Numerical Issues in Randomized Algorithms: Effect of Sampling on Condition Numbers

Ilse Ipsen

Joint work with Thomas Wentworth

North Carolina State University
Raleigh, NC, USA

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This Talk

Given:

- Real $m \times n$ matrix Q with orthonormal columns, $Q^T Q = I$
- Real $c \times m$ "sampling" matrix S with $c \ll m$
- Desired error $0 < \epsilon < 1$

Want: Probability that

$$\|(SQ)^T(SQ) - I\|_2 \le \epsilon$$
$$\kappa(SQ) = \|SQ\|_2 \, \|(SQ)^\dagger\|_2 \le \sqrt{\tfrac{1+\epsilon}{1-\epsilon}}$$

Motivation: Randomized preconditioned LS solver *Blendenpik*
[Avron, Maymounkov & Toledo 2010]

$\kappa(SQ) =$ Condition number of preconditioned matrix

Outline

1. Exactly(c) sampling
2. Sampling rows from matrices with orthonormal columns
3. Important property: Coherence
4. Probabilistic condition number bound for sampled matrices
5. Improving on coherence: Leverage scores
6. Summary

Exactly(c) Sampling [Drineas, Kannan & Mahoney 2006]

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

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

- S is $c \times m$, and samples *exactly* c rows
- Expected value $\mathbf{E}(S^T S) = I$
- S can sample a row more than once

Sampling from Matrices with Orthonormal Columns

Example: $m = 6,\ n = 2,\ c = 3$

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

Prob$[SQ$ has full rank$] \approx 11\%$

$$Q = \begin{pmatrix} 1/\sqrt{6} & -1/\sqrt{6} \\ 1/\sqrt{6} & 1/\sqrt{6} \\ 1/\sqrt{6} & -1/\sqrt{6} \\ 1/\sqrt{6} & 1/\sqrt{6} \\ 1/\sqrt{6} & -1/\sqrt{6} \\ 1/\sqrt{6} & 1/\sqrt{6} \end{pmatrix}$$

Prob$[SQ$ has full rank$] = 50\%$

Coherence = Largest Row Norm Squared

Q is $m \times n$ with orthonormal columns: $\mu = \max_{1 \leq k \leq m} \|e_k^T Q\|_2^2$

$$Q = \begin{pmatrix} 1 & 0 \\ 0 & 1 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \end{pmatrix} \qquad \text{high coherence: } \mu = 1$$

$$Q = \begin{pmatrix} 1/\sqrt{6} & -1/\sqrt{6} \\ 1/\sqrt{6} & 1/\sqrt{6} \\ 1/\sqrt{6} & -1/\sqrt{6} \\ 1/\sqrt{6} & 1/\sqrt{6} \\ 1/\sqrt{6} & -1/\sqrt{6} \\ 1/\sqrt{6} & 1/\sqrt{6} \end{pmatrix} \qquad \text{low coherence } \mu = \frac{1}{3}$$

Properties of Coherence

Coherence of $m \times n$ matrix Q with $Q^T Q = I$

$$\mu = \max_{1 \le k \le m} \|e_k^T Q\|_2^2$$

- $n/m \le \mu(Q) \le 1$
- Maximal coherence: $\mu(Q) = 1$
  At least one column of Q is a canonical vector
- Minimal coherence: $\mu(Q) = n/m$
  Columns of Q are columns of a Hadamard matrix
- Coherence measures "correlation with canonical basis"

Coherence in General

- 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

Different Definitions

- Coherence of subspace
  $\mathcal{Q}$ is subspace of $\mathbb{R}^m$ of dimension n
  P orthogonal projector onto $\mathcal{Q}$

$$\mu_0(\mathcal{Q}) = \frac{m}{n} \max_{1 \le k \le m} \|e_k^T P\|_2^2 \qquad \left(1 \le \mu_0(\mathcal{Q}) \le \tfrac{m}{n}\right)$$

- Coherence of full rank matrix
  A is $m \times n$ with $\mathrm{rank}(A) = n$
  Columns of Q are orthonormal basis for $\mathcal{R}(A)$

$$\mu(A) = \max_{1 \le k \le m} \|e_k^T Q\|_2^2 \qquad \left(\tfrac{n}{m} \le \mu(A) \le 1\right)$$

- Reflects difficulty of recovering the matrix from sampling

Sampling from Matrices with Orthonormal Columns

- Given: $m \times n$ matrix Q with orthonormal columns
- Sampling: $c \times m$ matrix

$$S = \sqrt{\frac{m}{c}} \begin{pmatrix} e_{k_1}^T \\ \vdots \\ e_{k_c}^T \end{pmatrix}$$

