & 0 \\
0 & 0 \\
0 & 0 \\
0 & 0
\end{pmatrix}
\quad Q = \frac{1}{\sqrt{8}} \begin{pmatrix}
1 & 1 \\
1 & 1 \\
1 & 1 \\
1 & 1 \\
1 & -1 \\
1 & -1 \\
1 & -1 \\
1 & -1
\end{pmatrix}
\]

\[ \max_j \| e_j^T Q \|_2^2 = 1 \quad \max_j \| e_j^T Q \|_2^2 = \frac{1}{4} \]

Sampling is hard

Sampling is easy

Largest row norm distinguishes matrices with orthonormal columns

Use it to quantify difficulty of sampling
Probabilistic Bound for Deviation from Orthonormality
Deviation of $SQ$ from Orthonormality

Given $0 \leq \epsilon < 1$, want sampling amount $c \geq n$ so that

$$\| (SQ)^T (SQ) - I \|_2 \leq \epsilon$$

This implies for the singular values of $SQ \in \mathbb{R}^{c \times n}$

$$1 - \epsilon \leq \sigma_j(SQ)^2 \leq 1 + \epsilon, \quad 1 \leq j \leq n$$

Therefore

- **$SQ$ has full column-rank:** $\min_j \sigma_j(SQ) \geq \sqrt{1 - \epsilon} > 0$
- **Left inverse exists and is bounded**

$$\| (SQ)^\dagger \|_2 = \frac{1}{\min_j \sigma_j(SQ)} \leq \frac{1}{\sqrt{1 - \epsilon}}$$

- **Condition number is bounded**

$$\kappa_2(SQ) = \| SQ \|_2 \| (SQ)^\dagger \|_2 = \frac{\max_j \sigma_j(SQ)}{\min_j \sigma_j(SQ)} \leq \frac{\sqrt{1 + \epsilon}}{\sqrt{1 - \epsilon}}$$
Matrix Bernstein Concentration Inequality  [Recht 2011]

Assume

- Zero-mean: Independent random $n \times n$ matrices $Y_t$ with $\mathbb{E}[Y_t] = 0_{n \times n}$
- Boundedness: $\|Y_t\|_2 \leq \tau$ almost surely
- Variance: $\rho_t \equiv \max\{\|\mathbb{E}[Y_t Y_t^T]\|_2, \|\mathbb{E}[Y_t^T Y_t]\|_2\}$
- Desired error tolerance: $0 < \epsilon < 1$
- Failure probability: $\delta = 2n \exp \left( -\frac{3}{2} \frac{\epsilon^2}{3 \sum_t \rho_t + \tau \epsilon} \right)$

Then with probability at least $1 - \delta$

$$\left\| \sum_t Y_t \right\|_2 \leq \epsilon \quad \{\text{Deviation from mean}\}$$
Apply the Concentration Inequality

Sampled matrix

\[
Q^T S^T SQ = X_1 + \cdots + X_c, \quad X_t = \frac{m}{c} Q^T e_{kt} e_{kt}^T Q
\]

Zero-mean version

\[
Q^T S^T SQ - I_n = Y_1 + \cdots + Y_c, \quad Y_t = X_t - \frac{1}{c} I_n
\]

Check assumptions

- Zero mean: \( \mathbb{E}[Y_t] = 0 \) \{by construction\}
- Boundedness: \( \|Y_t\|_2 \leq \frac{m}{c} \mu \)
- Variance: \( \|\mathbb{E}[Y_t^2]\|_2 \leq \frac{m}{c^2} \mu \)

Largest row norm squared: \( \mu = \max_{1 \leq j \leq m} \|e_j^T Q\|_2^2 \)

Deviation of \( SQ \) from orthonormality:
With probability at least \( 1 - \delta \),
\[ \|(SQ)^T (SQ) - I_n\|_2 \leq \epsilon \]
Assume

- $m \times n$ matrix $Q$ with $Q^T Q = I_n \quad \{\text{orthonormal columns}\}$
- Largest row norm squared: $\mu = \max_{1 \leq j \leq m} \|e_j^T Q\|_2^2$
- Number of sampled rows: $c \geq n$
- Desired error tolerance: $0 < \epsilon < 1$
- Failure probability

$$\delta = 2n \exp \left(-\frac{c}{m \mu} \frac{\epsilon^2}{3 + \epsilon} \right)$$

