

SVD approximations for large-scale inverse problems

Clarissa Garvey Chang Meng James Nagy

Department of Mathematics and Computer Science



EMORY
UNIVERSITY

ccgarve@emory.edu

September 12, 2017

Supported by



1 SVD Approximation Background

- SVDs
- Error Amplification
- Filtering

2 SVD Approximation via Kronecker Product Decomposition

- Kronecker Product Decompositions
- Algorithm Derivation

3 Approximation Quality

- Qualitative Quality

Singular Value Decomposition (SVD)



A real, $N \times N$ (with $n^2 = N$) matrix K can be decomposed into a singular value decomposition (SVD):

$$K = U\Sigma V^T$$

where

Singular Value Decomposition (SVD)

A real, $N \times N$ (with $n^2 = N$) matrix K can be decomposed into a singular value decomposition (SVD):

$$K = U\Sigma V^T$$

where

- $U^T U = U U^T = \mathbb{1}$ (the identity matrix)
- $V^T V = V V^T = \mathbb{1}$
- Σ is a non-negative diagonal matrix with diagonal elements σ_i ordered so that $\sigma_1 \geq \sigma_2 \geq \dots \geq \sigma_N$.

Singular Value Decomposition (SVD)

A real, $N \times N$ (with $n^2 = N$) matrix K can be decomposed into a singular value decomposition (SVD):

$$K = U\Sigma V^T$$

where

- $U^T U = U U^T = \mathbb{1}$ (the identity matrix)
- $V^T V = V V^T = \mathbb{1}$
- Σ is a non-negative diagonal matrix with diagonal elements σ_i ordered so that $\sigma_1 \geq \sigma_2 \geq \dots \geq \sigma_N$.

The columns of U and V are the left and right singular vectors of A , respectively.

The σ_i are the singular values of A .

Our linear problems are of the form

$$\mathbf{b} = K\mathbf{x} + \mathbf{e}$$

where

Our linear problems are of the form

$$\mathbf{b} = K\mathbf{x} + \mathbf{e}$$

where

- $\mathbf{b} \in \mathbb{R}^N$ is the measured data,
- $\mathbf{x} \in \mathbb{R}^N$ is the desired, unknown solution,
- $K \in \mathbb{R}^{N \times N}$ is a matrix relating the true solution to observation, and
- $\mathbf{e} \in \mathbb{R}^N$ is unknown error.

Our linear problems are of the form

$$\mathbf{b} = K\mathbf{x} + \mathbf{e}$$

where

- $\mathbf{b} \in \mathbb{R}^N$ is the measured data,
- $\mathbf{x} \in \mathbb{R}^N$ is the desired, unknown solution,
- $K \in \mathbb{R}^{N \times N}$ is a matrix relating the true solution to observation, and
- $\mathbf{e} \in \mathbb{R}^N$ is unknown error.

If the singular values of K tend to zero without a gap, K is ill-conditioned.

Our linear problems are of the form

$$\mathbf{b} = K\mathbf{x} + \mathbf{e}$$

where

- $\mathbf{b} \in \mathbb{R}^N$ is the measured data,
- $\mathbf{x} \in \mathbb{R}^N$ is the desired, unknown solution,
- $K \in \mathbb{R}^{N \times N}$ is a matrix relating the true solution to observation, and
- $\mathbf{e} \in \mathbb{R}^N$ is unknown error.

If the singular values of K tend to zero without a gap, K is ill-conditioned.

Then direct solution using the SVD may amplify noise:

$$K^{-1}\mathbf{b} = \mathbf{x} + K^{-1}\mathbf{e} = \mathbf{x} + V\Sigma^{-1}U^T\mathbf{e}$$

Filtering can avoid this issue.

Filtering can avoid this issue.

$$\begin{aligned} K^{-1} &= V\Sigma^{-1}U^T \\ &= V\mathit{diag}\left(\frac{1}{\sigma_1}, \dots, \frac{1}{\sigma_N}\right)U^T \end{aligned}$$

Filtering can avoid this issue.

$$\begin{aligned} K^{-1} &= V\Sigma^{-1}U^T \\ &= V\mathit{diag}\left(\frac{1}{\sigma_1}, \dots, \frac{1}{\sigma_N}\right)U^T \end{aligned}$$

$$K_F^{-1} = V\mathit{diag}\left(\frac{\phi_1}{\sigma_1}, \dots, \frac{\phi_N}{\sigma_N}\right)U^T$$

Filtering can avoid this issue.

$$\begin{aligned} K^{-1} &= V\Sigma^{-1}U^T \\ &= V\text{diag}\left(\frac{1}{\sigma_1}, \dots, \frac{1}{\sigma_N}\right)U^T \end{aligned}$$

$$K_F^{-1} = V\text{diag}\left(\frac{\phi_1}{\sigma_1}, \dots, \frac{\phi_N}{\sigma_N}\right)U^T$$

$\{\phi_i\}$ are weights such that, for small σ_i , $\phi_i = 0$.