- Unbiased estimator: $\mathbf{E}\left[Q^T S^T S Q\right] = Q^T Q = I$
- Sum of c random matrices:

$$Q^T S^T S Q = \frac{m}{c}\, Q^T e_{k_1} e_{k_1}^T Q + \cdots + \frac{m}{c}\, Q^T e_{k_c} e_{k_c}^T Q$$

Matrix Bernstein Inequality [Recht 2011]

- X_t independent random $n \times n$ matrices
- Expected value: $\mathbf{E}[X_t] = 0$
- Uniform boundedness: $\|X_t\|_2 \leq \tau$ almost surely
- Variance: $\rho_t \equiv \max\{\|\mathbf{E}[X_t X_t^T]\|_2, \|\mathbf{E}[X_t^T X_t]\|_2\}$
- Desired error $0 < \epsilon < 1$
- Failure probability $\delta = 2n \exp\left(-\frac{3}{2}\frac{\epsilon^2}{3\sum_t \rho_t + \tau\,\epsilon}\right)$

With probability at least $1 - \delta$

$$\left\|\sum_t X_t\right\|_2 \leq \epsilon$$

Assumptions for Our Problem

- $m \times n$ matrix Q with orthonormal columns
- Coherence $\mu = \max_{1 \le k \le m} \|e_k^T Q\|_2^2$
- Sum of c matrices

$$(SQ)^T(SQ) - I = \sum_{t=1}^{c} X_t \qquad X_t = \frac{m}{c} Q^T e_{k_t} e_{k_t}^T Q - \frac{1}{c} I$$

- Expected value: $\mathbf{E}[X_t] = 0$
- Uniform boundedness: $\|X_t\|_2 \le m\,\mu/c$
- Variance: $\mathbf{E}[X_t^2] \le m\,\mu/c^2$

Condition Number Bound

- Desired error $0 < \epsilon < 1$
- Failure probability

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

With probability at least $1-\delta$: $\|(SQ)^T(SQ) - I\|_2 \leq \epsilon$

This implies

With probability at least $1-\delta$: $\kappa(SQ) \leq \sqrt{\frac{1+\epsilon}{1-\epsilon}}$

Implications of Bound

- Coherence must be sufficiently low

$$\mu < \tfrac{3}{8} \frac{c}{m \ln(2n/\delta)}$$

{Follows from $\epsilon < 1$}

- Amount of sampling must be sufficiently large

$$c \geq \tfrac{8}{3} \frac{m\,\mu}{\epsilon^2} \ln(2n/\,\delta)$$

Minimal coherence $\mu = n/m$:

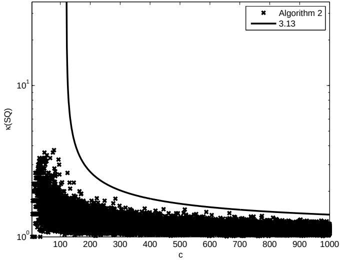
$$c \gtrsim (n \ln n)/\epsilon^2$$

Tightness of Condition Number Bound

Q is $m \times n$ with orthonormal columns, $m = 10^4$, $n = 5$

Coherence $\mu = 1.5n/m$, success probability $1 - \delta = .99$

Little sampling: $n \leq c \leq 1000$



Bound holds for $c \geq 144 \approx \frac{8}{3}\,\frac{m\mu}{\epsilon^2}\ln(2n/\delta)$

Predictive for $c \geq 200$

Coherence is not Enough

$$G_{ood} = \begin{pmatrix} 1/2 & 0 \\ 1/2 & 0 \\ 1/2 & 0 \\ 1/2 & 0 \\ 0 & -1/2 \\ 0 & -1/2 \\ 0 & 1/\sqrt{2} \end{pmatrix} \qquad B_{ad} = \begin{pmatrix} 1/\sqrt{2} & 0 \\ -1/\sqrt{2} & 0 \\ 0 & 1/\sqrt{2} \\ 0 & -1/\sqrt{2} \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \end{pmatrix}$$

- Same coherence: $\mu(G_{ood}) = \mu(B_{ad}) = 1/2$
- Sampling $c = 3$ rows

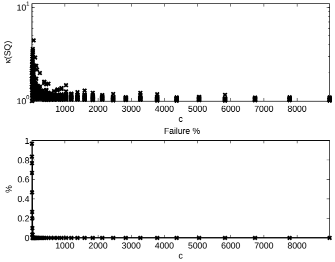
$$\textbf{Prob}[SG_{ood} \text{ has full rank}] \geq 73\%$$
$$\textbf{Prob}[SB_{ad} \text{ has full rank}] < 35\%$$

