Accuracy and Stability Issues for Randomized Matrix Algorithms: Sensitivity of Leverage Scores

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Statistical Leverage Scores

Hoaglin & Welsch 1978
Velleman & Welsch 1981
Chatterjee & Hadi 1986

Given: Real $m \times n$ matrix A, $m \geq n$, $\text{rank}(A) = n$
Want: Potential outliers in $\min_x \|Ax - b\|$ (two-norm)

- Hat matrix: Orthogonal projector onto range(A)

$$H = A\,(A^T A)^{-1}\,A^T$$

- Leverage scores of A

$$\ell_j(A) = H_{jj} \qquad 1 \leq j \leq m$$

- Least squares fit: $\hat{b} = Hb$

  If $\ell_k(A) = 1$ then b_k has maximal leverage: $\hat{b}_k = b_k$
  If $\ell_k(A) = 0$ then b_k has zero leverage over $\hat{b}_k$

Overview

1. Computation, and use of leverage scores
2. Coherence: Largest leverage score
3. Sensitivity of leverage scores to subspace angles

   Coherence

   Large leverage scores

4. Sensitivity of leverage scores to matrix perturbations

Computation, and Use of Leverage Scores

Computation of Leverage Scores

Real $m \times n$ *matrix* A *with* $\text{rank}(A) = n$

Hat matrix $H = A\,(A^T A)^{-1}\,A^T$

Leverage scores $\ell_j(A) = H_{jj} \qquad 1 \leq j \leq m$

- Singular Value Decomposition $A = U\,\Sigma V^T \quad U^T U = I_n$
  Hat matrix $H = UU^T$

$$\ell_j(A) = \|e_j^T\, U\|^2 \qquad 1 \leq j \leq m$$

- QR decomposition $A = Q\,R \quad Q^T Q = I_n$
  Hat matrix $H = QQ^T$

$$\ell_j(A) = \|e_j^T\, Q\|^2 \qquad 1 \leq j \leq m$$

Leverage Scores for Randomized Algorithms

[Drineas, Mahoney et al. 2006-2013]

Use of leverage scores:

As sampling probabilities
To analyze performance of uniform sampling strategies

Randomized subset selection [Boutsidis, Mahoney & Drineas 2010]

Given: $m \times n$ *matrix* A *with* $\text{rank}(A) = n$
Want: k *most important rows of* A

Idea: Sample row j of A with probability $p_j = \ell_j(A)/n$

Coherence: Largest Leverage Score

Coherence

Donoho & Huo 2001: *Mutual coherence of two bases*
Candés, Romberg & Tao 2006
Candés & Recht 2009: *Matrix completion*

Coherence of $m \times n$ matrix A with $\text{rank}(A) = n$

$$\mu(A) = \max_{1 \leq j \leq m} \ell_j(A)$$

Low coherence $\Rightarrow$ uniform leverage scores

- $n/m \leq \mu(A) \leq 1$
- Maximal coherence: $\mu(A) = 1$

  At least one basis vector for range(A) is a canonical vector
- Minimal coherence: $\mu(A) = n/m$

  Orthonormal bases for range(A) are like columns of a Hadamard matrix
- Coherence measures correlation with a standard basis

Sensitivity of Leverage Scores to Subspace Angles

Exact and Perturbed Leverage Scores

- Exact matrix: $\mathcal{A}$ is $m \times n$ with $\text{rank}(\mathcal{A}) = n$

  Exact leverage scores

  $$\ell_j(A) = \|e_j^T A\|^2 \qquad 1 \leq j \leq m$$

  where A is orthonormal basis for $\text{range}(\mathcal{A})$

- Perturbed matrix: $\mathcal{B}$ is $m \times n$ with $\text{rank}(\mathcal{B}) = n$

  Perturbed leverage scores

  $$\ell_j(B) = \|e_j^T B\|^2 \qquad 1 \leq j \leq m$$

  where B is orthonormal basis for $\text{range}(\mathcal{B})$

Question: How close is $\ell_j(B)$ to $\ell_j(A)$?

Principal Angles between Column Spaces

A and B are $m \times n$ with orthonormal columns, $A^T A = B^T B = I_n$

- SVD of $n \times n$ matrix $A^T B = U \Sigma V^T$

$$\Sigma = \operatorname{diag}\begin{pmatrix}\cos\theta_1 & \cdots & \cos\theta_n\end{pmatrix}$$

