

Chapter 10: SVD Analysis of Tomography Problems Feryal Ezgi Aşkın

Seminar: Computational Methods of X-ray Computed Tomography 21.07.2023

Overview

The Singular Value Decomposition

Intuitive Interpretations of the SVD

Matrix 2-Norm and Condition Number

What SVD looks like

Similarities to Singular Functions of the Radon Transform

Image Reconstruction using SVD

Picard plot and what Picard plot looks like

Ill-Conditioned Problems and Noisy Data

Spectral Filtering and TSVD

SVD Analysis for a limited-angle problem

The Role of the Null Space

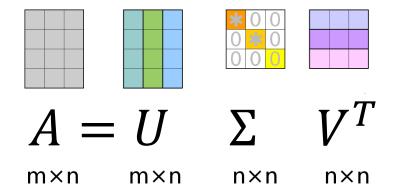
Goal

The goal of this presentation is to give an insight on

- what the Singular Value Decomposition is,
- what it can be used for regarding CT problems,
- how we can tackle ill-conditioned problems through SVD Analysis and
- what happens for when the data is discretized or limited.

The Singular Value Decomposition

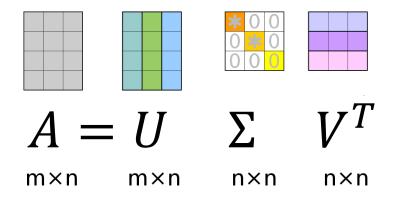
It is <u>always</u> possible to decompose a real matrix *A* into



where

- $U \in \mathbb{R}^{mxn}$ is a unitary matrix containing the left singular vectors,
- $\Sigma \in \mathbb{R}^{nxn}$ is a diagonal matrix with the singular values σ_i , where $\sigma_i \geq \sigma_{i+1} \geq \sigma_n \geq 0$,
- $V \in \mathbb{R}^{n \times n}$ is a unitary matrix containing the right singular vectors.

The Singular Value Decomposition

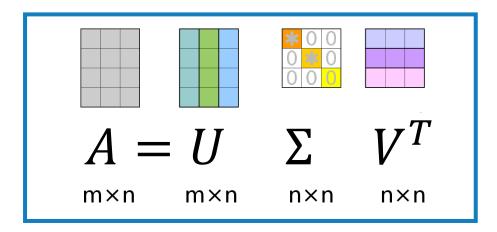


Both matrices *U* and *V* have columns that are orthogonal and have unit 2-norm, i.e.,

•
$$u_i^T u_j = v_i^T v_j = \begin{cases} 1 & for \ i = j, \\ 0 & else. \end{cases}$$
, meaning $U^T U = V^T V = I$

• For inverse problems, the singular vectors u_i and v_i tend to have more oscillations the greater the i is due to the Gibbs phenomenon, which we will refer to later.

The Singular Value Decomposition



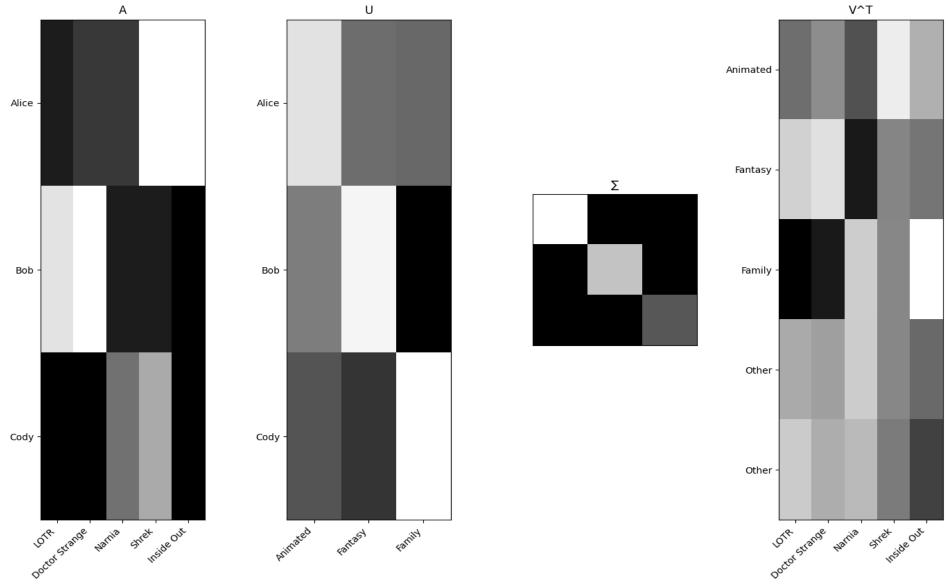
Economy-sized SVD or thin SVD with the assumption $m \ge n$

