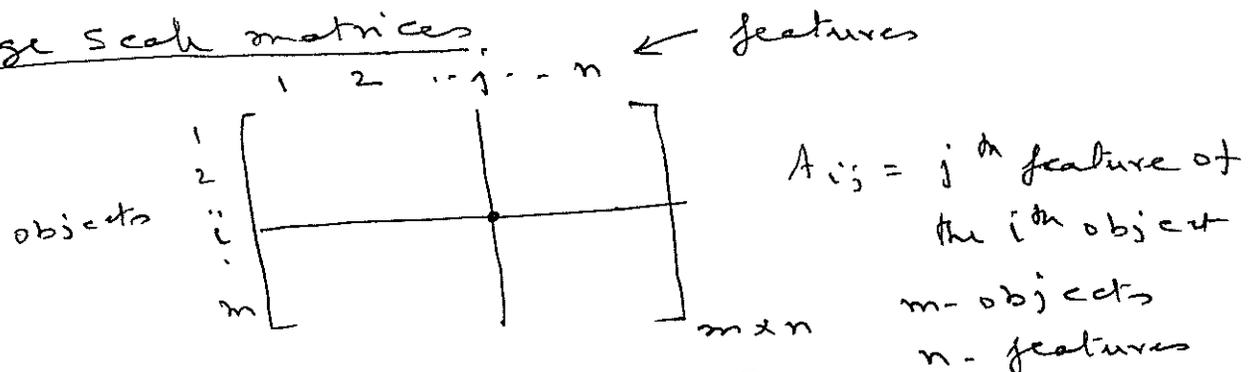


1) Large Scale matrices



• Geometrically: m objects in \mathbb{R}^n . $m < n$
points

1) Astronomy:

objects: Different angular regions in space

Features: Elements from frequency bands

2) Genetics

objects: list of genes

Features: level A_{ij} of the i^{th} gene in j^{th} individual

3) Document / Text

objects: list of documents

Features: A_{ij} = frequency of j^{th} term in i^{th} document

4) Discretization of ODE / PDE

5) Kernel matrices when describing pairwise relations

Properties of these matrices

• Singular values decay quickly suggesting the potential to compress or reduce dimension

Finding structures with randomness

Two step process

- 1) construct a low-dimensional subspace that captures the action of a matrix
- 2) Project / restrict the matrix to this subspace and process that matrix using standard factorization - QR, SVD, CUR of the resulting reduced matrix.

Stage 1: Compute an approximate basis for the range of the input matrix $A \in \mathbb{R}^{m \times n}$ consisting of columns of Q which are orthonormal: $Q \in \mathbb{R}^{m \times r}$:

$$A \approx Q Q^T A \quad \longrightarrow \quad (1)$$

where r is small but large enough to capture the actions of A

Stage 2: Given Q that satisfies (1), use Q to get standard factorization of A .

- Stage 1 is implemented by randomized approach - random sampling and random projection
- Stage 2 uses std. deterministic approach
- This separation is key to the success of this approach.

An example: SVD computation

1) From (1): $A \approx Q Q^T A$. Set $B = Q^T A \rightarrow (2)$

$Q \in \mathbb{R}^{m \times n}$ - n is the rank of Approx. $n \times n$

$Q^T Q = I_n$, $Q Q^T$ - Projection

This gives a low-rank factorization

$$A \approx Q B$$

2) Compute SVD of $B = \tilde{U} \Sigma \tilde{V}^T$

3) Set $U = Q \tilde{U}$ and $A \approx Q B$
 $= Q \tilde{U} \Sigma \tilde{V}^T$
 $= U \Sigma \tilde{V}^T$

Two ways

1) Fixed Precision Approximation

Statement

Given A and $\epsilon > 0$, seek a Q with ~~orthogonal columns~~ orthogonal columns and $k = k(\epsilon)$:
$$\|A - Q Q^T A\| \leq \epsilon \rightarrow (3)$$

Dimension k of the range of Q captures the action of A .

