Introduction to randomization and sketching techniques

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Plan

Some background

Random sketching

Randomization for least-squares problem

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Singular value decomposition

For any given $A \in \mathbb{R}^{m \times n}$, $m \ge n$ its singular value decomposition is

$$A = U\Sigma V^{T} = \begin{pmatrix} U_1 & U_2 & U_3 \end{pmatrix} \cdot \begin{pmatrix} \Sigma_1 & 0 \\ 0 & \Sigma_2 \\ 0 & 0 \end{pmatrix} \cdot \begin{pmatrix} V_1 & V_2 \end{pmatrix}^{T}$$

where for a given k,

- $U \in \mathbb{R}^{m \times m}$ is orthogonal matrix, the left singular vectors of A, U_1 is $m \times k$, U_2 is $m \times n k$, U_3 is $m \times m n$
- $\Sigma \in \mathbb{R}^{m \times n}$, its diagonal is formed by $\sigma_1(A) \ge ... \ge \sigma_n(A) \ge 0$ Σ_1 is $k \times k$, Σ_2 is $n - k \times n - k$
- $V \in \mathbb{R}^{n \times n}$ is orthogonal matrix, the right singular vectors of A, V_1 is $n \times k$, V_2 is $n \times n k$

Eigenvalues of a symmetric matrix

Symmetric Schur Decomposition

if $A \in \mathbb{R}^{n \times n}$ is symmetric, there exists a real orthogonal Q such that

$$Q^T A Q = diag(\lambda_1, ..., \lambda_n), \text{ for } k = 1, ..., n$$

 $AQ(:, k) = \lambda_k Q(:, k)$

Courant-Fischer Minimax Theorem

If $A \in \mathbb{R}^{n \times n}$ is symmetric, then

$$\lambda_k(A) = \max_{\dim(S)=k} \min_{0 \neq y \in S} \frac{y^T A y}{y^T y}, \text{ for } k = 1, \dots, n$$

Properties of SVD

Given $A = U\Sigma V^T$, we have

- $A^T A = V \Sigma^T \Sigma V^T$, the right singular vectors of A are a set of orthonormal eigenvectors of $A^T A$.
- $AA^T = U\Sigma^T\Sigma U^T$, the left singular vectors of A are a set of orthonormal eigenvectors of AA^T .
- The non-negative singular values of A are the square roots of the non-negative eigenvalues of A^TA and AA^T .
- If $\sigma_k \neq 0$ and $\sigma_{k+1}, \dots, \sigma_n = 0$, then $Range(A) = span(U_1)$, $Null(A) = span(V_2)$, $Range(A^T) = span(V_1)$, $Null(A) = span(U_2 \ U_3)$.

Norms and condition number

$$||A||_{2} = \sigma_{max}(A) = \sigma_{1}(A)$$

$$||A||_{F} = \sqrt{\sum_{i=1}^{m} \sum_{j=1}^{n} |a_{ij}|^{2}} = \sqrt{\sigma_{1}^{2}(A) + \dots \sigma_{n}^{2}(A)}$$

$$||A||_{*} = \sigma_{1}(A) + \dots \sigma_{n}(A)$$

$$\kappa(A) = \frac{\sigma_{max}(A)}{\sigma_{min}(A)} = \sqrt{||A^{T}A||_{2} ||(A^{T}A)^{-1}||_{2}}$$

Some properties:

$$\max_{i,j} |A(i,j)| \leq ||A||_2 \leq \sqrt{mn} \max_{i,j} |A(i,j)|$$
$$||A||_2 \leq ||A||_F \leq \sqrt{min(m,n)} ||A||_2$$

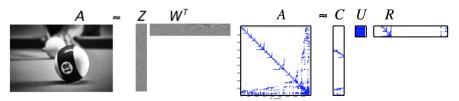
Orthogonal Invariance: If $Q \in \mathbb{R}^{m \times m}$ and $Z \in \mathbb{R}^{n \times n}$ are orthogonal, then

$$||QAZ||_F = ||A||_F$$

 $||QAZ||_2 = ||A||_2$

Low rank matrix approximation

■ Problem: given $A \in \mathbb{R}^{m \times n}$, compute rank-k approximation ZW^T , where Z is $m \times k$ and W^T is $k \times n$.