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Intuitive Interpretations of the SVD



The 2-norm of a matrix is defined as

$$||A||_2 = \max_{||v||_2 = 1} ||Av||_2$$

It is the largest "magnification" of a unit vector and simply the largest singular value of any matrix A.

$$||A||_2 = \sigma_1$$

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The singular values of A^TA are the squares of the singular values of A.

$$A^T A = V \Sigma^2 V^T \quad \rightarrow \quad \| A^T A \|_2 = \quad \sigma_1^2$$

Condition Number

If the matrix *A* is invertible, then we have

$$A^{-1} = V \Sigma^{-1} U^T$$

Hence the largest singular value of A^{-1} is the smallest singular value of A.

$$||A^{-1}||_2 = \sigma_n^{-1}$$

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The condition number of *A* is defined as

$$cond(A) = ||A||_2 ||A^{-1}||_2 = \frac{\sigma_1}{\sigma_n}$$

It indicates how much the output changes if there are small changes to (or perturbations in) the input. This number plays an important role for studies of sensitivity and for convergence analysis of iterative methods (in Chapter 11).

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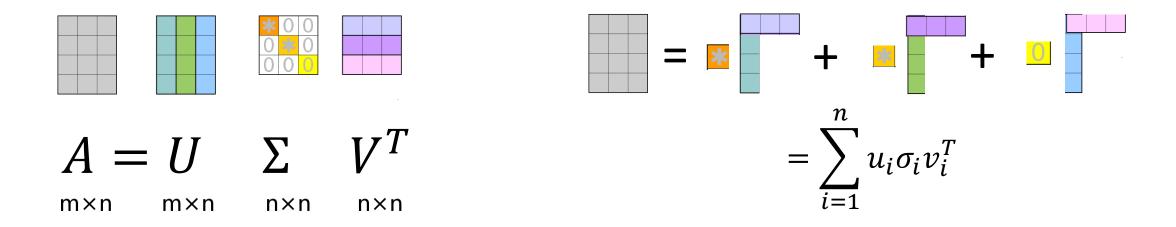
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With it, we can assess the accuracy of our methods and the impact of noisy data.

A smaller condition number indicates a well-posed problem, whereas a larger one indicates an ill-posed problem, where small errors in the input can lead to significant changes in the output.

Intuitive Interpretations of the SVD



- A as the summation of rank 1 matrices
- σ_1 is the 2-norm of matrix A, meaning its largest singular value
- Let us analyze the distribution and significance of all singular values

What the SVD looks like

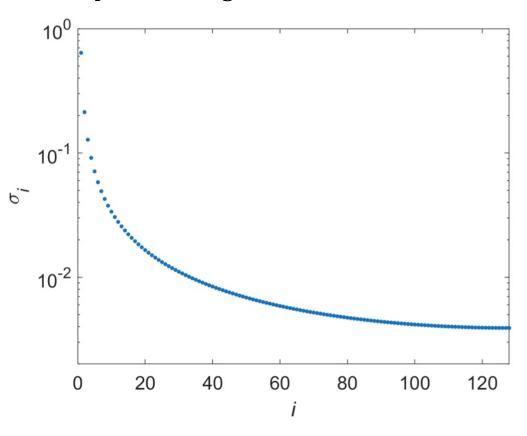
Let us consider a simple inverse problem: determine the elements of the vector $x \in \mathbb{R}^n$ from its cumulative sums:

$$b_i = \frac{1}{n} \sum_{j=1}^i x_j$$
, $i = 1, 2, ..., n$

We can think of b_i as elements of a vector b. Then we have a relation A x = b with a nxn triangular coefficient matrix

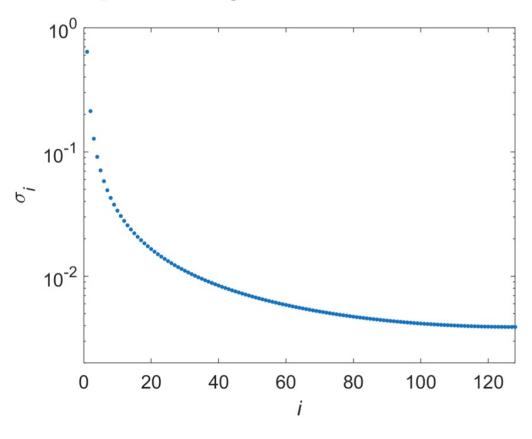
$$m{A} = rac{1}{n} egin{bmatrix} 1 & 0 & 0 & 0 & \cdots \ 1 & 1 & 0 & 0 & \cdots \ 1 & 1 & 1 & 0 & \cdots \ 1 & 1 & 1 & 1 & \cdots \ \vdots & \vdots & \vdots & \vdots & \ddots \end{bmatrix}$$

If we plot the singular values of the matrix *A*, we see that they decay to zero.