Pathway to Soln

SVD furnishes an optimal answer to this fixed precision problem. For each j
$$\min_{\text{rank}(X) \leq j} \|A - X\| \leq \sigma_{j+1} \rightarrow (4)$$

choosing $X = Q Q^T A$ where $Q_{m \times k}$ has k orthogonal left singular vectors of A which guarantees (3)

~~which guarantees~~

2) Fixed rank approx: Given A and k and an over sampling parameter $p > 0$, Construct Q with $(k+p)$ orthonormal columns

~~$\|A - Q Q^T A\|$~~ $\|A - Q Q^T A\| = \min_{\text{rank}(X) \leq k} \|A - X\| \rightarrow (5)$

Remark
~~Note~~

How randomness helps to solve fixed rank problem?

- Seek a basis for Range(A) with rank k:
- Let w be a random vector. ~~and $y = Aw$~~
Then $y = Aw$ is a random sample from Range(A)
- Build $Y = \{y_1, y_2, \dots, y_k\}$: $y_i = Aw_i$
- This set Y is in general position.
- Then orthogonalize Y .

Note:
oversampling
 $w_i \in \mathbb{R}^n$

Let $A = B + E$ $\begin{cases} B - \text{rank } k \\ E - \text{Perturbation} \end{cases}$
 $y_i = Aw_i = Bw_i + Ew_i \quad 1 \leq i \leq k+p \rightarrow (6)$

- Goal is to find a basis that covers B
- E shifts the direction sample vectors outside of the range of B which can prevent the $\text{Span}(Y)$ to cover the $\text{Range}(B)$
- The enriched set in (6) can reduce the leak outside of $\text{Range}(B)$

- Small p helps $p = 5$ to 10 .

- This is the basis for randomized algorithm.

Fixed Rank Algorithm: Proto-type

Given: $A \in \mathbb{R}^{m \times n}$ Target-Rank = k ,
over sampling parameter p .

output: $Q \begin{vmatrix} \\ \\ \end{vmatrix}_{m \times (k+p)}$

- 1) Draw $n \times (k+p)$ random matrix $R \begin{vmatrix} \\ \\ \end{vmatrix}_{n \times (k+p)}$
- 2) Compute $Y \begin{vmatrix} \\ \\ \end{vmatrix}_{m \times (k+p)} = A \begin{vmatrix} \\ \\ \end{vmatrix}_{m \times n} R \begin{vmatrix} \\ \\ \end{vmatrix}_{n \times (k+p)} = [y_1, y_2, \dots, y_{k+p}]$
- 3) orthonormalize the columns of $Y = QR$ and get $Q \begin{vmatrix} \\ \\ \end{vmatrix}_{m \times (k+p)}$. This is the basis for Range (A)

Gram-Schmidt
Householder
QR

Performance Analysis:

Theorem 1.1 $A \in \mathbb{R}^{m \times n}$, select a target-rank $k \geq 2$ and an oversize parameter $p \geq 2$ where $(k+p) < \min\{m, n\}$. Execute the prototype algorithm with $R = [R_i]$, $R_i \sim \text{i.i.d } N(0, 1)$ to obtain $Q \begin{vmatrix} \\ \\ \end{vmatrix}_{m \times (k+p)}$ with orthonormal columns.

Then

$$E \|A - QQ^T A\| \leq \left\{ \left[1 + \frac{4\sqrt{k+p}}{p-1} \right] (m \wedge n)^{1/2} \right\} \sigma_{k+1}$$

↓
(w.r. to random R) → (7)

known as a sharper than deterministic
analog based on RRR algorithm of
Gu and Eisenstat (1996)

Thanks to measure concentration: The
following holds:

$$\|A - QQ^T A\| \leq \left[1 + 11 \sqrt{k+p} \cdot (mn)^{1/2} \right] \sigma_{k+1}$$

holds with ^{probability} at least $(1 - 6p^{-p})$. $p=5$ gives
good result.

Historical Facts. (Existence)

Existence

1) Column selection: Every $A \in \mathbb{R}^{m \times n}$
contains a ~~submatrix~~ C with k ~~columns~~
columns s.t.

$$\|A - CC^+ A\| \leq \sqrt{1 + k(n-k)} \|A - A_{(k)}\|$$

where $A_{(k)}$ is the ~~best~~ k -rank approximation
to A . $\rightarrow (8)$

[A. F. Ruston (1964) "Auerbach's Theorem",
Math. Proc. Cambridge Phil. Society vol 56
(1964) pp 476-480

Note: Column selection is NP-hard.