- Problem with diverse applications
 - □ from scientific computing: fast solvers for integral equations, H-matrices
 - □ to data analytics: principal component analysis, image processing, ...

$$Ax \to ZW^T x$$
Flops $2mn \to 2(m+n)k$

Low rank matrix approximation

■ Best rank-k approximation $A_{opt,k} = U_k \Sigma_k V_k^T$ is rank-k truncated SVD of A [Eckart and Young, 1936]



$$\min_{rank(A_k) \le k} ||A - A_k||_2 = ||A - A_{opt,k}||_2 = \sigma_{k+1}(A)$$
 (1)

$$\min_{rank(A_k) \le k} ||A - A_k||_F = ||A - A_{opt,k}||_F = \sqrt{\sum_{j=k+1}^n \sigma_j^2(A)}$$
 (2)

Image, size 1190×1920



Rank-10 approximation, SVD



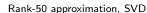




Image source: https://pixabay.com/photos/billiards-ball-play-number-half-4345870/

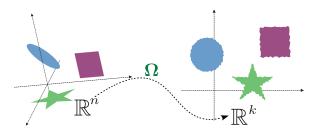
Plan

Some background

Random sketching

Randomization for least-squares problem

Random sketching



Sketching: embedding of a high dimensional subspace into a low dimensional one, while preserving some geometry, with high probability

Applications: least squares problems, low rank matrix approximation, data compression, column subset selection, orthogonalization of set of vectors, Krylov subspace methods, . . .

References: [Johnson and Lindenstrauss, 1984, Dasgupta and Gupta, 2003], [Martinsson and Tropp, 2020]

Image courtesy of O. Balabanov

RandBLAS and RandLAPACK

Ongoing effort to define standards similar to BLAS/LAPACK, organized as

- drivers: few and simple
- computational routines: building blocks for the drivers

RandBLAS - data-oblivious sketching routines

- generate a sketching operator
- apply a sketching operator to a matrix

RandLAPACK: linear algebra problems solved through randomization, e.g.

- least squares
- low rank approximation
- linear solvers
- advanced sketching: leverage scores, sketching operators with tensor product structures

RandBLAS and RandLAPACK

Randomized Numerical Linear Algebra: A Perspective on the Field With an Eye to Software, R. Murray et al, describes:

- basic sketching: dense and sparse sketching operators
- least squares and optimization
- low rank approximation
- full rank matrix decompositions
- kernel methods as arising in machine learning models
- linear solvers and trace estimation
- advanced sketching: leverage scores, sketching operators with tensor product structures

References on RandNLA

Many references available, as:

- Sketching As a Tool for Numerical Linear Algebra [Woodruff, 2014]
- Finding Structure with Randomness: Probabilistic Algorithms for Constructing Approximate Matrix Decompositions [Halko et al., 2011]
- Randomized Numerical Linear Algebra: Foundations and Algorithms [Martinsson and Tropp, 2020]

ε -subspace embedding property

For a given subspace $\mathcal{V} \subset \mathbb{R}^m$ and $\varepsilon \in (0,1)$, a sketching matrix $\Omega \in \mathbb{R}^{l \times m}$ is an ε -embedding for \mathcal{V} if for all $x_i, x_i \in \mathcal{V}$, we have

$$|\langle \Omega x_i, \Omega x_j \rangle - \langle x_i, x_j \rangle| \le \epsilon ||x_i||_2 ||x_j||_2 \tag{3}$$

- If $x_i = x_j$ we obtain $\|\Omega x_i\|_2^2 = (1 \pm \epsilon) \|x_i\|_2^2$.
- It can also be expressed as: given all vectors $x_i, x_j \in V$ are rescaled to be unit vectors, then for all $x_i, x_i \in V$ we require to hold:

$$\|\Omega(x_i + x_j)\|_2^2 = (1 \pm \epsilon) \|x_i + x_j\|_2^2$$
 (4)

Proof that we obtain relation (3):

$$\langle \Omega x_{i}, \Omega x_{j} \rangle = (\|\Omega(x_{i} + x_{j})\|_{2}^{2} - \|\Omega x_{i}\|_{2}^{2} - \|\Omega x_{j}\|_{2}^{2})/2$$

$$= ((1 \pm \epsilon)\|x_{i} + x_{j}\|_{2}^{2} - (1 \pm \epsilon)\|x_{i}\|_{2}^{2} - (1 \pm \epsilon)\|x_{j}\|_{2}^{2})/2$$

$$= \langle x_{i}, x_{j} \rangle \pm O(\epsilon)$$

ε -subspace embedding property

Let W be a matrix whose columns form a basis for $\mathcal V$. For simplicity, we refer to an ε -subspace embedding for $\mathcal V$ as an ε -embedding for W.