Why is this a significant quality of the SVD?

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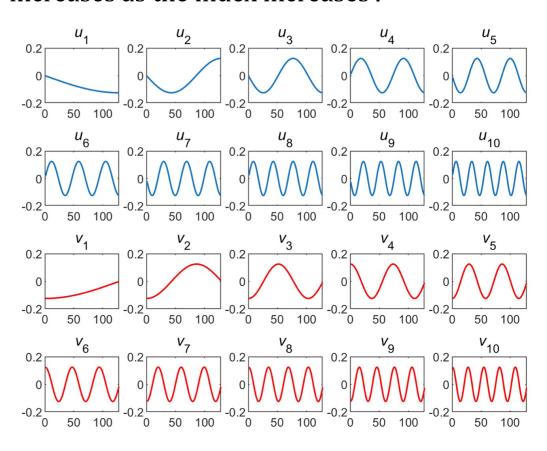
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This is a significant quality of SVD, as it enables efficient data compression.

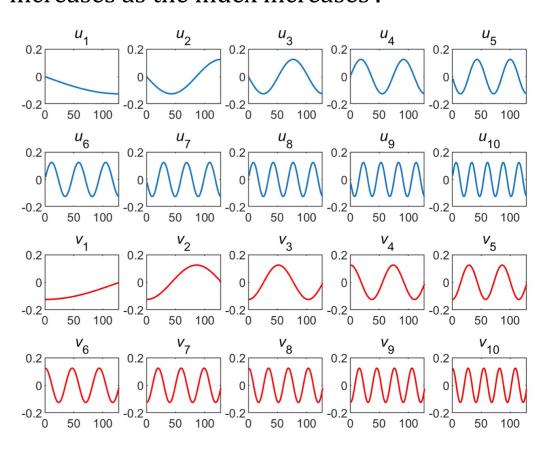
The Radon transform does this by reducing an image to its line integrals in the sinogram domain, while keeping the reconstruction of the image possible.

The SVD, on the other hand, can achieve data compression and image reconstruction by retaining only the dominant (larger) singular values.

Another remark is that the number of oscillations in the corresponding left and right singular vectors increases as the index increases.

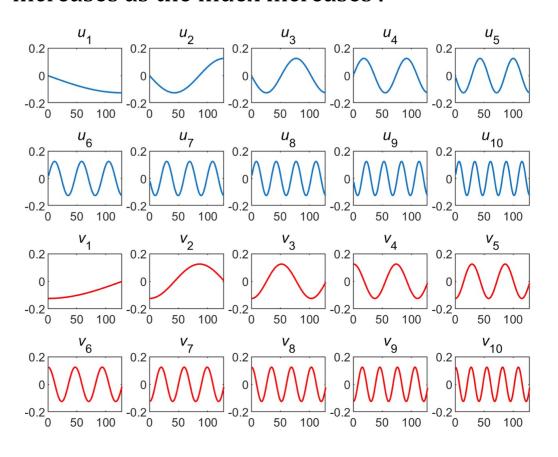


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The singular vectors with higher indices capture finer variations in the data, which can be interpreted as detailed structures and sharp corners or edges.

However, artifacts and noise in the data can easily contribute to the higher number of oscillations.

Thus, an intricate analysis of the singular values and vectors is necessary to understand the data.

Image Reconstruction using SVD in Python

To reconstruct the Shepp-Logan phantom, first the SVD of the phantom is calculated. The matrices U, Σ, V^T are then truncated by including only the first n singular values and their corresponding singular vectors.