Efficient deterministic RRR method
will achieve the above bound in (8)

2) using this there exists randomized
algorithm for fixed rank approximation:

$$\|A - QQ^T A\| \leq \min_{\text{rank}(X) \leq k} \|A - X\| \rightarrow (9)$$

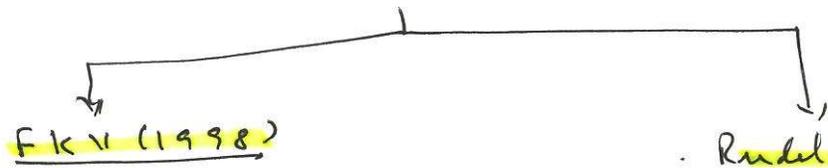
Column Selection

This approach use sampling probabilities based on

- (1) Squared 2-norms of rows / columns
- (2) Leverage Score that reflects the relative importance of columns

Columns are selected using this distribution

Earliest method for randomized column selection is by Frieze, Kannan, Vempala (1998)



Given A and $k(\epsilon, k)$ select B :

$$\|A - B\|_F \leq \|A - A_{(k)}\|_F + \epsilon \|A\|_F$$

Rudelson + Vershynin (2007)
 using the same sampling, proved $\| \cdot \|_2$ bounds

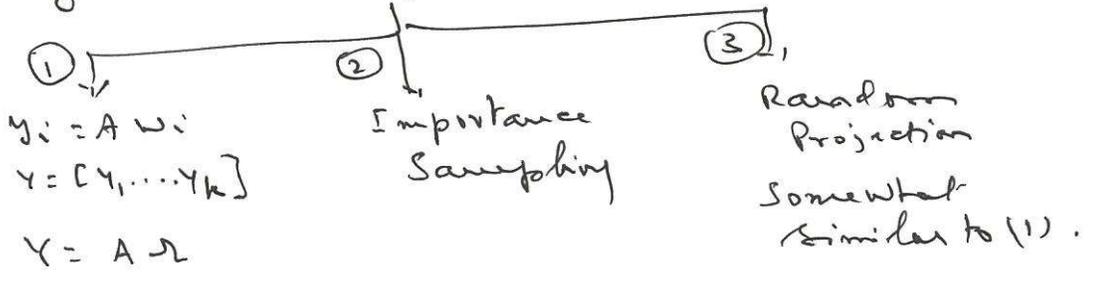
Deshpande et al (2006)
 $\|A - B\|_F \leq (1 + \epsilon) \|A - A_{(k)}\|_F$

3 Dimension reduction using random projection

- Started in 1984 - Johnson-Lindenstrauss
- l_2 embedding

Summary:-

Stage 1 is realized in one of 3 ways



Sampling based randomized algorithms

Fact $x \in \mathbb{R}^n$ a random vector

$\cdot E(x) \in \mathbb{R}^n$ → (1)

$\cdot \text{Var}(x) = E[\|x - E(x)\|^2]$

$= E[(x - E(x))^T (x - E(x))]$

$= \sum_i E(x_i - E(x_i))^2$ - Total Variance

$\cdot \text{Cov}(x) = E[(x - E(x))(x - E(x))^T]$ → (2)

$\cdot \text{Var}(x) = \text{tr}[\text{Cov}(x)]$ → (3)

$$E[xx^T - x^T E(x) - E(x)^T x + E^T(x)E(x)]$$

$$= E[xx^T] - E^T(x)E(x)$$

$$= E[\|x\|^2] - \|E(x)\|^2$$

(2a)

Problem 1

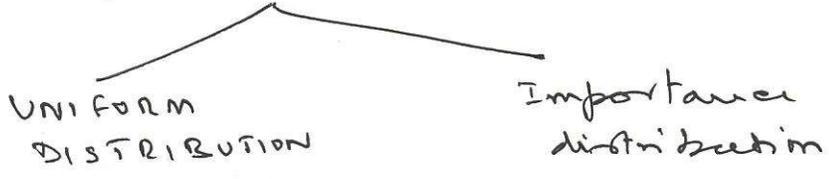
Matrix-vector product

$\cdot A \in \mathbb{R}^{m \times n}, v \in \mathbb{R}^n, Av = \sum_j A_{x_j} v_j \rightarrow (4)$
= sum of n vectors.