- Sampled B_{ad} matrices more likely to be rank deficient

Good Matrices

Q is $m \times n$ with orthonormal columns, $m = 10^4$, $n = 5$

Coherence $\mu = .05 = 100n/m$



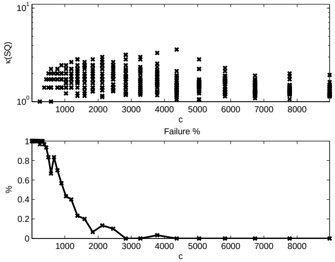
If SQ has full rank, then $\kappa(SQ) \ll 10$

Low percentage of rank deficient SQ for $c \geq n$

Bad Matrices

Q is $m \times n$ with orthonormal columns, $m = 10^4$, $n = 5$

Coherence $\mu = .05 = 100n/m$



High percentage of rank deficient SQ for $c \leq 2000 = m/n$

Distinguishing Good and Bad Matrices with Same Coherence

Idea: Use all row norms

- Q is $m \times n$ with orthonormal columns
- Leverage scores $=$ row norms squared

$$\ell_k = \|e_k^T Q\|_2^2, \qquad 1 \leq k \leq m$$

- Coherence $\mu = \max_k \ell_k$
- Low coherence $\approx$ uniform leverage scores

- Leverage scores of full column rank matrix A:
  Columns of Q are orthonormal basis for $\mathcal{R}(A)$

$$\ell_k(A) = \|e_k^T Q\|_2^2, \qquad 1 \leq k \leq m$$

Statistical Leverage Scores

Hoaglin & Welsch 1978
Chatterjee & Hadi 1986

- Identify potential outliers in $\min_x \|Ax - b\|_2$
- Orthogonal projector onto $\mathcal{R}(A)$: $H = A(A^T A)^{-1} A^T$
- Leverage score H_{kk}: Influence of kth data point on LS fit

Statistical Leverage Scores

Hoaglin & Welsch 1978
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- Identify potential outliers in $\min_x \|Ax - b\|_2$
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- Leverage score H_{kk}: Influence of kth data point on LS fit

- QR decomposition: $A = QR$

$$H_{kk} = \|e_k^T Q\|_2^2 = \ell_k(A)$$

Application to randomized algorithms:
Drineas, Mahoney & al. 2006–2012

Assumptions for Our Problem

- $m \times n$ matrix Q with orthonormal columns
- Leverage scores $\ell_k = \|e_k^T Q\|_2^2$, $\quad \mu = \max_{1 \le k \le m} \ell_k$

$$L = \mathrm{diag}\begin{pmatrix} \ell_1 & \dots & \ell_m \end{pmatrix}$$

- Sum of c matrices

$$(SQ)^T(SQ) - I = \sum_{t=1}^{c} X_t \qquad X_t = \frac{m}{c} Q^T e_{k_t} e_{k_t}^T Q - \frac{1}{c} I$$

- Expected value: $\mathbf{E}[X_t] = 0$
- Uniform boundedness: $\|X_t\|_2 \le m\,\mu/c$
- Variance: $\mathbf{E}[X_t^2] \le m\,\|Q^T L Q\|_2/c^2$

Condition Number Bound with Leverage Scores

- Desired error $0 < \epsilon < 1$
- Failure probability

$$\delta = 2n\,\exp\left(-\frac{3}{2}\,\frac{c\,\epsilon^2}{m\,(3\,\|Q^T L Q\|_2 + \mu\,\epsilon}\right)$$

With probability at least $1-\delta$: $\quad \|(SQ)^T(SQ) - I\|_2 \leq \epsilon$

This implies

With probability at least $1-\delta$: $\quad \kappa(SQ) \leq \sqrt{\frac{1+\epsilon}{1-\epsilon}}$

Leverage Scores vs. Coherence

Failure probability

$$\delta = 2n\ \exp\left(-\frac{3}{2}\,\frac{c\,\epsilon^2}{m\,(3\,\|Q^T L Q\|_2 + \mu\,\epsilon}\right)$$

- Bounds in terms of coherence:

$$\mu^2 \leq \|Q^T L Q\|_2 \leq \mu$$

- Estimation in terms of largest leverage scores
  If $k = 1/\mu$ is an integer then

$$\|Q^T L Q\|_2 \leq \mu \sum_{j=1}^{k} \ell_{[j]}$$

where $\ell_{[1]} \geq \cdots \geq \ell_{[m]}$

Summary

- Randomized sampling of rows from matrices with orthonormal columns
- Sampling strategy: Exactly(c)
  {Bernoulli sampling is very similar}
- Coherence: *Largest* row norm squared
- Bounds for condition number of sampled matrices

  Explicit and non-asymptotic

  Realistic even for small matrix dimensions
- Leverage scores: Row norms squared
- Tighter bounds: Replace coherence by leverage scores

How much tighter???