

EE270

Large scale matrix computation, optimization and learning

Instructor : Mert Pilanci

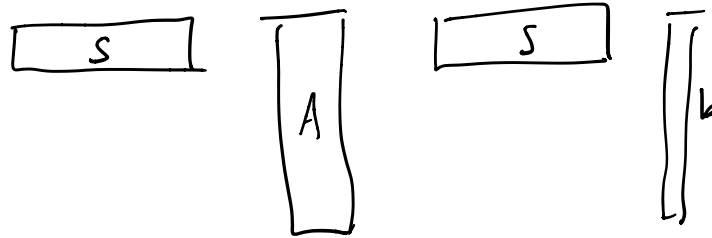
Stanford University

Tuesday, Feb 9 2021

Randomized Linear Algebra

Lecture 9: High-dimensional Problems, Least-norm Solutions and Randomized Methods

Faster Least Squares Optimization: Random Projection



► Left-sketching

Form SA and Sb where $S \in \mathbb{R}^{m \times n}$ is a random projection matrix

► Solve the smaller problem

$$\min_{x \in \mathbb{R}^d} \|SAx - Sb\|_2^2$$

► using any classical method.

Direct method complexity md^2

Gaussian Sketch

- ▶ Let S be $\frac{1}{m} \times$ i.i.d. Gaussian. $\mathbb{E}[S^T S] = I$

$$\tilde{x} = \arg \min_{x \in \mathbb{R}^d} \|SAx - Sb\|_2^2$$

- ▶ Unbiased $\mathbb{E}[\tilde{x}] = x_{LS}$

$$\text{since } \tilde{x} = x_{LS} + \underbrace{(A^T S^T S A)^{-1} A^T S^T S b^\perp}_{\text{zero mean}}$$

Gaussian Sketch

$$f(x) = \|Ax - b\|_2^2$$

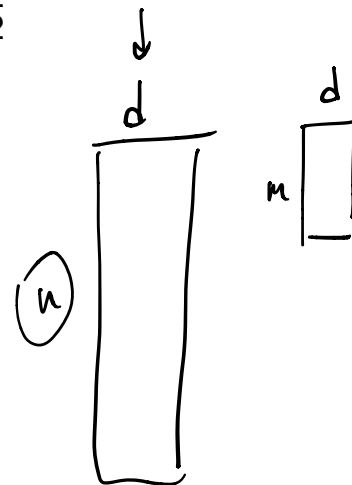
$$f(x) =$$

- Let S be $\frac{1}{m} \times$ i.i.d. Gaussian. $\mathbb{E}[S^T S] = I$

$$\tilde{x} = \arg \min_{x \in \mathbb{R}^d} \|SAx - Sb\|_2^2$$

- Unbiased $\mathbb{E}[\tilde{x}] = x_{LS}$

since $\tilde{x} = x_{LS} + \underbrace{(A^T S^T S A)^{-1} A^T S^T S b^\perp}_{\text{zero mean}}$



- Variance

$$\mathbb{E}\|A(\tilde{x} - x_{LS})\|_2^2 = f(x_{LS}) \frac{d}{m-d-1}$$

valid for $m > d + 1$ where $f(x) = \|Ax - b\|_2^2$

Gaussian Sketch

- ▶ Let S be $\frac{1}{m} \times$ i.i.d. Gaussian. $\mathbb{E}[S^T S] = I$

$$\tilde{x} = \arg \min_{x \in \mathbb{R}^d} \|SAx - Sb\|_2^2$$

- ▶ Unbiased $\mathbb{E}[\tilde{x}] = x_{LS}$

$$\text{since } \tilde{x} = x_{LS} + \underbrace{(A^T S^T SA)^{-1} A^T S^T Sb^\perp}_{\text{zero mean}}$$

- ▶ Variance

$$\mathbb{E}\|A(\tilde{x} - x_{LS})\|_2^2 = f(x_{LS}) \frac{d}{m-d-1}$$

valid for $m > d + 1$ where $f(x) = \|Ax - b\|_2^2$

- ▶ Function value

$$f(\tilde{x}) = \|A\tilde{x} - b\|_2^2 = \|A(\tilde{x} - x_{LS})\|_2^2 + \|Ax_{LS} - b\|_2^2$$