$\cdot (Av)$ can be estimated using a sample of column vectors of A

\cdot Error in the estimate is measured by the variance of the estimate.

\cdot Two ways to sample the columns:



Motivating

Exercise 1

Scaled Random Variable

A case for data dependent sampling

Let x be a r.v. and $x = \frac{a_i}{p_i}$ with prob = p_i with $\sum_{i=1}^n p_i = 1$. Let $n=2$ for simplicity

$$\begin{aligned}
 E(x) &= \frac{a_1}{p_1} \cdot p_1 + \frac{a_2}{p_2} \cdot p_2 = a_1 + a_2 \triangleq \bar{a} \\
 \text{Var}(x) &= p_1 \left[\frac{a_1}{p_1} - \bar{a} \right]^2 + p_2 \left[\frac{a_2}{p_2} - \bar{a} \right]^2 \\
 &= p_1 \left[\frac{a_1^2}{p_1^2} - \frac{2a_1\bar{a}}{p_1} + \bar{a}^2 \right] + p_2 \left[\frac{a_2^2}{p_2^2} + \bar{a}^2 - \frac{2a_2\bar{a}}{p_2} \right] \\
 &= \frac{a_1^2}{p_1} + \frac{a_2^2}{p_2} + (p_1 + p_2) \bar{a}^2 - (2a_1\bar{a} + 2a_2\bar{a}) \\
 &= \frac{a_1^2}{p_1} + \frac{a_2^2}{p_2} + \bar{a}^2 - 2\bar{a}(a_1 + a_2) \\
 &= \frac{a_1^2}{p_1} + \frac{a_2^2}{p_2} - (a_1 + a_2)^2
 \end{aligned}$$

Special Case Set $p_1 = p_2 = 1/2$ - uniform sampling

$$\begin{aligned}
 E(x) &= a_1 + a_2 \\
 \text{Var}(x) &= 2a_1^2 + 2a_2^2 - (a_1^2 + 2a_1a_2 + a_2^2) \\
 &= a_1^2 - 2a_1a_2 + a_2^2 = (a_1 - a_2)^2 > 0
 \end{aligned}$$

This is higher than the sampling below.

optimal p_1 & p_2 } What choice of p_i 's will min. $\text{Var}(x)$?
 $\text{Min} \left(\frac{a_1^2}{p_1} + \frac{a_2^2}{p_2} \right)$ when $p_1 + p_2 = 1$

$$L(p, \lambda) = \frac{a_1^2}{p_1} + \frac{a_2^2}{p_2} + \lambda (p_1 + p_2 - 1)$$

$$\frac{\partial L}{\partial p_1} = -\frac{a_1^2}{p_1^2} + \lambda = 0 \Rightarrow \lambda = \frac{a_1^2}{p_1^2} \Rightarrow \boxed{p_1 = \frac{a_1}{\lambda}}$$

$$\frac{\partial L}{\partial p_2} = -\frac{a_2^2}{p_2^2} + \lambda = 0 \Rightarrow \lambda = \frac{a_2^2}{p_2^2} \Rightarrow \boxed{p_2 = \frac{a_2}{\lambda}}$$

• But $p_1 + p_2 = 1 \Rightarrow \frac{a_1}{\sqrt{\lambda}} + \frac{a_2}{\sqrt{\lambda}} = 1 \Rightarrow a_1 + a_2 = \sqrt{\lambda}$

\therefore optimal $p_1^* = \frac{a_1}{a_1 + a_2}$ $p_2^* = \frac{a_2}{a_1 + a_2}$

$$\begin{aligned} \text{Var}(x) &= \frac{a_1^2}{p_1} + \frac{a_2^2}{p_2} - (a_1 + a_2)^2 \\ &= \frac{a_1^2 (a_1 + a_2)}{a_1} + \frac{a_2^2 (a_1 + a_2)}{a_2} - (a_1 + a_2)^2 \\ &= a_1 (a_1 + a_2) + a_2 (a_1 + a_2) - (a_1 + a_2)^2 \\ &= (a_1 + a_2)^2 - (a_1 + a_2)^2 = 0 \end{aligned}$$

