Update 1

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1 Postive Definiteness, SVD and Eigendecomposition

Suppose $A \in \mathbb{C}^{n\times n}$, and Λ is the diagonal matrix with eigenvalues of A lies on its diagonal in arbitrary order. Denote $\Lambda(A)$ as all the eigenvalues of A, and $\Sigma(A)$ as all the singular values of A. We use SVD to denote "Singular Value Decomposition".

1. We know that if A is normal, then it can be unitarily diagaonlizable, i.e. $A = Q\Lambda Q^*$, where Q is a unitary matrix.

2. If A is Hermitian, then its eigenvalues are all real and $\Sigma(A) = |\Lambda(A)|$. If the SVD of A is $U\Sigma V^*$, then $|U| = |V|$. They are not agreed when the eigenvalues and "corresponding" singular values are not agreed.

3. A is Hermitian, then its eigenvalues are all real. (one can easily prove this by using 1).

4. If A is normal, and $\Lambda(A) \subset \mathbb{R}$, then $A^* = A$.

   Proof. Since A is normal, then by 1, A is unitarily diagonalizable, $A = Q\Lambda Q^*$. Then $A^* = Q\Lambda^* Q^* = Q\Lambda Q^*$. The final equality uses $\Lambda(A) \subset \mathbb{R}$, i.e. $\overline{\Lambda(A)} = \Lambda(A)$. □

5. The previous two points can be concluded as: *If A is normal, then A is Hermitian if and only if its eigenvalues are all real.*

6. Using 4, we conclude that a normal matrix that is not Hermitian must have complex eigenvalues. E.g.

$$A = \begin{bmatrix} 1 & 1+\mathrm{i} & 1 \\ -1+\mathrm{i} & 1 & 1 \\ -1 & -1 & 1 \end{bmatrix}$$

   This matrix is normal, but not Hermitian, and $\Lambda(A) = \{1+2.21\mathrm{i}, 1-1.68\mathrm{i}, 1-0.54\mathrm{i}\}$. Then I wondering, why these complex eigenvalues does not comes in conjugate pairs.

7. Complex eigenvalues of matrices with *real* entries come as conjugate pairs.

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Lemma 1.1 (SVD and Eigendecomposition)**.** *Suppose $A \in \mathbb{R}^{n\times n}$ has a SVD $U\Sigma V^*$. Then, we have the following*

$$AA^* = U\Sigma V^* V\Sigma^* U^* = U(\Sigma^2)U^*,$$
$$A^*A = V\Sigma^* U^* U\Sigma V^* = V(\Sigma^2)V^*.$$

1. *Hence the singular values $\sigma_1, \ldots, \sigma_n$ are the positive square roots of the eigenvalues of AA^* or A^*A. Moreover, since AA^* and A^*A are positive semi-definite, hence the square roots are real and non-negative.*

2. *The left singular vectors, columns of U are the eigenvectors of AA^*.*

3. *The right singular vectors, columns of V are the eigenvectors of A^*A.*

Proposition 1.2 ([8, Theorem 5.5])**.** *If $A = A^* \in \mathbb{C}^{n\times n}$, then the singular values of A are the absolute values of the eigenvalues of A.*

Proof. This proof is done by construction of SVD. A is Hermitian, hence we have $A = Q\Lambda Q^*$, where $\Lambda \in \mathbb{R}^{n\times n}$, and Q is unitary. We can write the eigendecomposition as

$$A = Q\Lambda Q^* = Q|\Lambda|\text{sign}(\Lambda)Q^* =: Q|\Lambda|P^*, \tag{1}$$

where $|\Lambda|$ and $\text{sign}(\Lambda)$ denote the diagonal matrices whose entries are $|\lambda_i|$ and $\text{sign}(\lambda_i)$, respectively. Notice that P is unitary by noticing $\text{sign}(\Lambda)$ is unitary. Therefore, (1) is a SVD of A, with singular values equal to $|\lambda_i|$. One can easily order the diagonal entries of $|\Lambda|$ by applying suitable permutation matrices to Q and $\text{sign}(\Lambda)Q^*$. $\square$

Corollary 1.3. *If $A = A^* \in \mathbb{C}^{n\times n}$, and it has a singular value decomposition $A = U\Sigma V^*$. Then $|U| = |V|$.*

Proof. ([1, Section 3.1]) Let $A \in \mathbb{R}^{n\times n}$ be a symmetric matrix with SVD $A = U\Sigma V^T$. Then $V^TAV = V^TU\Sigma$, and $V^TU\Sigma$ is orthogonally similar to A, with V^TU is orthogonal.