- Principal angles θ_j between range(A) and range(B)

$$1 \geq \cos\theta_1 \geq \ldots \geq \cos\theta_n \geq 0$$

$$0 \leq \theta_1 \leq \cdots \leq \theta_n \leq \pi/2$$

- Special cases

  If $A = B$ then $\Sigma = I_n$ and all $\theta_j = 0$

  If $A^T B = 0$ then $\Sigma = 0$ and all $\theta_j = \pi/2$

Sensitivity of Leverage Scores to Angles

- Angles between range(A) and range(B)

$$0 \leq \theta_1 \leq \cdots \leq \theta_n \leq \pi/2$$

- Leverage score bounds

$$\begin{aligned} \ell_j(B) &\leq \left(\cos\theta_1 \sqrt{\ell_j(A)} + \sin\theta_n \sqrt{1-\ell_j(A)}\right)^2 \\ \ell_j(A) &\leq \left(\cos\theta_1 \sqrt{\ell_j(B)} + \sin\theta_n \sqrt{1-\ell_j(B)}\right)^2 \qquad 1 \leq j \leq m \end{aligned}$$

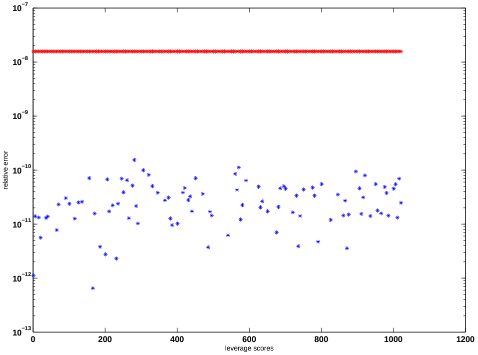
Leverage scores of A and B are close,
if all angles between range(A) and range(B) are small

Uniform Leverage Scores

$\mathcal{A}$ is $m \times n$ Hadamard $\quad m = 1024,\ n = 50,$ leverage scores are n/m

Angles: $\quad \cos\theta_1 = 1 \quad \sin\theta_n \approx 10^{-8}$

Relative error: $(\ell_j(B) - \ell_j(A))/\ell_j(A)$ $\qquad$ Relative bound



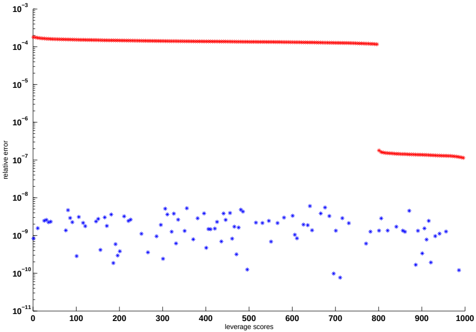
Bound reflects behaviour of errors

20% Large Leverage Scores

$\mathcal{A}$ is $m \times n$ $\quad m = 1000,\ n = 50$, and 200 large leverage scores

Angles: $\cos\theta_1 = 1 \quad \sin\theta_n \approx 10^{-8}$

Relative error: $(\ell_j(B) - \ell_j(A))/\ell_j(A)$ $\qquad$ Relative bound



Bound tighter for large leverage scores

Large Leverage Scores, and Angles

- Assume: Bounded angles

$$0 \leq \theta_1 \leq \cdots \leq \theta_n \leq \pi/4$$

- Large leverage score: $\ell_k(A) \geq 1/2$ for some k
- Bound for perturbed leverage scores

$$\left(1 - \sqrt{2}\sin\theta_n\right)^2 \ell_k(A) \leq \ell_k(B) \leq (1 + \sin\theta_n)^2 \ell_k(A)$$

Upper and lower bounds for large leverage scores

Coherence and Angles

- Angles between range(A) and range(B)

$$0 \leq \theta_1 \leq \cdots \leq \theta_n \leq \pi/2$$

- Coherence: $\mu(A) = \max_{1 \leq j \leq m} \ell_j(A)$
- Bound for perturbed coherence

$$\mu(A)/\gamma \leq \mu(B) \leq \gamma\, \mu(A)$$

where

$$\gamma = \left(\cos\theta_1 + \sin\theta_n \sqrt{\tfrac{m}{n}}\right)^2$$

Coherence is sensitive if

Large aspect ratio: $m \gg n$

Large angles between range(A) *and* range(B)

Sensitivity of Leverage Scores to Matrix Perturbations

Bound for Angles in terms of Perturbations

- $\mathcal{A}$ and $\mathcal{A}+\mathcal{E}$ are $m \times n$ of rank n
- Condition number and relative perturbation

$$\kappa = \|\mathcal{A}\| \, \|\mathcal{A}^\dagger\| \qquad \epsilon = \|\mathcal{E}\|/\|\mathcal{A}\|$$

- Largest angle between range($\mathcal{A}$) and range($\mathcal{A}+\mathcal{E}$): θ_n
- Assume: Perturbation $\epsilon < .5/\kappa$
- Bound for largest angle

$$\sin\theta_n \leq 2\,\kappa\,\epsilon$$

All angles between range($\mathcal{A}$) and range($\mathcal{A}+\mathcal{E}$) are small
if $\mathcal{A}$ is well-conditioned with respect to inversion