- ▶ $\mathbb{E}f(\tilde{x}) - f(x_{LS}) = f(x_{LS}) \frac{d}{m-d-1}$

Variance Reduction by Averaging



- ▶ Let S_1, \dots, S_r be $\frac{1}{\sqrt{m}} \times$ i.i.d. Gaussian. $\mathbb{E}[S_i^T S_i] = I$

$$\tilde{x}_i = \arg \min_{x \in \mathbb{R}^d} \|S_i A x - S_i b\|_2^2$$

- ▶ let $\tilde{x} = \frac{1}{r} \sum_{i=1}^r x_i$ $\mathbb{E} \tilde{x} = \frac{1}{r} \sum \underbrace{\mathbb{E} x_i}_{x_{LS}} = x_{LS}$

- ▶ Unbiased $\mathbb{E}[\tilde{x}] = x_{LS}$

- ▶ Variance is reduced by $\frac{1}{r}$

- ▶ $\mathbb{E} \|A(\tilde{x} - x_{LS})\|_2^2 = f(x_{LS}) \frac{1}{r} \frac{d}{m-d-1}$

$$\begin{aligned} \text{Var} \left(\frac{1}{r} \sum_{i=1}^r x_i \right) &= \frac{1}{r^2} \frac{\text{Var}(\sum_{i=1}^r x_i)}{\sum_{i=1}^r \text{Var}(x_i)} \\ &= \frac{1}{r^2} \cdot \frac{\sum_{i=1}^r \text{Var}(x_i)}{\sum_{i=1}^r \text{Var}(x_i)} \\ &= \frac{1}{r} \cdot \text{Var}(x_1) \end{aligned}$$

Variance Reduction by Averaging

$$b = Ax_{LS} + b^\perp$$

$$f(x) = \|Ax - b\|_2^2 = \|A(x - x_{LS}) - \overbrace{b^\perp}^{f(x_{LS})}\|_2^2$$

$$= \|A(x - x_{LS})\|_2^2 + \underbrace{\|b^\perp\|_2^2}_{f(x_{LS})}$$

- Let S_1, \dots, S_r be $\frac{1}{m} \times$ i.i.d. Gaussian. $\mathbb{E}[S^T S] = I$

$$\tilde{x}_i = \arg \min_{x \in \mathbb{R}^d} \|S_i A x - S_i b\|_2^2$$

$$\|Ax_{LS} - b\|_2^2$$

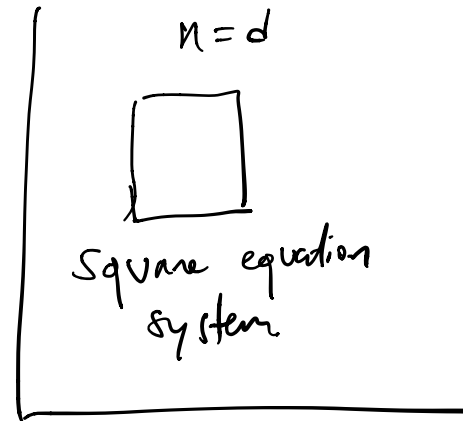
- let $\tilde{x} = \frac{1}{r} \sum_{i=1}^r x_i$
- Unbiased $\mathbb{E}[\tilde{x}] = x_{LS}$
- Variance is reduced by $\frac{1}{r}$
- $\mathbb{E}\|A(\tilde{x} - x_{LS})\|_2^2 = f(x_{LS}) \frac{1}{r} \frac{d}{m-d-1}$
- $\mathbb{E}f(\tilde{x}) - \underbrace{f(x_{LS})}_{\rightarrow} = f(x_{LS}) \frac{1}{r} \frac{d}{m-d-1}$

$$f(x_{LS}) \leq \mathbb{E} f(\tilde{x}) \leq f(x_{LS}) \cdot \left(1 + \frac{1}{r} \frac{d}{m-d-1}\right)$$

High-dimensional Least Squares Problems

Right sketching.