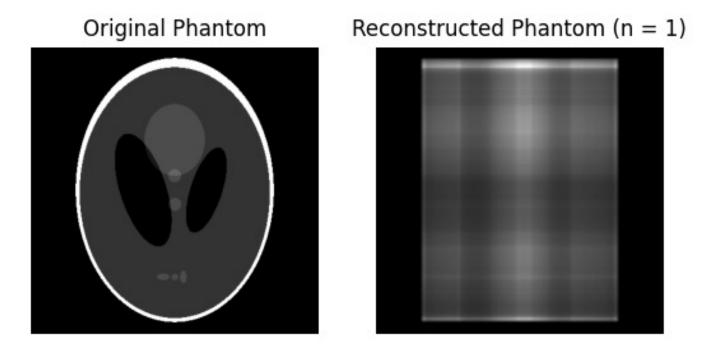


Image Reconstruction using SVD in Python

By including the first n singular values & their singular vectors and omitting the rest, we focus on the most significant components of the original phantom. The higher number n is, the better the reconstruction.

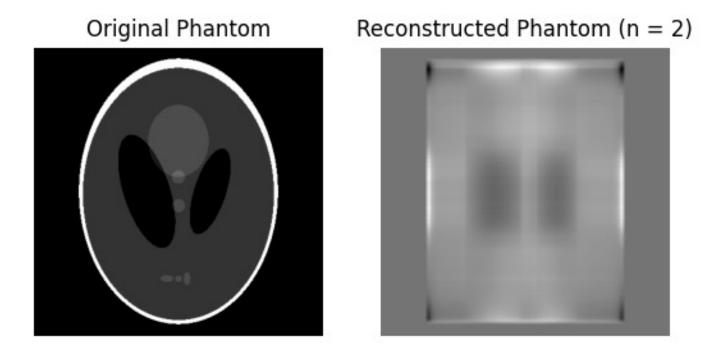
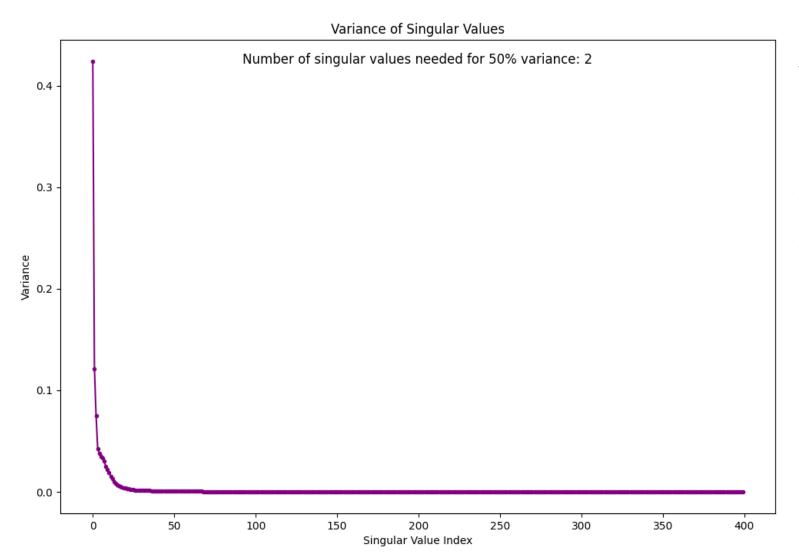


Image Reconstruction using SVD



A useful metric for the similarity between the original and the reconstructed phantom is the variance of the singular values, i.e., the proportion of the total variance by each singular value.

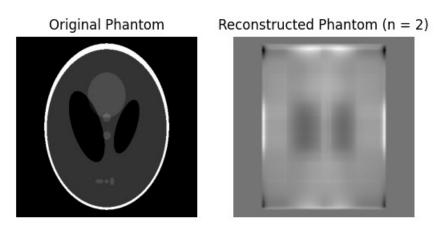
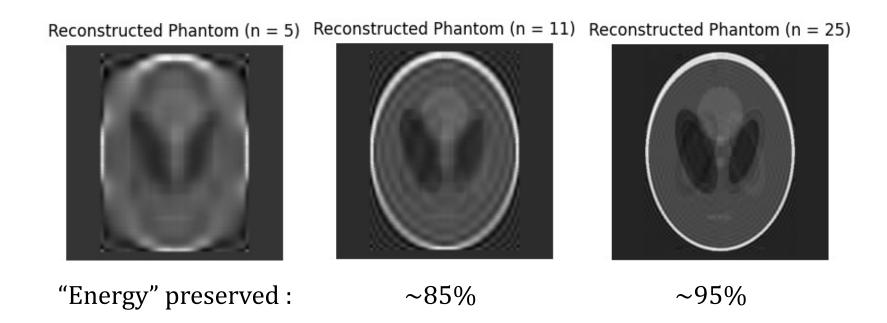


Image Reconstruction using SVD

There are certain tradeoffs to consider while selecting the most appropriate n value. Two of the most apparent being accuracy vs. computational effort and detail vs. noise.