Corollary 1 (Corollary 2.2 in [Balabanov and Grigori, 2022])

If $\Omega \in \mathbb{R}^{l \times m}$ is an ε -embedding for W, then the singular values of W are bounded by

$$(1+\varepsilon)^{-1/2}\sigma_{\min}(\Omega W) \leq \sigma_{\min}(W) \leq \sigma_{\max}(W) \leq (1-\varepsilon)^{-1/2}\sigma_{\max}(\Omega W).$$

Proof.

Let $a \in \mathbb{R}^{\dim(\mathcal{V})}$ be an arbitrary vector and x = Wa. By definition of Ω ,

The statement of proposition then follows by using definitions of the minimal and the maximal singular values of a matrix.

Oblivious subspace embedding

Aim: construct Ω such that for any n-dimensional subspace $\mathcal{V} \subset \mathbb{R}^m$

$$\mathbb{P}(\Omega \text{ is } \varepsilon\text{-embedding for } \mathcal{V}) \geq 1 - \delta$$

Definition: oblivious subspace embedding

A random matrix $\Omega \in \mathbb{R}^{l \times m}$ is an oblivious subspace embedding with parameters $\mathsf{OSE}(n,\epsilon,\delta)$ if with probability at least $1-\delta$ for any n-dimensional subspace $\mathcal{V} \subset \mathbb{R}^m$, for all $x_i, x_i \in \mathcal{V}$, we have

$$|\langle \Omega x_i, \Omega x_j \rangle - \langle x_i, x_j \rangle| \le \epsilon ||x_i||_2 ||x_j||_2$$
(5)

Oblivious subspace embedding (contd)

With high probability, OSEs have bounded norm.

Corollary 2 (Corollary 2.4 in [Balabanov and Grigori, 2022])

If $\Omega \in \mathbb{R}^{l \times m}$ is a $(\varepsilon, \delta/m, 1)$ oblivious ℓ_2 -subspace embedding, then with probability at least $1 - \delta$, we have

$$\|\Omega\|_F \leq \sqrt{(1+\varepsilon)m}$$
.

Proof.

It directly follows from the definition of oblivious embedding, (5), and the union bound argument that Ω is an ε -embedding for each canonical (Euclidean) basis vector. This implies that the ℓ_2 -norms of the columns of Ω are bounded from above by $\sqrt{1+\varepsilon}$. The statement of the corollary then follows immediately.

Random sketching matrices

- $\Omega \in \mathbb{R}^{I \times m}$ whose entries are independent standard normal random variables, multiplied by $1/\sqrt{I}$
 - \square Ω is $OSE(n, \epsilon, \delta)$ with $I = \mathcal{O}(\epsilon^{-2}(n + \log \frac{1}{\delta}))$
 - □ Cost of computing ΩW , $W \in \mathbb{R}^{m \times n}$: 2mnl flops
 - \square Relies on BLAS3 operations when W is dense
- Easy to parallelize, $\Omega W = \sum_{i=1}^{P} \Omega_i W_i$

$$\Omega W = \begin{pmatrix} \Omega_1 & \dots & \Omega_P \end{pmatrix} \begin{pmatrix} W_1 \\ \vdots \\ W_P \end{pmatrix} = \sum_{i=1}^P \Omega_i W_i$$

- □ Each processor i owns a block $\Omega_i \in \mathbb{R}^{l \times m/P}$ and a block $W_i \in \mathbb{R}^{m/P \times n}$
- □ Each processor computes $\Omega_i W_i \in \mathbb{R}^{I \times n}$
- □ Sum-Reduce among all processors to compute $\Omega W = \sum_{i=1}^{P} \Omega_i W_i$
- Cost of the algorithm

$$(2mnI/P)\gamma + \log_2 P\alpha + \ln\log_2 P\beta$$

Fast Johnson-Lindenstrauss transform

Find sparse or structured Ω such that computing ΩW is cheap, e.g. a subsampled random Hadamard transform (SRHT).