$A \cdot S$



► $A \in \mathbb{R}^{n \times d}$ where $d > n$

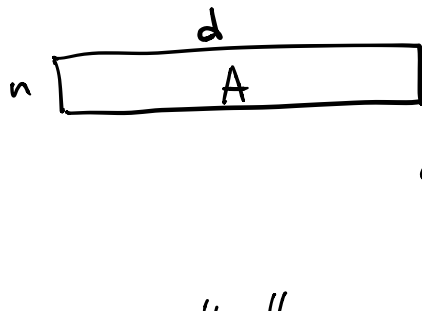
► no unique solution

tall LS



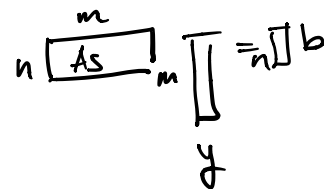
$n \gg d$

wide LS (high-dim)



$\min \|x\|_2$

s.t. $Ax = b$



$\min \|y\|_2$

$ASy = b$

High-dimensional Least Squares Problems

$$A = U \Sigma V^T \quad A^+ = A^T (A A^T)^{-1}$$

$$\min_x \frac{1}{2} \|x\|_2^2 + \lambda^T (Ax - b) = \frac{1}{2} \|A^T \lambda\|_2^2 - \lambda^T A A^T \lambda - \lambda^T b$$

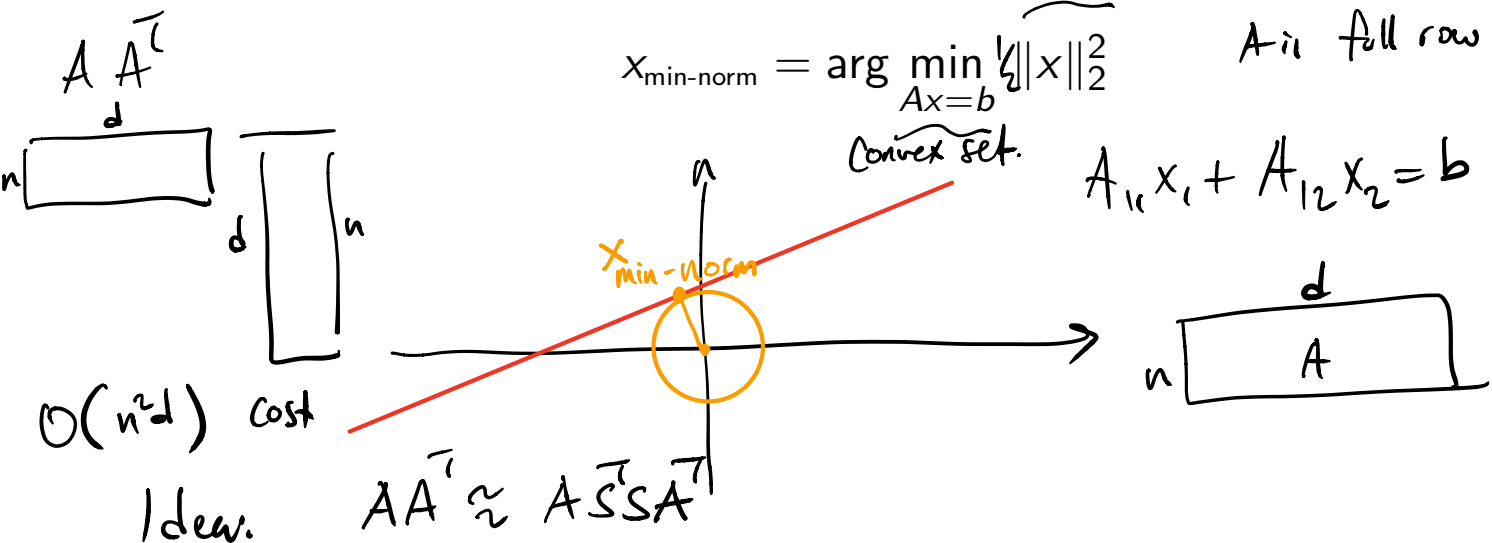
$$x + A^T \lambda = 0 \Rightarrow x = -A^T \lambda = A^T (A A^T)^{-1} b = A^+ b$$

- ▶ $A \in \mathbb{R}^{n \times d}$ where $d > n$
- ▶ no unique solution
- ▶ minimum (ℓ_2) norm solution is unique

$$-A A^T \lambda - b = 0$$

$$\lambda = -(A A^T)^{-1} b$$

invertible iff
A is full row rank



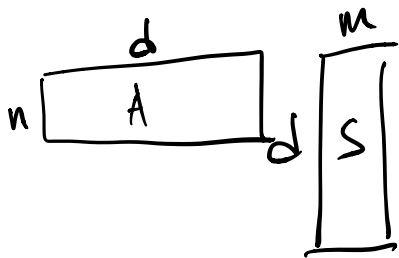
Minimum norm solution and SVD

$$x_{\text{min-norm}} = \arg \min_{Ax=b} \|x\|_2^2$$

Random projection to reduce dimension: Right Sketch

$$x_{\text{min-norm}} = \arg \min_{Ax=b} \|x\|_2^2$$

- We can right multiply A and form AS where $S \in \mathbb{R}^{d \times m}$ and solve