In a truncated SVD, $\phi_i = 0$ if $i > k$, a cutoff index.

The Kronecker product of matrices $A_{m \times m}$ and B is

$$A \otimes B = \begin{bmatrix} a_{1,1}B & \dots & a_{1,m}B \\ \vdots & & \vdots \\ a_{m,1}B & \dots & a_{m,m}B \end{bmatrix}$$

The Kronecker product of matrices $A_{m \times m}$ and B is

$$A \otimes B = \begin{bmatrix} a_{1,1}B & \dots & a_{1,m}B \\ \vdots & & \vdots \\ a_{m,1}B & \dots & a_{m,m}B \end{bmatrix}$$

Given $A = U_A \Sigma_A V_A^T$ and $B = U_B \Sigma_B V_B^T$,

The Kronecker product of matrices $A_{m \times m}$ and B is

$$A \otimes B = \begin{bmatrix} a_{1,1}B & \dots & a_{1,m}B \\ \vdots & & \vdots \\ a_{m,1}B & \dots & a_{m,m}B \end{bmatrix}$$

Given $A = U_A \Sigma_A V_A^T$ and $B = U_B \Sigma_B V_B^T$,

$$A \otimes B = (U_A \otimes U_B)(\Sigma_A \otimes \Sigma_B)(V_A \otimes V_B)^T$$

Arbitrary $N \times N$ matrices may not be writeable as $A_{n \times n} \otimes B_{n \times n}$

Arbitrary $N \times N$ matrices may not be writeable as $A_{n \times n} \otimes B_{n \times n}$

But all $N \times N$ matrices K can be represented as

$$K = \sum_{i=1}^R A_i \otimes B_i$$

where all A_i, B_i are $n \times n$ with $n^2 = N$ in size and the index R is the Kronecker rank. (See *Van Loan and Pitsiannis, 1993* [?])

Suppose we have $K = \sum_{i=1}^R A_i \otimes B_i$, and

Suppose we have $K = \sum_{i=1}^R A_i \otimes B_i$, and

- $A_1 = U_{A_1} \Sigma_{A_1} V_{A_1}^T$
- $B_1 = U_{B_1} \Sigma_{B_1} V_{B_1}^T$

Suppose we have $K = \sum_{i=1}^R A_i \otimes B_i$, and

- $A_1 = U_{A1} \Sigma_{A1} V_{A1}^T$
- $B_1 = U_{B1} \Sigma_{B1} V_{B1}^T$
- $U_1 = U_{A1} \otimes U_{B1}$
- $\Sigma_1 = \Sigma_{A1} \otimes \Sigma_{B1}$
- $V_1 = V_{A1} \otimes V_{B1}$

Suppose we have $K = \sum_{i=1}^R A_i \otimes B_i$, and

- $A_1 = U_{A1} \Sigma_{A1} V_{A1}^T$
- $B_1 = U_{B1} \Sigma_{B1} V_{B1}^T$
- $U_1 = U_{A1} \otimes U_{B1}$
- $\Sigma_1 = \Sigma_{A1} \otimes \Sigma_{B1}$
- $V_1 = V_{A1} \otimes V_{B1}$

Then $A_1 \otimes B_1 = U_1 \Sigma_1 V_1^T$.

Suppose we have $K = \sum_{i=1}^R A_i \otimes B_i$, and

- $A_1 = U_{A1} \Sigma_{A1} V_{A1}^T$
- $B_1 = U_{B1} \Sigma_{B1} V_{B1}^T$
- $U_1 = U_{A1} \otimes U_{B1}$
- $\Sigma_1 = \Sigma_{A1} \otimes \Sigma_{B1}$
- $V_1 = V_{A1} \otimes V_{B1}$

Then $A_1 \otimes B_1 = U_1 \Sigma_1 V_1^T$.