If A has distinct singular values $\sigma_1 > \sigma_2 > \cdots > \sigma_p$ with respective multiplicities m_i, $i = 1, \ldots, p$. ($\sum_i^p m_i = n$). Partitioning U and V into

$$U = [U_1 \mid \cdots \mid U_p], \qquad V = [V_1 \mid \cdots \mid V_p]$$

where $U_i, V_i \in \mathbb{R}^{n\times m_i}$ corresponding to each distinct singular value. Since, due to the symmetry of A and Lemma 1.1, both its left and right singular vectors (columns of U and V) are eigenvectors of A^2. Consequently,

$$V^TU = \text{diag}(V_1^TU_1, \ldots, V_p^TU_p)$$

is block diagonal, where each diagonal block $V_i^TU_i \in \mathbb{R}^{m_i\times m_i}$ is itself *orthogonal*. Furthermore, since

$$V^TAV = V^TU\Sigma = \text{diag}(\sigma_1V_1^TU_1, \ldots, \sigma_pV_p^TU_p)$$

is symmetric, we conclude that each $V_i^TU_i$ is not only orthogonal but also symmetric, therefore, its eigenvalues are ±1. The ±1 are precisely the signs of those eigenvalues of A having modulus σ_i.

Example 1.4. Suppose A has an eigendecomposition

$$A = \widetilde{V} \begin{bmatrix} 4 & & & \\ & -3 & & \\ & & 3 & \\ & & & 5 \end{bmatrix} \widetilde{V}^T,$$

then the SVD of A have the form

$$A = U \begin{bmatrix} 5 & & & \\ & 4 & & \\ & & 3 & \\ & & & 3 \end{bmatrix}.$$

Since $V^T U \Sigma$ is orthogonally similar to A, therefore,

$$V^T U = \begin{bmatrix} 1 & & & \\ & 1 & & \\ & & -1 & \\ & & & 1 \end{bmatrix}$$

(END OF EXAMPLE)

In the simplest case when $m_i = 1$, then eigenvalues are just $v_i^T u_i \sigma$. In the general case, a simple calculation shows that if the spectrum (eigenvalues) of $V_i^T U_i$ contains m_i^+ eigenvalues equal to 1 and m_i^- equal to -1, ($m_i = m_i^+ + m_i^-$), then

$$m_i^{\pm} = \frac{m_i \pm \operatorname{trace}(V_i^T U_i)}{2}, \tag{2}$$

i.e. the multiplicity of the eigenvalues $\pm\sigma_i$ can be easily recovered from the trace of $V_i^T U_i$.

Now, in order to obtain eigenvectors of A, we split into the following three cases:

1. If $m_i = 1$, then right singular vectors v_i itself is an eigenvector.
2. If $m_i > 1$, but $\operatorname{trace}(V_i^T U_i) = m_i$ (the eigenvalues of $V_i^T U_i^T$ are all positive 1 by (2)), then all the m_i eigenvalues are all equal to σ_i, and the eigenvectors are the columns of V_i. Analog applies to $\operatorname{trace}(V_i^T U_i) = -m_i$.
3. Generally, if $m_i > 1$ and $m_i \neq m_i^{\pm}$, consider for each $i = 1, \ldots, p$, we have an orthogonalization $V_i^T U_i = W_i J_i W_i^T$, with $J_i = \operatorname{diag}(I_{m_i^+}, -I_{m_i^-})$ and $W_i = [W_i^+ \mid W_i^-] \in \mathbb{R}^{m_i \times m_i}$ partitioned accordingly. Then, denoting $W = [W_1, \ldots, W_p]$, we have

$$V^T U \Sigma = \begin{bmatrix} \Sigma_1^+ & & & & \\ & \Sigma_1^- & & & \\ & & \ddots & & \\ & & & \Sigma_p^+ & \\ & & & & \Sigma_p^- \end{bmatrix} =: \widetilde{\Sigma}.$$

Therefore, we successfully recover the eigenvalues from the singular values by using the left and right singular vectors. Then by the relation $V^T A V = V^T U \Sigma$, we have

$$A = V \widetilde{\Sigma} V^T.$$

□

For this interesting mathematical analysis, we need to do a numerical test.

```
>> rng = 1; A = randn(10); A = A + A'; % generate symmetric
   matrix
>> [U,S,V] = svd(A); D = V'*U*S;
>> disp(norm(A*V - V*D)/norm(A));
  1.1880e-15
```

The numerical experiment shows that $V^T U \Sigma$ indeed "apporoximate" the eigenvalues.