Then with probability at least $1 - \delta$

Condition number of sampled matrix $\kappa(SQ) \leq \sqrt{\frac{1+\epsilon}{1-\epsilon}}$
Tightness of Condition Number Bound

Input: $m \times n$ matrix $Q$ with $Q^T Q = I_n$ \{orthonormal columns\}

$$m = 10^4, \quad n = 5, \quad \mu = 1.5 \frac{n}{m}$$

Investigate: $c \times n$ matrix $SQ$ \{sampling with replacement\}

Little sampling: $n \leq c \leq 1000$
A lot of sampling: $1000 \leq c \leq m$

Plots:

1. Exact condition number $\kappa(SQ)$

2. Bound $\kappa(SQ) \leq \sqrt{\frac{1 + \epsilon}{1 - \epsilon}}$ with probability $1 - \delta \equiv .99$

$$\epsilon \equiv \frac{1}{2c} \left( \ell + \sqrt{12c\ell + \ell^2} \right)$$

$$\ell \equiv \frac{2}{3} \left( m \mu - 1 \right) \ln\left(2n/\delta\right) = \Omega \left( m \mu \ln n \right)$$
Little sampling \((n \leq c \leq 1000)\)

Exact condition numbers \(\kappa(SQ)\)

Bound holds starting from \(c \geq 93 \approx 3\ell = \Omega(m\mu\ln n)\)
A lot of sampling \((1000 \leq c \leq m)\)

Bound predicts correct magnitude of condition numbers
Conclusions for Condition Number Bound

Given: $m \times n$ matrix $Q$ with $Q^T Q = I_n$ \{orthonormal columns\}
Sampling: $c \times n$ matrix $SQ$

Bound on condition number $\kappa(SQ)$ of sampled matrix:

- Correct magnitude
- Informative even for small matrix dimensions and stringent success probabilities
- Implies lower bound on number of sampled rows

$$c = \Omega (m \mu \ln n)$$

- Depends on coherence of $Q$: $\mu = \max_{1 \leq j \leq m} \| e_j^T Q \|_2^2$
  Largest squared row norm of $Q$
  Reveals distribution of mass in $Q$
Coherence
Properties of Coherence

Coherence of $m \times n$ matrix $Q$ with $Q^TQ = I_n \quad \{\text{orthonormal columns}\}$

$$\mu = \max_{1 \leq j \leq m} \|e_j^TQ\|_2^2$$

- $n/m \leq \mu(Q) \leq 1$
- **Maximal coherence:** $\mu(Q) = 1$
  At least one column of $Q$ is column of identity
- **Minimal coherence:** $\mu(Q) = n/m$
  Columns of $Q$ are columns of Hadamard matrix

Definition can be extended to: general matrices, subspaces
Properties of Coherence

Coherence of $m \times n$ matrix $Q$ with $Q^T Q = I_n$ \{orthonormal columns\}

$$\mu = \max_{1 \leq j \leq m} \|e_j^T Q\|_2^2$$

- $n/m \leq \mu(Q) \leq 1$
- **Maximal** coherence: $\mu(Q) = 1$
  At least one column of $Q$ is column of identity
- **Minimal** coherence: $\mu(Q) = n/m$
  Columns of $Q$ are columns of Hadamard matrix

Coherence
- Measures **correlation with standard basis**
- Reflects difficulty of **recovering** the matrix from **sampling**
The Origins of Coherence

- Donoho & Huo 2001
  Mutual coherence of two bases

- Candés, Romberg & Tao 2006

- Candés & Recht 2009
  Matrix completion: Recovering a low-rank matrix by sampling its entries

- Mori & Talwalkar 2010, 2011
  Estimation of coherence

- Avron, Maymounkov & Toledo 2010
  Randomized preconditioners for least squares

- Drineas, Magdon-Ismail, Mahoney & Woodruff 2011
  Fast approximation of coherence
Effect of Coherence on Sampling

Input: $m \times n$ matrix $Q$ with $Q^T Q = I_n$ \{orthonormal columns\}  
$m = 10^4, \ n = 5$

Investigate: $c \times n$ matrix $SQ$ \{sampling with replacement\}

Question: How does coherence of $Q$ affect sampling?