Further, $K = U_1 \Sigma_1 V_1^T + \sum_{i=2}^R U_1 U_1^T K_i V_1 V_1^T$

Suppose we have $K = \sum_{i=1}^R A_i \otimes B_i$, and

- $A_1 = U_{A1} \Sigma_{A1} V_{A1}^T$
- $B_1 = U_{B1} \Sigma_{B1} V_{B1}^T$
- $U_1 = U_{A1} \otimes U_{B1}$
- $\Sigma_1 = \Sigma_{A1} \otimes \Sigma_{B1}$
- $V_1 = V_{A1} \otimes V_{B1}$

Then $A_1 \otimes B_1 = U_1 \Sigma_1 V_1^T$.

$$\begin{aligned} \text{Further, } K &= U_1 \Sigma_1 V_1^T + \sum_{i=2}^R U_1 U_1^T K_i V_1 V_1^T \\ &= U_1 \left(\Sigma_1 + \sum_{i=2}^R U_1^T K_i V_1 \right) V_1^T \end{aligned}$$

See Nagy, Ng, and Perrone (2006) [?] and Kamm and Nagy (2000) [?]

$$K = U_1 \left(\Sigma_1 + \sum_{i=2}^R U_1^T K_i V_1 \right) V_1^T$$

$$\begin{aligned} K &= U_1 \left(\Sigma_1 + \sum_{i=2}^R U_1^T K_i V_1 \right) V_1^T \\ &= U_1 \left(\begin{bmatrix} \Sigma_{1,k} & 0 \\ 0 & \hat{\Sigma}_0 \end{bmatrix} + \begin{bmatrix} W_{11} & W_{12} \\ W_{21} & W_{22} \end{bmatrix} \right) V_1^T \end{aligned}$$

$$\begin{aligned} K &= U_1 \left(\Sigma_1 + \sum_{i=2}^R U_1^T K_i V_1 \right) V_1^T \\ &= U_1 \left(\begin{bmatrix} \Sigma_{1,k} & 0 \\ 0 & \hat{\Sigma}_0 \end{bmatrix} + \begin{bmatrix} W_{11} & W_{12} \\ W_{21} & W_{22} \end{bmatrix} \right) V_1^T \\ &= U_1 \left(\begin{bmatrix} \Sigma_{1,k} + W_{11} & 0 \\ 0 & \hat{\Sigma}_0 \end{bmatrix} + \begin{bmatrix} 0 & W_{12} \\ W_{21} & W_{22} \end{bmatrix} \right) V_1^T \end{aligned}$$

$$\begin{aligned} K &= U_1 \left(\Sigma_1 + \sum_{i=2}^R U_1^T K_i V_1 \right) V_1^T \\ &= U_1 \left(\begin{bmatrix} \Sigma_{1,k} & 0 \\ 0 & \hat{\Sigma}_0 \end{bmatrix} + \begin{bmatrix} W_{11} & W_{12} \\ W_{21} & W_{22} \end{bmatrix} \right) V_1^T \\ &= U_1 \left(\begin{bmatrix} \Sigma_{1,k} + W_{11} & 0 \\ 0 & \hat{\Sigma}_0 \end{bmatrix} + \begin{bmatrix} 0 & W_{12} \\ W_{21} & W_{22} \end{bmatrix} \right) V_1^T \\ &= U_1 \left(\begin{bmatrix} U_k \hat{\Sigma}_k V_k^T & 0 \\ 0 & \hat{\Sigma}_0 \end{bmatrix} + \begin{bmatrix} 0 & W_{12} \\ W_{21} & W_{22} \end{bmatrix} \right) V_1^T \end{aligned}$$

$$K = U_1 \left(\begin{bmatrix} U_k \hat{\Sigma}_k V_k^T & 0 \\ 0 & \hat{\Sigma}_0 \end{bmatrix} + \begin{bmatrix} 0 & W_{12} \\ W_{21} & W_{22} \end{bmatrix} \right) V_1^T$$

$$\begin{aligned} K &= U_1 \left(\begin{bmatrix} U_k \widehat{\Sigma}_k V_k^T & 0 \\ 0 & \widehat{\Sigma}_0 \end{bmatrix} + \begin{bmatrix} 0 & W_{12} \\ W_{21} & W_{22} \end{bmatrix} \right) V_1^T \\ &= U_1 \begin{bmatrix} U_k & 0 \\ 0 & \mathbf{1} \end{bmatrix} \left(\begin{bmatrix} \widehat{\Sigma}_k & 0 \\ 0 & \widehat{\Sigma}_0 \end{bmatrix} + \begin{bmatrix} 0 & U_k^T W_{12} \\ W_{21} V_k & W_{22} \end{bmatrix} \right) \begin{bmatrix} V_k^T & 0 \\ 0 & \mathbf{1} \end{bmatrix} V_1^T \end{aligned}$$