$$\arg \min_{ASz=b} \|z\|_2^2$$

$$\underline{z = (AS)^+ b} \quad m\text{-dimensional}$$

$$\text{Idea 1) let } \hat{x} = S (AS)^+ b$$

Random projection to reduce dimension: Right Sketch

$$x_{\text{min-norm}} = \arg \min_{Ax=b} \|x\|_2^2$$

- ▶ We can right multiply A and form AS where $S \in \mathbb{R}^{d \times m}$ and solve

$$\arg \min_{ASz=b} \|z\|_2^2$$

- ▶ How do we use $z \in \mathbb{R}^m$?

Right Sketch

$$x_{\text{min-norm}} = \arg \min_{Ax=b} \underbrace{\|x\|_2^2}_{f(x)}$$

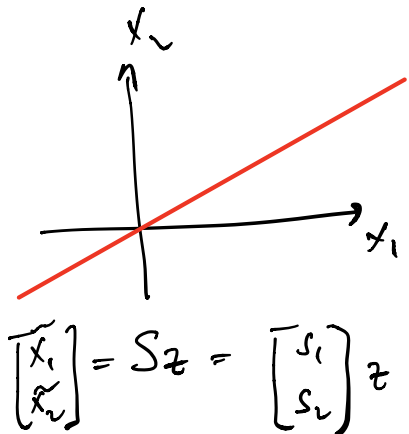
approximation $\tilde{x} = S\tilde{z}$

where $\tilde{z} := \arg \min_{ASz=b} \|z\|_2^2$

Feasible estimate for x :

$$\begin{aligned} A\tilde{x} &= AS\tilde{z} \\ &= b \end{aligned}$$

Right Sketch



$$x_{\text{min-norm}} = \arg \min_{Ax=b} \underbrace{\|x\|_2^2}_{f(x)}$$

approximation $\tilde{x} = S\tilde{z}$

where $\tilde{z} := \arg \min_{ASz=b} \|z\|_2^2$

- ▶ Let S be i.i.d. Gaussian $N(0, \frac{1}{\sqrt{m}})$
- ▶ Is \tilde{x} unbiased, i.e., $\mathbb{E}\tilde{x} \stackrel{?}{=} x_{\text{min-norm}}$

Right Sketch

$$\underline{x_{\min\text{-norm}}} = \arg \min_{Ax=b} \underbrace{\|x\|_2^2}_{f(x)}$$

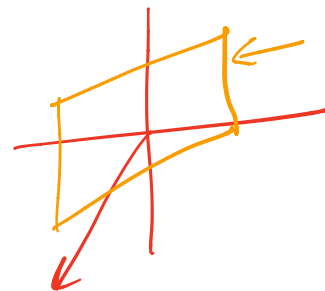
approximation $\tilde{x} = S\tilde{z}$

where $\tilde{z} := \arg \min_{ASz=b} \|z\|_2^2$

- ▶ Let S be i.i.d. Gaussian $N(0, \frac{1}{\sqrt{m}})$
- ▶ Is \tilde{x} unbiased, i.e., $\mathbb{E}\tilde{x} \stackrel{?}{=} x_{\min\text{-norm}}$
- ▶ Yes, conditioned on SA

$$\tilde{x} \sim N(x_{\min\text{-norm}}, V_z V_z^T b^T (AS^T SA^T)^{-1} b)$$

- ▶ $V_z V_z^T$ is the projection onto the null space of A
- ▶ error $\tilde{x} - x_{\min\text{-norm}} \in \text{Null}(A)$



$$Ax = b$$

$$A\tilde{x} = b$$

$$A(x - \tilde{x}) = 0$$

$$x - \tilde{x} \in \text{Null}(A)$$

$$\boxed{A}$$

$$\begin{aligned} A &= U \Sigma V^T \\ &= U \begin{bmatrix} \Sigma & 0 \end{bmatrix} \begin{bmatrix} v_1 & v_2 \end{bmatrix}^T \end{aligned}$$