Given $m = 2^q, l < m$, the SRHT ensemble embedding \mathbb{R}^m into \mathbb{R}^l is defined as

$$\Omega = \sqrt{\frac{m}{I}} \cdot P \cdot H \cdot D, \text{ where}$$
 (6)

- $D \in \mathbb{R}^{m \times m}$ is diagonal matrix of uniformly random signs, random variables uniformly distributed on ± 1
- lacksquare $H \in \mathbb{R}^{m imes m}$ is the normalized Walsh-Hadamard transform
- $P \in \mathbb{R}^{I \times m}$ formed by subset of I rows of the identity, chosen uniformly at random (draws I rows at random from HD).

References: Sarlos'06, Ailon and Chazelle'06, Liberty, Rokhlin, Tygert and Woolfe'06.

Fast Johnson-Lindenstrauss transform (contd)

Definition of Normalized Walsh-Hadamard Matrix

For given $m = 2^q$, $H_m \in \mathbb{R}^{m \times m}$ is the non-normalized Walsh-Hadamard transform defined recursively as,

$$H_2 = \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}, \quad H_m = \begin{pmatrix} H_{m/2} & H_{m/2} \\ H_{m/2} & -H_{m/2} \end{pmatrix}.$$
 (7)

The normalized Walsh-Hadamard transform is $H = m^{-1/2}H_m$.

Cost of matrix vector multiplication:

For $w \in \mathbb{R}^m$ and $\Omega \in \mathbb{R}^{l \times m}$, computing Ωw costs $2m \log_2 m$ flops.

Random sketching matrices - SRHT

• $\Omega \in \mathbb{R}^{I \times m}$ is a fast Johnson-Lindenstrauss transform, e.g. a subsampled randomized Hadamard transform (SRHT)¹

$$\Omega = \sqrt{\frac{m}{I}} \cdot R \cdot H \cdot D, \text{ where}$$
 (8)

 $D \in \mathbb{R}^{m \times m}$ is diagonal with independent random signs, $H \in \mathbb{R}^{m \times m}$ is normalized Walsh-Hadamard matrix, $R \in \mathbb{R}^{l \times m}$ draws l rows uniformly at random from HD.

- $\ \square$ $\ \Omega$ is $\mathsf{OSE}(n,\epsilon,\delta)$ with $I = \mathcal{O}(\epsilon^{-2} \left(n + \ln \frac{m}{\delta}\right) \ln \frac{n}{\delta})$
- □ Cost of computing ΩW , $W \in \mathbb{R}^{m \times n}$ on P processors:

$$\frac{2mn\log_2 m}{P}\gamma + \log_2 P\alpha + \frac{mn}{P}\log_2 P\beta$$

^{1.} Ailon and Chazelle'06, Liberty, Rokhlin, Tygert and Woolfe'06, Sarlos'06.

Block SRHT for parallelization on P processors

• Ω as in (9) is $OSE(n, \epsilon, \delta)$ with $I = \mathcal{O}(\epsilon^{-2} \left(n + \ln \frac{m}{\delta}\right) \ln \frac{n}{\delta})$

$$\Omega = [\Omega_1 \quad \Omega_2 \quad \dots \quad \Omega_P] = \sqrt{\frac{m}{Pl}} \cdot \begin{bmatrix} D_{L1} & \dots & D_{LP} \end{bmatrix} \begin{bmatrix} RH & & & \\ & \ddots & & \\ & & RH \end{bmatrix} \begin{bmatrix} D_{R1} & & & \\ & \ddots & & \\ & & D_{RP} \end{bmatrix}, \tag{9}$$

where $\Omega_i = \sqrt{\frac{m}{P!}} D_{Li} R H D_{Ri}$, D_{Li} , $D_{Ri} \in \mathbb{R}^{m/P \times m/P}$ are diagonal with independent random signs, $H \in \mathbb{R}^{m/P \times m/P}$ is normalized Walsh-Hadamard matrix, $R \in \mathbb{R}^{l \times m/P}$ is uniform sampling matrix.

Parallelize as [Balabanov et al., 2022]:

$$\Omega W = \sqrt{\frac{m}{Pl}} \sum_{i=1}^{P} D_{Li} R H D_{Ri} W_i$$

Parallelization of block SRHT

Considering each processor i owns a block $W_i \in \mathbb{R}^{m/P \times n}$, parallelize as:

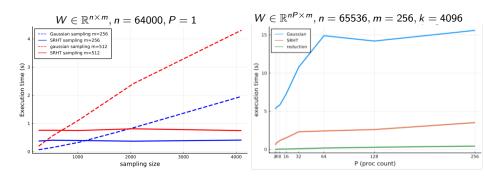
$$\begin{split} \Omega W &= \left(\Omega_1 \quad \dots \quad \Omega_P\right) \begin{pmatrix} W_1 \\ \vdots \\ W_P \end{pmatrix} = \left(\sqrt{\frac{m}{Pl}} D_{L1} R H D_{R1} \quad \dots \quad \sqrt{\frac{m}{Pl}} D_{LP} R H D_{RP} W_P\right) \begin{pmatrix} W_1 \\ \vdots \\ W_P \end{pmatrix} \\ &= \sum_{i=1}^{P} \sqrt{\frac{m}{Pl}} D_{Li} R H D_{Ri} W_i \end{split}$$

- Root processor broadcasts seed of R
- Each processor i draws R, D_{Li}, D_{Ri}
- Each processor computes $\Omega_i W_i = \sqrt{\frac{m}{Pl}} D_{Li} RH D_{Ri} W_i$, $\Omega_i W_i \in \mathbb{R}^{l \times n}$
- Sum-Reduce among all processors to compute $\Omega W = \sum_{i=1}^{P} \Omega_i W_i$

Cost of the algorithm (some lower order terms ignored)

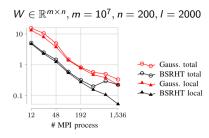
$$2mn\log_2 m/P\gamma + \log_2 P\alpha + ln\log_2 P\beta$$

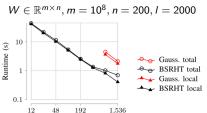
Performance of Gaussian vs block SRHT



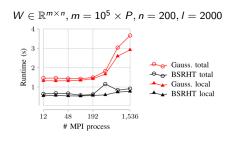
 Results obtained in Julia on nodes formed by 2 Cascade Lake Intel Xeon 5218, 16 cores each, 2.4GHz/core

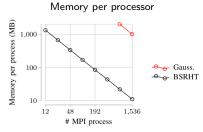
Performance of Gaussian vs SRHT





MPI process



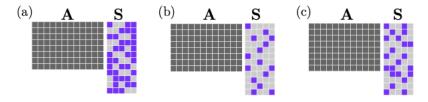


Machine: Intel Skylake 2.7GHz (AVX512), 48 cores per node

Sparse sketching operators

Can be grouped into three categories:

- Short-axis-sparse sketching operators (SASOs)
- Long-axis-sparse sketching operators (LASOs)
- lid-sparse sketching operators



(a) SASO with 3 nnz per row, (b) LASO with 3 nnz per column, and (c) an iid-sparse sketching operator with iid non-zero entries.

For a more detailed description, see section 2.4 of [Murray et al., 2023], figure from that book, S is the sketching matrix.

Short-axis-sparse sketching operators

Suppose the sketching matrix $S \in \mathbb{R}^{m \times l}$, with $l \ll m$. The short-axis vectors of a SASO should be independent of one another.

Select the locations of *k* nonzero elements as:

- sample k indices uniformly from [m] without replacement, once for each column, or
- divide [m] into k contiguous subsets of equal size, and then for each column select one index (independently and uniformly) from each of the k index sets.

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Solving least squares problems

Given $W \in \mathbb{R}^{m \times n}$ full-rank and $b \in \mathbb{R}^m$, with $n \ll m$, solve

$$y := \arg\min_{x \in \mathbb{R}^n} \|Wx - b\|_2$$

The unique solution is

$$y = W^+ b, \quad W^+ = (W^T W)^{-1} W^T$$

Solve by using the QR factorization of W (see lecture on dense QR)

$$W = QR = \begin{pmatrix} \tilde{Q} & \bar{Q} \end{pmatrix} \begin{pmatrix} \tilde{R} \\ 0 \end{pmatrix} \tag{10}$$

We obtain

$$||r||_{2}^{2} = ||b - Wx||_{2}^{2} = ||b - (\tilde{Q} \quad \bar{Q}) \begin{pmatrix} R \\ 0 \end{pmatrix} x||_{2}^{2}$$

$$= ||(\tilde{Q}^{T}) b - (\tilde{R}) x||_{2}^{2} = ||(\tilde{Q}^{T} b - \tilde{R} x) ||_{2}^{2}$$

$$= ||\tilde{Q}^{T} b - \tilde{R} x||_{2}^{2} + ||\tilde{Q}^{T} b||_{2}^{2}$$

Solve $\tilde{R}x = \tilde{Q}^T b$ to minimize $||r||_2$.