$$\begin{aligned}
 K &= U_1 \left(\begin{bmatrix} U_k \widehat{\Sigma}_k V_k^T & 0 \\ 0 & \widehat{\Sigma}_0 \end{bmatrix} + \begin{bmatrix} 0 & W_{12} \\ W_{21} & W_{22} \end{bmatrix} \right) V_1^T \\
 &= U_1 \begin{bmatrix} U_k & 0 \\ 0 & \mathbf{1} \end{bmatrix} \left(\begin{bmatrix} \widehat{\Sigma}_k & 0 \\ 0 & \widehat{\Sigma}_0 \end{bmatrix} + \begin{bmatrix} 0 & U_k^T W_{12} \\ W_{21} V_k & W_{22} \end{bmatrix} \right) \begin{bmatrix} V_k^T & 0 \\ 0 & \mathbf{1} \end{bmatrix} V_1^T \\
 &= \widehat{U} \left(\begin{bmatrix} \widehat{\Sigma}_k & 0 \\ 0 & \widehat{\Sigma}_0 \end{bmatrix} + \begin{bmatrix} 0 & \widehat{W}_{12} \\ \widehat{W}_{21} & W_{22} \end{bmatrix} \right) \widehat{V}^T.
 \end{aligned}$$

Given

$$K = \hat{U} \left(\begin{bmatrix} \hat{\Sigma}_k & 0 \\ 0 & \hat{\Sigma}_0 \end{bmatrix} + \begin{bmatrix} 0 & \hat{W}_{12} \\ \hat{W}_{21} & W_{22} \end{bmatrix} \right) \hat{V}^T$$

Given

$$K = \hat{U} \left(\begin{bmatrix} \hat{\Sigma}_k & 0 \\ 0 & \hat{\Sigma}_0 \end{bmatrix} + \begin{bmatrix} 0 & \hat{W}_{12} \\ \hat{W}_{21} & W_{22} \end{bmatrix} \right) \hat{V}^T$$

partition $\hat{U} = [\hat{U}_k \quad \hat{U}_0]$ and $V = [\hat{V}_k \quad \hat{V}_0]$.

Given

$$K = \hat{U} \left(\begin{bmatrix} \hat{\Sigma}_k & 0 \\ 0 & \hat{\Sigma}_0 \end{bmatrix} + \begin{bmatrix} 0 & \hat{W}_{12} \\ \hat{W}_{21} & W_{22} \end{bmatrix} \right) \hat{V}^T$$

partition $\hat{U} = [\hat{U}_k \quad \hat{U}_0]$ and $V = [\hat{V}_k \quad \hat{V}_0]$.

Then we can construct a truncated SVD

$$K \approx \hat{U}_k \hat{\Sigma}_k \hat{V}_k^T$$



observed image



SVD approx
1 Kron term



SVD approx
5 Kron terms

In this example:

- K is $N \times N$, with $N = 65,536 \times 65,536$.
- K_{TSVD} uses $k = 2,601$ for truncation.



observed image



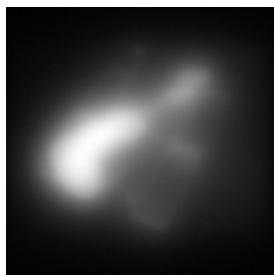
SVD approx
1 Kron term



SVD approx
10 Kron terms

In this example:

- K is $N \times N$, with $N = 65,536 \times 65,536$.
- K_{TSVD} uses $k = 2,601$ for truncation.



observed image



SVD approx
1 Kron term







SVD approx
67 Kron terms

In this example:

- K is $N \times N$, with $N = 65,536 \times 65,536$.
- K_{TSVD} uses $k = 2,601$ for truncation.

- We created an algorithm for approximating a truncated SVD.
- Kronecker products help keep computational costs down.
- We can compute the TSVD on larger problems than traditional methods allow.
- This method is fast (seconds) and produces reasonable solutions.

-  C.F. Van Loan and N. Pitsianis. Approximation with Kronecker Products. *Linear Algebra for Large Scale and Real-time Applications*, Springer Netherlands 293-314, 1993.
-  J. Nagy, M.K. Ng, L. Perrone. Kronecker Product Approximations for Image Restoration with Reflexive Boundary Conditions. *SIAM Journal on Matrix Analysis and Applications*, 25(3), 829-841, 2006.
-  J. Kamm, and J. Nagy. Optimal Kronecker Product Approximation of Block Toeplitz Matrices. *SIAM Journal on Matrix Analysis and Applications* 22.1, 155-172, 2000.
-  N. Halko, P.G. Martinsson, and J.A. Tropp. Finding Structure with Randomness: Probabilistic Algorithms for Constructing Approximate Matrix Decompositions. *SIAM Review* 53.2, 217-288, 2011.

Acknowledgement: This work is supported by the National Science Foundation under grant number DMS-1522760.

Thank you!