This leads us to the questions:

How do we select the optimal *n* value? What if noise comes into play?



Picard plot

To figure this out we must first go back to mathematical foundations of the SVD. But for the sake of simplicity, we have the following expression, which is obtained through the properties of the SVD.

$$x = A^{-1} b = \sum_{i=1}^{n} \frac{u_i^T b}{\sigma_i} v_i$$

The Picard plot is a plot of the ingredients in this equation, namely

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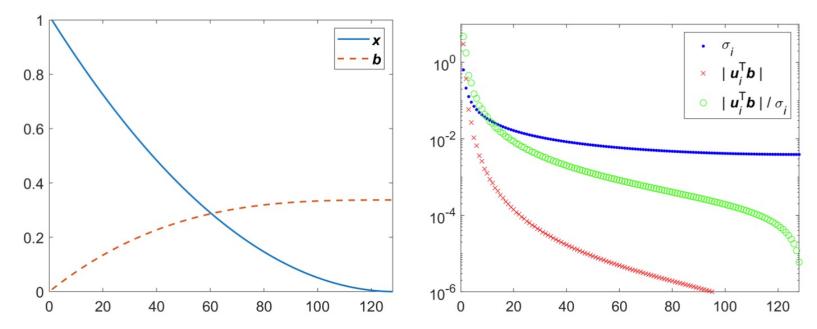
The Picard plot is a plot of the ingredients in this equation, namely

- the singular values σ_i ,
- the absolute values of the coefficients for the right-hand side $\left|u_i^T b\right|$
- the absolute values of the solution's coefficients $\left| \frac{u_i^T b}{\sigma_i} \right|$

What the Picard plot looks like

Let us return to the cumulative sum problem, where we observed singular values decaying to zero.

This time with a solution vector x whose decaying elements are given by



$$x_i = ((n-i+1)/n)^2$$

 $i = 1, 2, ..., n$.

Figure 10.3. Results for the cumulative sum problem in Example 10.3 with a solution given by (10.18). Left: The solution \mathbf{x} and the corresponding noise-free right-hand side \mathbf{b} . Right: The Picard plot for this particular example; we see that the singular values decay rather slowly and that the right-hand side's coefficients $|\mathbf{u}_i^T \mathbf{b}|$ decay faster than the singular values σ_i .

From now on we define the naive solution as either the solution A^{-1} b when m=n or the least-squares solution when m>n . In both cases it has the same SVD expansion.

$$x^{naive} = \sum_{i=1}^{n} \frac{u_i^T b}{\sigma_i} v_i$$

The condition number is a measure of how sensitive the solution is to errors in the data i.e., the right-hand side b. We now define the exact solution \bar{x} and the perturbed solution x as:

$$A\bar{x} = \bar{b}, \quad Ax = b = \bar{b} + e$$

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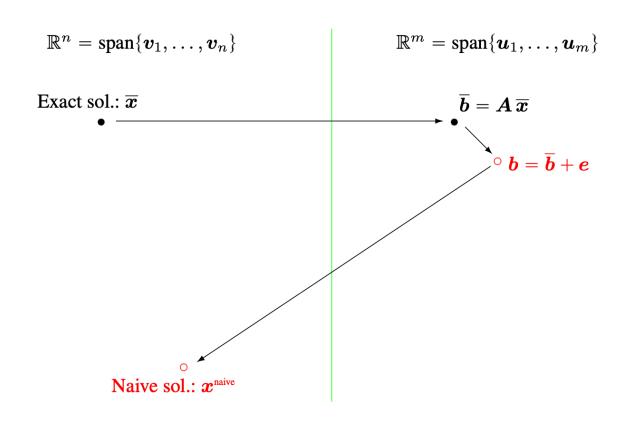
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Here e denotes the errors and the noise in the data. Therefore,

$$\frac{\|\boldsymbol{x} - \overline{\boldsymbol{x}}\|_2}{\|\overline{\boldsymbol{x}}\|_2} \leqslant \operatorname{cond}(\boldsymbol{A}) \frac{\|\boldsymbol{e}\|_2}{\|\overline{\boldsymbol{b}}\|_2}$$

The larger the condition number $cond(A) = \sigma_1/\sigma_n$, the further the perturbed solution x^{naive} can be from the exact solution \bar{x} .