Least squares problems

Solve by using the normal equations,

$$W^T W x = W^T b$$

- 1. with direct methods multiply W^TW and compute the Cholesky factorization of the result
- 2. or with iterative methods without computing explicitely W^TW use a Krylov subspace solver and at each iteration multiply W^TW with a vector

Randomized least squares - sketch and solve

Solve by using randomization, with $\Omega \in \mathbb{R}^{I \times m}$ being $\mathsf{OSE}(n+1,\epsilon,\delta)$ for $\mathcal{V} = \mathit{range}([W,b])$

$$y_s := arg \min_{x \in \mathbb{R}^n} \|\Omega(Wx - b)\|_2$$

or $y_s = (\Omega W)^{\dagger}(\Omega b)$ We obtain with probability $1 - \delta$:

$$||Wy_s - b||_2^2 \le (1 + \varepsilon)||Wy - b||_2^2$$

Proof omitted, but can be found in [Sarlos, 2006]. It can be easily proven that:

$$egin{aligned} \min_{x \in \mathbb{R}^n} \|\Omega(\mathit{W}x - b)\|_2 &= \|\Omega(\mathit{W}y_s - b)\|_2 \leq \|\Omega(\mathit{W}y - b)\|_2 \ &\leq (1 + arepsilon) \|\mathit{W}y - b\|_2 \end{aligned}$$

Randomized least squares - sketch and precondition

Sketch the least squares problem to obtain a preconditioner, and solve a preconditioned least squares problem [Rokhlin and Tygert, 2008], that is

- Compute $S = \Omega W$, $S \in \mathbb{R}^{I \times n}$
- Compute the (rank revealing) QR factorization $S = Q_s R_s \Pi$, $P_s = R_s \Pi$, where Π is a permutation matrix, $Q_s \in \mathbb{R}^{l \times n}$ has orthonormal columns
- Use P_s as a preconditioner and solve $\arg\min_{z\in\mathbb{R}^n}\|WP_s^{-1}z-b\|_2$, with WP_s^{-1} being a well conditioned matrix
- Compute the solution to $arg \min_{x \in \mathbb{R}^n} \|Wx b\|_2$ as $x = P_s^{-1}z$

A more detailed discussion on rank revealing QR will be provided in a future lecture.

Sketch and precondition (contd)

The following results hold:

$$\kappa(WP_{S}^{-1}) = \frac{\sigma_{max}(WP_{s}^{-1})}{\sigma_{min}(WP_{s}^{-1})} \le \frac{1+\varepsilon}{1-\varepsilon}$$

Sketch of the proof from [Rokhlin and Tygert, 2008]. Consider the following SVD decompositions of $W \in \mathbb{R}^{m \times n}$ and $(\Omega U) \in \mathbb{R}^{l \times n}$:

$$\begin{array}{lll} W & = & U \Sigma V^T, \, U \in \mathbb{R}^{m \times n}, \, \Sigma \in \mathbb{R}^{n \times n}, \, V \in \mathbb{R}^{n \times n} \\ \Omega U & = & \tilde{U} \tilde{\Sigma} \tilde{V}^T, \, \tilde{U} \in \mathbb{R}^{m \times n}, \, \tilde{\Sigma} \in \mathbb{R}^{n \times n}, \, \tilde{V} \in \mathbb{R}^{n \times n} \end{array}$$

It can be shown that $\tilde{U}=Q_s\tilde{Q}$, where $\tilde{Q}\in\mathbb{R}^{n\times n}$ is orthogonal. We obtain:

$$P_{s} = W\tilde{\Sigma}\tilde{V}^{T}\Sigma V^{T}$$

$$WP_{s}^{-1} = U\tilde{V}\tilde{\Sigma}^{-1}\tilde{Q}^{T}$$

$$\|(WP_{s}^{-1})^{T}(WP_{s}^{-1})\|_{2} = \|\tilde{\Sigma}^{-1}\|_{2}$$

$$\|((WP_{s}^{-1})^{T}(WP_{s}^{-1}))^{-1}\|_{2} = \|\tilde{\Sigma}\|_{2}$$

This allows to deduce that $\kappa(WP_s^{-1}) = \kappa(\Omega U)$

Sketch and precondition (contd)

$$\kappa(WP_s^{-1}) = \kappa(\Omega U)$$

and since U is orthonormal, Corollary 1 can be applied, from which the bound is obtained.

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