\therefore Variance reduction is possible using a data dependent sampling distribution

• Return to Matrix-Vector multiply

• What is a good sampling distribution for the columns of A ?

key step

• Define a random vector $x = \frac{A_{*j} N_j}{p_j}$
with probability p_j , $1 \leq j \leq n$

• scaled random vector scaled by p_j

$$E(x) = \sum_j p_j \frac{A_{*j} N_j}{p_j} = \sum A_{*j} N_j = AN \rightarrow (4)$$

(ii) x is an unbiased random vector

$$\text{Var}(x) = E \|x\|^2 - \|E(x)\|^2 \quad \text{from (2a) in page 10}$$

$$= \sum_j \frac{\|A_{xj} v_j\|^2}{p_j^2} p_j - \|AV\|^2 \quad \text{From (4)}$$

$$(\because \|a\| = |a| \|x\|)$$

$$= \sum_j \frac{N_j \|A_{xj}\|^2}{p_j} - \underbrace{\|AV\|^2}_{\substack{\downarrow \\ \text{Constant} \\ \text{w.r. to } p_j}} \rightarrow (5)$$

Similar to the example

choice of p_j depends on the first term on the r. h. s. of (5).

LS_{col}(A) - [Distribution that depends on the squared length of columns of A]

choice of p_j

$$\begin{aligned} \text{column } j \text{ is picked with prob. } p_j &= \frac{\|A_{xj}\|^2}{\sum_j \|A_{xj}\|^2} \\ &= \frac{\|A_{xj}\|^2}{\|A\|_F^2} \rightarrow (6) \end{aligned}$$

Substitute (6) in (5)

$$\text{Var}(x) = \sum_j N_j \frac{\|A_{xj}\|^2}{\|A_{xj}\|^2} \cdot \|A\|_F^2 - \|AV\|^2$$

$$= \|A\|_F^2 \sum_j N_j - \|AV\|^2$$

$$= \|A\|_F^2 \|N\|_2 - \|AV\|^2$$

$$\leq \|A\|_F^2 \|N\|_2 \rightarrow (7)$$

useful when $\|AV\|$ is comparable to $\|A\|_F \|N\|_2$

$$\mathcal{S}_{\text{sol}}(A) = \{p_1, p_2, \dots, p_m \mid \sum p_j = 1, p_j \text{ is in (6)}\}$$

To approximate AV :

- Perform λ trials (with replacement) and take the average

$$Y = \frac{1}{\lambda} \sum_{t=1}^{\lambda} \left[\frac{A \cdot j_t \cdot \mathbb{1}_{j_t}}{p_{j_t}} \right] \approx AV$$

$$= \frac{1}{\lambda} \sum_{t=1}^{\lambda} x_t = \sum_t \left(\frac{x_t}{\lambda} \right)$$

$$\therefore E(Y) = \frac{1}{\lambda} \sum_{t=1}^{\lambda} E(x_t) = \frac{\lambda(AV)}{\lambda} = AV$$

$$\text{Var}(Y) = \frac{1}{\lambda^2} \sum_t \text{Var}(x_t) \quad [\text{using (7)}]$$

$$\leq \frac{1}{\lambda^2} \cdot \left[\sum_{j=1}^m \|A\|_F \|N\|_2^2 \right]$$

$$= \frac{1}{\lambda} \|A\|_F^2 \|N\|_2^2 \rightarrow (8)$$

Note:-

(1) We could row sampling as well using a similar argument to get $RS(A)$ distribution.

Problem 2

MATRIX-MATRIX Product

$$C = A | B |$$

$m \times n \quad n \times k$

Three ways of multiplying Matrices

$$C = AB = (AB_{*1}, AB_{*2}, \dots, AB_{*k})$$

- Apply Matrix-Vector product routine k times and collate the result.

claim: $[n$ is the common # of columns of A and rows of B .