Corollary 1.5. *Let $A \in \mathbb{C}^{n\times n}$ be Hermitian positive definite, then its eigendecomposition coincide with its singular value decomposition.*

Proof. By noting if A is Hermitian positive definite, and its eigendecomposition is $Q\Lambda Q^*$, then $\operatorname{sign}(\Lambda) = I$. □

Notice that, previous construction does not care about the order of the diagonal entries of Λ, since we can always permute Q and Λ to make Λ sorted. This can be done using MATLAB.

```
1 % https://uk.mathworks.com/help/matlab/ref/eig.html
2 function [Vs,Ds] = myeig(A)
3 [V,D] = eig(A);
4 [~,ind] = sort(diag(abs(D)),'descend');
5 Ds = D(ind,ind);
6 Vs = V(:,ind);
7 end
```

On the 4th line of the code, I use `abs(D)` in order to sort the eigenvalues with respect to their absolute values, which is the singular values. We can then check the function via

```
>> rng(1); A = randn(5); A = A + A'; % symmetric matrix
>> [V,D] = myeig(A);
>> disp(diag(D)); disp('---'); disp(norm(A*V-V*D));
  -6.7126e+00
   4.9099e+00
  -4.3623e+00
  -1.1499e+00
   5.0084e-01
---
   2.4697e-15
```

The function `myeig` successfully create a sorted eigendecomposition in the sense that the eigenvalues are sorted in the descending order in modulus. Moreover, to support Proposition 1.2, we check by

```
>> svd(A) - abs(diag(D))
ans =
   8.8818e-16
   8.8818e-16
   3.5527e-15
   6.6613e-16
  -8.8818e-16
```

These numbers are around unit roundoff and considered as zeros.

Conclusion. To compute the matrix principal square roots for Hermitian positive definite matrix, we aim to compute it via eigendecomposition, since $A^{1/2} = Q\Lambda^{1/2}Q^*$.

By Corollary 1.5, we can simply compute the singular value decomposition via DV-SVD algorithm[1].

2 Path to Matrix Square Root of SPD Matrix

Normally, we can compute the principal square root of any positive definite matrix via the following algorithm proposed by Higham in [7, 2008, Algorithm 6.21].

Algorithm 1 Given a Hermitian positive definite matrix $A \in \mathbb{C}^{n\times n}$ this algorithm computes $H = A^{1/2}$.

1: Compute the Cholesky factorization $A = RR^T$.
2: Compute the Hermitian polar factor H of R by applying any method (exploiting the triangularity of R).

Algorithm 2 Given a Hermitian positive definite matrix $A \in \mathbb{C}^{n\times n}$ this algorithm computes $H = A^{1/2}$.

1: Compute the eigendecomposition $A = Q\Lambda Q^*$.
2: Compute the matrix square root $A^{1/2} = Q\Lambda^{1/2}Q^*$.

These two algorithms both compute the eigendecomposition of a positive definite matrix and, by previous section, we can compute the SVD instead of the eigendecomposition such that the accuracy of the one-sided Jacobi can be explored.

1. For Algorithm 1, we can compute the Hermitian polar factor of R using
   (a) Scaled Newton Method, [7, 2008, Algorithm 8.20]. This can make use of the existing code by Higham [5].
   (b) Newton–Schulz iteration.
   (c) The DV-SVD algorithm.
2. For Algorithm 2, the analysis of the DV-SVD algorithm is also required. This involves several papers by Drmač.

The aim of this stage is to compare different method for computing the matrix square root of a Hermitian positive definite matrix. This can also extend to – How to use mixed-precision one-sided Jacobi algorithm [4] to speed up the process without loss of accuracy.

3 Summary of Reading

1. [6][2]: Newton's method has been used for computing the matrix square root. However, this method is unstable. The paper rederive the stable DB iteration and derive the coupled Newton–Schulz iteration for matrix square root. Scaling method is briefly

[1]This algorithm refer to the SVD algorithm proposed by Drmač and Veselić in [2, 3]
[2]Detail notes can be found here url

discussed in context of the new derivation. A new way for computing the square root of the positive definite matrix is given.

References

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[4] Weiguo Gao, Yuxin Ma, and Meiyue Shao. A mixed precision Jacobi SVD algorithm, 2022. (Cited on p. 5.)

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[6] Nicholas J. Higham. Stable iterations for the matrix square root. *Numerical Algorithms*, 15(2):227–242, 1997. (Cited on p. 5.)

[7] Nicholas J. Higham. *Functions of Matrices: Theory and Computation*. Society for Industrial and Applied Mathematics, Philadelphia, PA, USA, 2008. xx+425 pp. ISBN 978-0-898716-46-7. (Cited on p. 5.)

[8] Lloyd N. Trefethen and David Bau III. *Numerical Linear Algebra*. Society for Industrial and Applied Mathematics, Philadelphia, PA, USA, 1997. xii+361 pp. ISBN 0898713617. (Cited on p. 2.)