Analogous to our previous definition of the

Picard plot $(\sum_{i=1}^n \frac{u_i^T b}{\sigma_i} v_i)$, we see that the perturbation of the solution is given by

$$oldsymbol{x} - \overline{oldsymbol{x}} = \sum_{i=1}^n rac{oldsymbol{u}_i^T oldsymbol{e}}{\sigma_i} \, oldsymbol{v}_i \; .$$

If A is ill-conditioned, it has some small singular values σ_i , hence there is a high risk that the perturbation of the solution will also be large.

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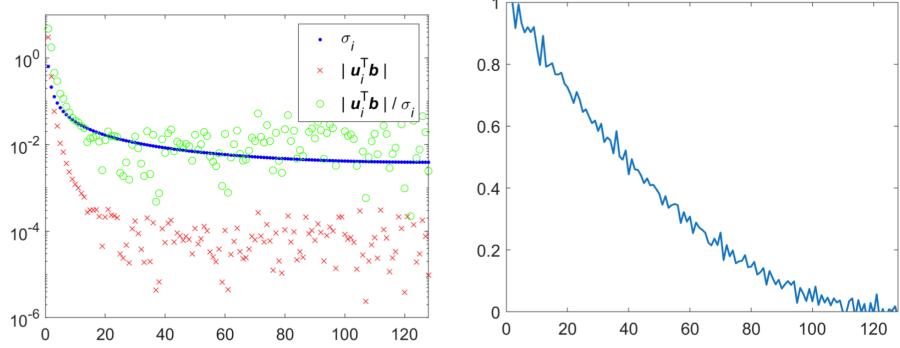
To dive further into this aspect, we assume there is white noise inferring with the data, meaning the expected values of $|u_i^T e|$ are independent of the index i. When such noise is present in the data $b = \bar{b} + e$ the coefficients of the noisy right-hand side satisfy

$$oldsymbol{u}_i^Toldsymbol{b} = oldsymbol{u}_i^Toldsymbol{ar{b}} + oldsymbol{u}_i^Toldsymbol{e} pprox \left\{egin{array}{c} oldsymbol{u}_i^Toldsymbol{ar{b}} & ext{when } |oldsymbol{u}_i^Toldsymbol{ar{b}}| > |oldsymbol{u}_i^Toldsymbol{e}| \ oldsymbol{u}_i^Toldsymbol{e} & ext{when } |oldsymbol{u}_i^Toldsymbol{ar{b}}| < |oldsymbol{u}_i^Toldsymbol{e}| \ . \end{array}
ight.$$

Recall from the Picard plot that the $u_i^T \bar{b}$ exhibits a decaying nature. For large singular values, the coefficients are dominated by noise-free coefficients. As the index increases and the singular values become smaller the coefficients become dominated by noise. These coefficients with $u_i^T b \approx u_i^T e$ are problematic.

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Solution: Spectral Filtering

A simple yet powerful approach for noise reduction is to retain the first SVD components with a small i, while removing the rest of the components with a large i.

$$x_{filt} = \sum_{i=1}^{n} \varphi_i \frac{u_i^T b}{\sigma_i} v_i$$

The scalars φ_i are the filter factors and these methods are called spectral filtering methods.

TSVD

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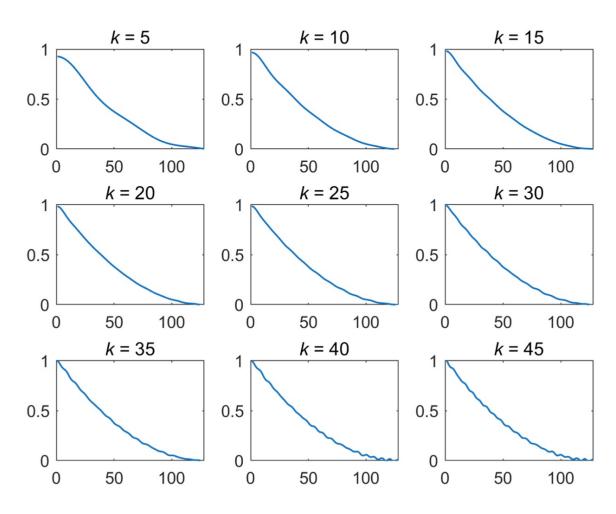
TSVD

We can easily discard SVD coefficients corresponding to small singular vectors by introducing "binary" filter factors.