Right Sketch

$$x_{\min\text{-norm}} = \arg \min_{Ax=b} \underbrace{\|x\|_2^2}_{f(x)}$$

$$A^+ b = A(AA^T)^{-1} b$$

approximation $\tilde{x} = S\tilde{z}$

where $\tilde{z} := \arg \min_{ASz=b} \|z\|_2^2$

$$(AS)^+ b = S^+ A^+ (AS S^+ A^+)^{-1} b$$

$n \times n$
matrix

- ▶ Let S be i.i.d. Gaussian $N(0, \frac{1}{\sqrt{m}})$
- ▶ Is \tilde{x} unbiased, i.e., $\mathbb{E}\tilde{x} = ? x_{\min\text{-norm}}$
- ▶ Yes, conditioned on SA

we need
at least
 $m \geq n$

$$\tilde{x} \sim N(x_{\min\text{-norm}}, VV^T b^T (AS^T SA^T)^{-1} b)$$

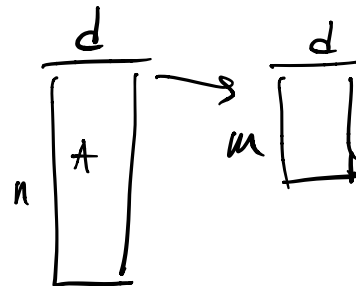
- ▶ VV^T is the projection onto the null space of A
- ▶ error $\tilde{x} - x_{\min\text{-norm}} \in \text{Null}(A)$
- ▶ Using $\mathbb{E}(AS^T SA^T)^{-1} = (AA^T)^{-1} \frac{m}{m-n-1}$

$$m > n+1$$

$$\mathbb{E}\|\tilde{x} - x_{\min\text{-norm}}\|_2^2 = \frac{d-n}{m-n-1} f(x_{\min\text{-norm}}) = \frac{d-n}{m-n-1} \|x_{\min\text{-norm}}\|_2^2$$

Left Sketch vs Right Sketch Summary

- ▶ Both are unbiased using Gaussian projections
- ▶ A is $n \times d$
- ▶ Left sketch $n \geq d$



$$\tilde{x} = \arg \min_{x \in \mathbb{R}^d} \|SAx - Sb\|_2^2$$

Variance: $\mathbb{E}\|A(\tilde{x} - x_{LS})\|_2^2 = f(x_{LS}) \frac{\overbrace{d}^{\text{dimension of the relevant subspace}}}{m-d-1}$

- ▶ Right sketch $d > n$

$$\tilde{x} = S\tilde{z} \quad \text{where } \tilde{z} := \arg \min_{ASz=b} \|z\|_2^2$$

Variance: $\mathbb{E}\|\tilde{x} - x_{\min\text{-norm}}\|_2^2 = f(x_{\min\text{-norm}}) \frac{\underbrace{d-n}_{\text{dimension of the relevant subspace}}}{m-n-1}$

The diagram shows a wide rectangle with 'n' on the left and 'd' on top. An arrow points to a square with 'n' on the left and 'n' on top.

Back to Left Sketch: Which sketching matrices are good?

- ▶ We need to find conditions to guarantee approximate optimality
- ▶ Let $A = U\Sigma V^T$ SVD in compact form

some deterministic options

- ▶ $S = U^T$ is $d \times n$
- ▶ $S = A^T$

high dim
 V_1^T
 $S = A$

- ▶ For random S matrices $A^T S^T S A$ needs to be invertible
we want it to be close to $A^T A$

Approximate Matrix Multiplication

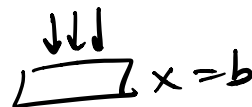
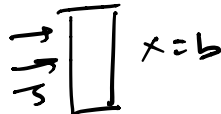
- ▶ Let the approximate product of AB be $C = AS^T SB$

$$\mathbb{P}[\|AB - C\|_F > \epsilon \|A\|_F \|B\|_F] \leq \delta$$

- ▶ Follows from JL Moment property
- ▶ $S \in \mathbb{R}^{m \times n} \sim \frac{1}{\sqrt{m}} \times \text{random i.i.d. sub-Gaussian, e.g., } \pm 1, \text{ or } N(0, 1) \text{ with } m = \frac{c_1}{\epsilon^2} \log \frac{1}{\delta}$
- ▶ $S \in \mathbb{R}^{m \times n} \sim \frac{1}{\sqrt{m}} \times \text{CountSketch matrix (one nonzero per column, which is } \pm 1 \text{ at a uniformly random location) with } m = \frac{c_2}{\epsilon^2 \delta}$
- ▶ $S \in \mathbb{R}^{m \times n} \sim \frac{1}{\sqrt{m}} \times \text{Fast JL Transform with } m = \frac{c_3}{\epsilon} \log \frac{1}{\delta}$