Perturbation of Coherence

- $\mathcal{A}$ and $\mathcal{A}+\mathcal{E}$ are $m \times n$ of rank n
- Condition number and relative perturbation

$$\kappa = \|\mathcal{A}\| \, \|\mathcal{A}^\dagger\| \qquad \epsilon = \|\mathcal{E}\|/\|\mathcal{A}\|$$

- Coherence: $\mu(\mathcal{A}) = \max_{1\leq j\leq m} \ell_j(\mathcal{A})$
- Assume: Perturbation $\epsilon < .5/\kappa$
- Bound for perturbed coherence

$$\mu(A)/\gamma \leq \mu(B) \leq \gamma\, \mu(A) \qquad \gamma = \left(1 + 2\sqrt{\frac{m}{n}}\,\kappa\,\epsilon\right)^2$$

Coherence is sensitive to perturbations if

Large aspect ratio: $m \gg n$
$\mathcal{A}$ *is ill-conditioned with respect to inversion*

Perturbation of Large Leverage Scores

- $\mathcal{A}$ and $\mathcal{A}+\mathcal{E}$ are $m \times n$ of rank n
- Condition number and relative perturbation

$$\kappa = \|\mathcal{A}\| \, \|\mathcal{A}^\dagger\| \qquad \epsilon = \|\mathcal{E}\|/\|\mathcal{A}\|$$

- Large leverage scores: $\ell_k(\mathcal{A}) \geq 1/2$ for some k
- Assume: Perturbation $\epsilon < .3/\kappa$
- Relative error for large leverage scores

$$\left| \frac{\ell_k(\mathcal{A}+\mathcal{E}) - \ell_k(\mathcal{A})}{\ell_k(\mathcal{A})} \right| \leq 4\,\kappa\epsilon\,(\kappa\epsilon + 1)$$

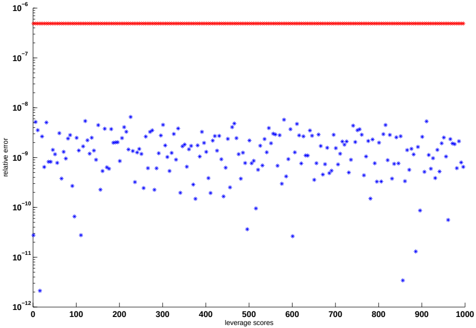
Large leverage scores are insensitive to perturbations
if $\mathcal{A}$ is well-conditioned with respect to inversion

Well-Conditioned Matrix

$\mathcal{A}$ is $m \times n$ $\quad m = 1000,\ n = 50$

Condition number: $\kappa \approx 23$ $\quad$ Relative perturbation: $\epsilon \approx 10^{-8}$

Relative error: $|\ell_j(B) - \ell_j(A)|/\ell_j(A)$ $\quad$ Bound



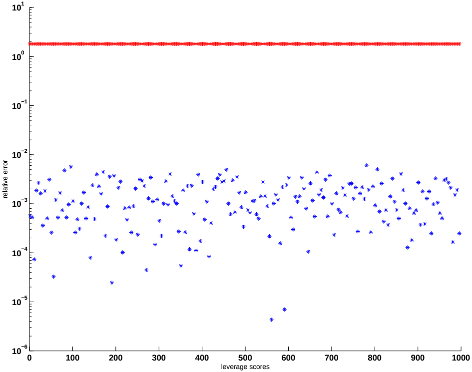
Bound informative even if matrix has no large leverage scores

Moderately Conditioned Matrix

$\mathcal{A}$ is $m \times n$ $\quad m = 1000,\ n = 50$

Condition number: $\kappa \approx 10^8$ $\quad$ Relative perturbation: $\epsilon \approx 10^{-8}$

Relative error: $|\ell_j(B) - \ell_j(A)|/\ell_j(A)$ $\quad$ Bound



Bound informative for all leverage scores (not just large ones)

Summary

Leverage scores

Two-norms of rows of $m \times n$ orthonormal matrices
Sampling probabilities in randomized algorithms

Coherence

Largest leverage score
Performance analysis of sampling strategies

Sensitivity analysis

Relative error bounds for leverage scores of exact and perturbed matrix

Angles between column spaces
Condition number and matrix perturbation

Leverage scores insensitive if

Angles are small
Matrix is well-conditioned

Coherence more sensitive if $m \gg n$

Future Work

- Sampling strategies only need the correct exponent
  Are relative error bounds too strong?

- Sampling strategies depend on large leverage scores
  Tighter bounds targeted at large leverage scores

- Extend sensitivity analysis to

  Rank deficient matrices
  Low-rank approximations
  Large perturbations (missing data)
  Structured perturbations (categorical data)