- Define p_i : $\sum_{i=1}^n p_i = 1$

- Define a random matrix $X_j = \frac{A_{*j} B_{j*}}{p_j} \rightarrow (1)$

with probability p_j , $1 \leq j \leq n$

$$E(X) = \sum_{j=1}^n X_j p_j = \sum_{j=1}^n A_{*j} B_{j*} = AB \rightarrow (2)$$

$$p_j = \frac{\|A_{*j}\|^2 \|B_{j*}\|^2}{\sum_{j=1}^n \|A_{*j}\|^2 \|B_{j*}\|^2} \quad 1 \leq j \leq n \rightarrow (3)$$

~~Define~~ Define $Y = \frac{1}{n} \sum_{t=1}^n X_t = \frac{1}{n} \sum_{t=1}^n \left(\frac{A_{*j_t} B_{j_t*}}{p_{j_t}} \right)$

$$E(Y) = AB \Rightarrow \text{unbiased} \rightarrow (4)$$

$$\text{Var}(Y) = \frac{1}{n} \sum_{t=1}^n \frac{\|A_{*j_t}\|^2 \|B_{j_t*}\|^2}{p_{j_t}} \rightarrow (5)$$

using p_j as in (3)

$$= \|AB\|_F^2$$

$$\leq \frac{1}{n} \|A\|_F^2 \|B\|_F^2 \rightarrow (6)$$

Implementation

• let k_1, k_2, \dots, k_s be s integers chosen in s trials.

• Then, ~~the~~

$$\frac{1}{s} \sum x_i = \frac{1}{s} \left[\frac{A_{\times k_1} B_{k_1 \times}}{p_{k_1}} + \frac{A_{\times k_2} B_{k_2 \times}}{p_{k_2}} + \dots + \frac{A_{\times k_s} B_{k_s \times}}{p_{k_s}} \right]$$

$$= [A_{\times k_1}, A_{\times k_2}, \dots, A_{\times k_s}] \begin{bmatrix} B_{k_1 \times} / s p_{k_1} \\ B_{k_2 \times} / s p_{k_2} \\ \vdots \\ B_{k_s \times} / s p_{k_s} \end{bmatrix}$$

$$= C \tilde{B}$$

↓
chosen columns of A

↙ chosen rows of \tilde{B}
scaled by $s p_k$

$$\begin{bmatrix} A \\ m \times n \end{bmatrix} \begin{bmatrix} B \\ n \times p \end{bmatrix} \approx \begin{bmatrix} C \\ m \times s \end{bmatrix} \begin{bmatrix} \tilde{B} \\ s \times p \end{bmatrix} \rightarrow \textcircled{7}$$

• Error bound is given by (6) above.

Special cases:

1) If $B = A^T$, we can approximate the Gramian AA^T and hence the singular values of A .

2) When $B = A^T$: start with

$$\begin{aligned} \text{var}(Y) &\leq \frac{1}{n} \sum \frac{\|A\|_F^2 \|A^T\|_F^2}{p_j} - \|AA^T\|_F^2 \\ &= \frac{1}{n} \sum \frac{\|A\|_F^4}{p_j} - \|AA^T\|_F^2 \rightarrow (8) \end{aligned}$$

minimize w.r. to p_j

Exercise 2 let a_1, a_2, \dots, a_n be \neq real numbers.

Prove that $\sum_{j=1}^n \frac{a_j}{x_j}$ when $\sum x_j = 1$ attains the minimum when $x_j = \frac{\sqrt{a_j}}{\sum \sqrt{a_j}}$. (See Exercise 1)

Problem 3. Low rank approximation for A is

Sketch

called sketch of A, where the columns and rows each picked in ~~individual~~ individual trials based on importance distribution based on squared lengths of columns/rows is a good sketch. let $A \in \mathbb{R}^{m \times n}$

- 1) Pick k columns of A and form $C \in \mathbb{R}^{m \times k}$ based on $LS_{col}(A)$
- 2) Pick r rows of A from $LS_{row}(A)$ and form $R \in \mathbb{R}^{r \times n}$
- 3) Using C and R express: $A \approx CUR$ by computing U

Note: You may think of using SVD to get a good sketch. While it is true, it takes a long time: $A = U \Sigma V^T$

A comparison with SVD

- Besides ^{in SVD} the columns of U and rows of V are ~~not or combinations of those of A~~ not directly ~~related to those of A~~ from A but are linear combinations.
- In here, we directly pick the columns and row of A by sampling and is called interpolative approximation
- SVD gives best approximation, the CUR is not optimal in that sense.