Two types of matrices $Q$

1. Low coherence: $\mu = 7.5 \cdot 10^{-4} = 1.5 \ n/m$
2. Higher coherence: $\mu = 7.5 \cdot 10^{-2} = 150 \ n/m$

Plots for $n \leq c \leq 1000$

1. Percentage of numerically rank-deficient $SQ$ \{$\kappa(SQ) \geq 10^{16}$\}
2. Condition number of full column-rank $SQ$

$$\kappa(SQ) = \| SQ\|_2 \| (SQ)^\dagger \|_2$$
Sampling Rows from $Q$ with Low Coherence

Only a single matrix $SQ$ is rank-deficient (for $c = 5$)

Full-rank matrices $SQ$ perfectly conditioned: $κ(SQ) < 4$
Sampling Rows from $Q$ with Higher Coherence

Sampling up to 10% of rows:

Most matrices $SQ$ are rank-deficient

Full-rank matrices $SQ$ perfectly conditioned: $\kappa(SQ) \leq 5$
Effect of Coherence on Sampling: Conclusions

Given: \( m \times n \) matrix \( Q \) with \( Q^T Q = I_n \) \{orthonormal columns\}

Investigate: \( c \times n \) sampled matrix \( SQ \)

\( Q \) has low coherence \( \mu \approx n/m \)
- Most \( SQ \) full-rank and perfectly conditioned \{even for small \( c \}\)
- Mass of \( Q \) uniformly distributed \{it does not matter what you pick\}
- Sampling is easy

\( Q \) has higher coherence \( \mu \approx 100n/m \)
- Most \( SQ \) rank-deficient \{even for larger \( c \}\)
- Mass of \( Q \) concentrated in a few spots \{you have to be lucky\}
- Sampling is hard
A Few Take Aways for Randomized Least Squares Solvers

\[ \min_x \|Ax - b\|_2 \]

- Sampling is effective if \( A \) has good coherence ('uniformity')
- Powerful matrix concentration inequalities are important
- Not discussed: Improving coherence with fast multiplication by random matrix
- The 'safe' randomized LS solver: *Blendenpik*
  Randomization confined to preconditioner

Research questions
- Numerical behavior in floating point arithmetic
- Effect of sampling on statistical model uncertainty
- Flexible preconditioners that can change in every iteration
- Regularization for ill-posed problems
Resources: Surveys and Books

- L. Devroye: *Nonuniform Random Variate Generation*  
  Springer-Verlag (1986)

- M. Mitzenmacher and E. Upfal:  

- R. Vershynin:  

- J. A. Tropp: *An Introduction to Matrix Concentration Inequalities*  

- N. Halko, P.G. Martinsson and J.A. Tropp:  
  *Finding Structure with Randomness: Probabilistic Algorithms for Constructing Approximate Matrix Decompositions*  

- M.W. Mahoney: *Randomized Algorithms for Matrices and Data*  
Resources: Papers Discussed in this Talk

- H. Avron, P. Maymounkov, and S. Toledo
  **Blendenpik: Supercharging Lapack’s Least-Squares Solver**

- P. Drineas, M.W. Mahoney, S. Muthukrishnan, and T. Sarlós
  **Faster Least Squares Approximation**

- I.C.F. Ipsen and T. Wentworth
  **The Effect of Coherence on Sampling from Matrices with Orthonormal Columns, and Preconditioned Least Squares Problems**

- J.T. Chi and I.C.F. Ipsen
  **Multiplicative Perturbation Bounds for Multivariate Multiple Linear Regression in Schatten p-Norms**
  Linear Algebra Appl. (to appear)

- J.T. Chi and I.C.F. Ipsen
  **A Projector-Based Approach to Quantifying Total and Excess Uncertainties for Sketched Linear Regression**
  arXiv:1808.0594