$$arphi_i^{ extstyle ext$$

TSVD

The TSVD solution can be defined as and looks like the following:



$$oxed{oldsymbol{x}_k = \sum\limits_{i=1}^n \, arphi_i^{ ext{ iny TSVD}} rac{oldsymbol{u}_i^T oldsymbol{b}}{\sigma_i} \, oldsymbol{v}_i = \sum\limits_{i=1}^k \, rac{oldsymbol{u}_i^T oldsymbol{b}}{\sigma_i} \, oldsymbol{v}_i \; , \qquad k < n \; .}$$

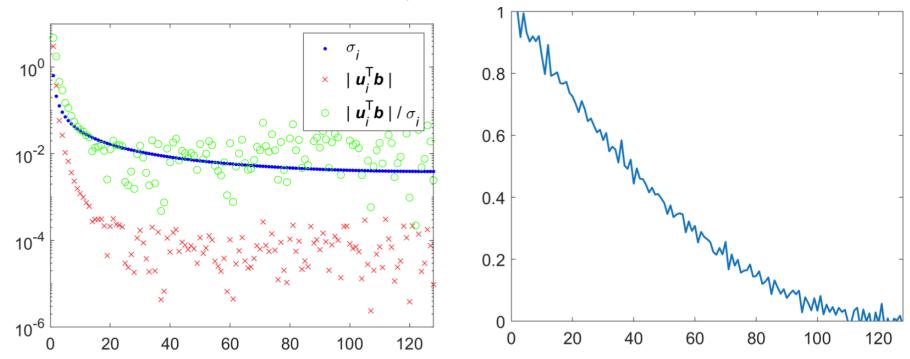
As we increase the truncation parameter k, we include more SVD components but also more noise in x_k . At some point the noise becomes visible and x_k starts to deteriorate.

The Role of the Truncation Parameter

- The optimal truncation parameter k for the TSVD solution x_k is determined by the noisy SVD coefficients u_i^T b but not the singular values.
- Why is this so?

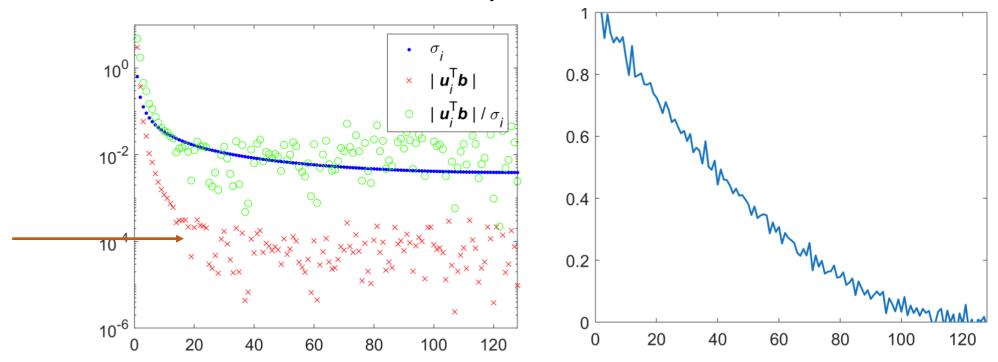
The Role of the Truncation Parameter

- The optimal truncation parameter k for the TSVD solution x_k is determined by the noisy SVD coefficients u_i^T b but not the singular values.
- Why is this so? Because the matrix isn't affected by the noise in the data.
- We should choose k as the index i, where u_i^T b starts to "level off" due to the noise.



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A x = b

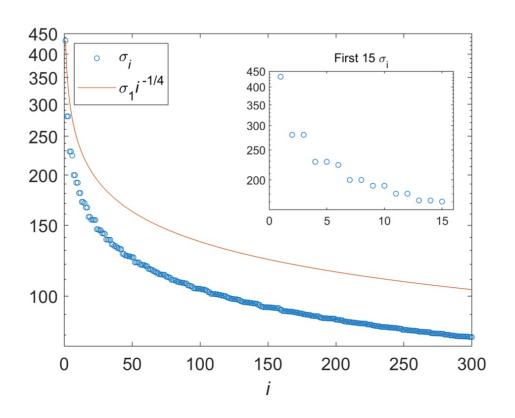
We are now ready to analyze CT problems formulated as a system of linear equations A x = b using SVD. In this context the linear equation represents the imaging process, in which