Fast JL Transform

→ row / column sampling



Approximate Matrix Multiplication

- ▶ Let the approximate product of AB be $C = AS^T SB$

$$\mathbb{P}[\|AB - C\|_F > \epsilon \|A\|_F \|B\|_F] \leq \delta$$

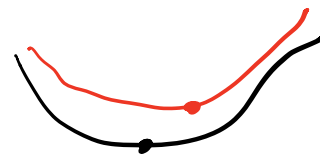
- ▶ Follows from JL Moment property
- ▶ $S \in \mathbb{R}^{m \times n} \sim \frac{1}{\sqrt{m}} \times \text{random i.i.d. sub-Gaussian, e.g., } \pm 1, \text{ or } N(0, 1) \text{ with } m = \frac{c_1}{\epsilon^2} \log \frac{1}{\delta}$
- ▶ $S \in \mathbb{R}^{m \times n} \sim \frac{1}{\sqrt{m}} \times \text{CountSketch matrix (one nonzero per column, which is } \pm 1 \text{ at a uniformly random location) with } m = \frac{c_2}{\epsilon^2 \delta}$
- ▶ $S \in \mathbb{R}^{m \times n} \sim \frac{1}{\sqrt{m}} \times \text{Fast JL Transform with } m = \frac{c_3}{\epsilon} \log \frac{1}{\delta}$
- ▶ Sparse JL and Fast JL are more efficient
- ▶ advantages: doesn't require any knowledge about matrices A and B (**oblivious**)
- ▶ optimal sampling probabilities depend on the column/row norms of A and B

Basic Inequality Method

used in statistics
ML

$\min f(x)$

$\min \tilde{f}(x)$



- second ineq. → We minimize $\tilde{x} = \arg \min \|S(Ax - b)\|_2^2$
- first ineq. → x_{LS} minimizes $\|Ax - b\|_2^2$
- How far is \tilde{x} from x_{LS} ?
- **Step 1.** Establish two optimality (in)equalities for these variables
- $\|Ax_{LS} - b\|_2^2 \leq \|Ax' - b\|_2^2$ for any x' , i.e., $A^T(Ax_{LS} - b) = 0$
- $\|S(A\tilde{x} - b)\|_2^2 \leq \|S(Ax_{LS} - b)\|_2^2$

Basic Inequality Method

$$b = Ax_{LS} + b^\perp$$

$$\|SA(\Delta + x_{LS}) - Sb\|_2^2 \leq \|SAx_{LS} - Sb\|_2^2$$

$$\|SA\Delta + \cancel{SAx_{LS}} - \cancel{SAx_{LS}} - Sb^\perp\|_2^2 \leq \|SAx_{LS} - SAx_{LS} - Sb^\perp\|_2^2$$

$$\Rightarrow \|SA\Delta\|_2^2 + \|Sb^\perp\|_2^2 - 2b^{\perp T} S^T SA\Delta \leq \|Sb^\perp\|_2^2$$

$$\Rightarrow \|Ax_{LS} - b\|_2^2 \leq \|Ax' - b\|_2^2 \text{ for any } x', \text{ i.e., } A^T(Ax_{LS} - b) = 0$$

$$\|S(A\tilde{x} - b)\|_2^2 \leq \|S(Ax_{LS} - b)\|_2^2$$

Step 1. Establish two optimality (in)equalities for these variables

$$\|S(A\tilde{x} - b)\|_2^2 \leq \|S(Ax_{LS} - b)\|_2^2$$

$$\|SA\Delta\|_2^2 \leq 2b^{\perp T} (S^T S - I) A \Delta$$

Step 2. Define error $\Delta = \tilde{x} - x_{LS}$ and re-write these inequalities in terms of Δ

$$\tilde{x} = \Delta + x_{LS}$$

$$\|SA\Delta\|_2^2 \leq 2b^{\perp T} (S^T S - I) A \Delta$$

Step 3. Argue $S^T S \approx I$

$$\underbrace{A^T A^T S^T S A}_{\approx I} \Delta = \|SA\Delta\|_2^2 \leq 2b^{\perp T} S^T SA\Delta = 2b^{\perp T} (\underbrace{S^T S - I}_{\approx I}) A \Delta \quad \text{since } b^{\perp T} A = 0$$

Leverage Scores

Questions?