How to choose U? $A \in \mathbb{R}^{m \times n}$

1) An Intuition: $A = AI$

- Sample s columns of A and get $C |_{m \times s}$
- Let w be the corresponding s rows of I scaled as w matrix-matrix product.

• $A = AI = CW \longrightarrow \textcircled{1}$

• From (b): $\|AI - CW\|_F^2 \leq \frac{\|A\|_F^2 \|I\|_F^2}{s}$
 $= \|A\|_F^2 \left(\frac{n}{s}\right) \rightarrow \textcircled{2}$

• Since we need $s > n$, this is not viable, but the idea stands.

2) modification: $A \in \mathbb{R}^{m \times n}$

• Consider $C |_{m \times s}$ and $R_{n \times n}$ that we selected earlier, where $s < m, r < n$.

• If R is of full-rank, then

$RR^T |_{n \times n}$ is SPD

$R^+ = R^T (RR^T)^{-1}$ is the Moore-Penrose inverse

$P = R^T (RR^T)^{-1} R$ is the projection onto the row space of R .

• Recall P acts as identity on the ~~row~~ row space of R .

Illustration

eg: $R = (1, 1) \quad RR^T = (1, 1) \begin{pmatrix} 1 \\ 1 \end{pmatrix} = 2$

$R^+ = R^T (RR^T)^{-1} = \frac{1}{2} \begin{pmatrix} 1 \\ 1 \end{pmatrix}$

$P = R^T (RR^T)^{-1} R = \frac{1}{2} \begin{pmatrix} 1 \\ 1 \end{pmatrix} (1, 1) = \frac{1}{2} \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}$

Row space of R $y = R^T a \Rightarrow Py = R^T (RR^T)^{-1} RR^T a = R^T a = y$
 $a = \begin{pmatrix} a_1 \\ a_2 \end{pmatrix}$

So we can replace i by P in the above analysis.

$$AP = A \underbrace{R^T (R R^T)^{-1} R}_{U} \approx CUR$$

$$U = R^T (R R^T)^{-1}$$

\therefore By the inequality (b):

$$E \left[\|AP - CUR\|_2^2 \right] \leq E \left[\|AP - CUR\|_F^2 \right]$$

$$\leq \frac{\|A\|_F^2 \|P\|_F^2}{\underbrace{\quad}} = \|A\|_F^2 \left(\frac{\lambda}{\lambda} \right)$$

$\rightarrow (3)$

where $\|P\|_F^2 = \lambda$. (why?)

Recall $\|A\|_F^2 = \text{tr}(A A^T)$

$$\Rightarrow \|P\|_F^2 = \text{tr}[P] = \text{tr}[R^T (R R^T)^{-1} R]$$

$$\boxed{\text{tr}(AB) = \text{tr}(BA)} = \text{tr}[R R^T (R R^T)^{-1}]$$

$$= \text{tr}[\Sigma_n] = n \rightarrow (4)$$

Combining:

$$A - CUR = A - AP + AP - CUR$$

$$\|A - CUR\|_2 \leq \|A - AP\|_2 + \|AP - CUR\|_2$$

Triangle inequality

Recall: $x \leq y + z$

$$\Rightarrow x^2 \leq (y + z)^2 = y^2 + 2yz + z^2 \leq 2(y^2 + z^2)$$

$$\Rightarrow 0 \leq (y^2 - 2yz + z^2) = (y - z)^2$$

$$\therefore \|A - CUR\|_2^2 \leq 2 \|A - AP\|_2^2 + 2 \|AP - CUR\|_2^2$$

$$\|A\|_2 \leq \|A\|_F$$

$R_{n \times n}$
 $R^T_{n \times n}$
 $P_{n \times n}$
 $(R R^T)_{n \times n}$