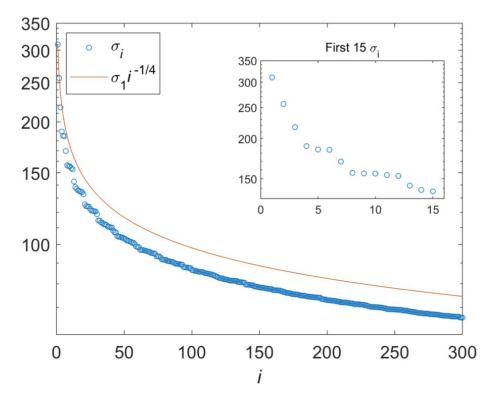
- *A* is the system matrix (on a square domain),
- *x* is the unknown vector representing the object to be reconstructed
- *b* is the measured data

Once we have computed the SVD of the system matrix $A = U \Sigma V^T$ we can plot the left and right singular vectors and their singular values. Here, the singular vectors represent the discretized versions of the left and right singular functions.

In examples 10.8 and 10.9 of the book ¹, we compare the insights that can be obtained by the SVD for full-angle and limited-angle data, respectively. We have the following conclusions:

• The limited-angle scenario does not influence the the overall behavior of the large singular values.



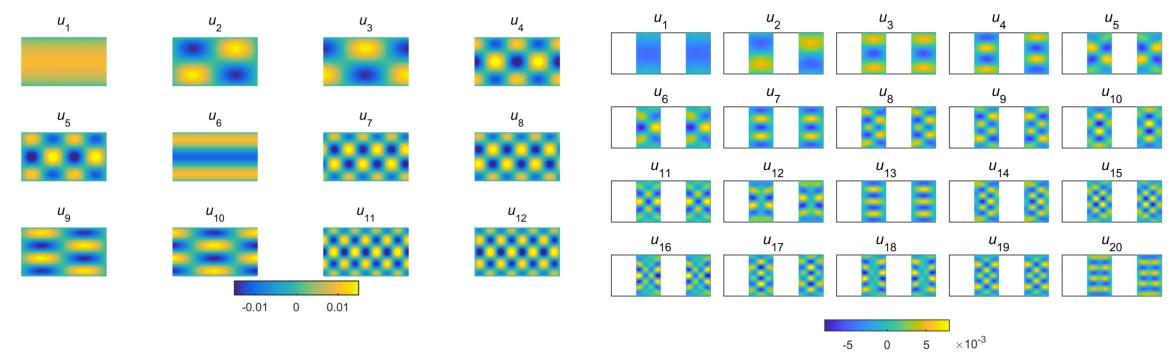


¹ Computed Tomography: Algorithms, Insight, and Just Enough Theory

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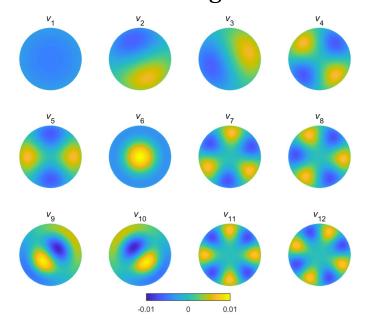
• The left singular vectors u_i in the sinogram domain have the same oscillatory features as the ones for the full-angle problem.

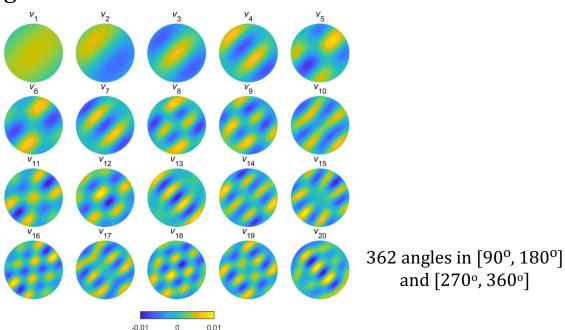


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In examples 10.8 and 10.9 of the book ¹, we compare the insights that can be obtained by the SVD for full-angle and limited-angle data, respectively. We have the following conclusions:

• The right singular vectors v_i of the limited-angle data on the other hand differ significantly from the full-angle data. All the reshaped vectors are dominated by features that are elongated at the angle 45° , while those of full-angle data have no dominating directions.





¹ Computed Tomography: Algorithms, Insight, and Just Enough Theory

To elaborate on this aspect, we consider the right singular vector v_{13} and its left singular vector u_{13} . They satisfy $\sigma_{13}u_{13}=A\ v_{13}$. Since the singular value $\sigma_{13}=143$ is large, the features associated with v_{13} should be apparent in the limited-data sinogram via u_{13} .

Which means it should be easy to reconstruct these features from the limited-data.

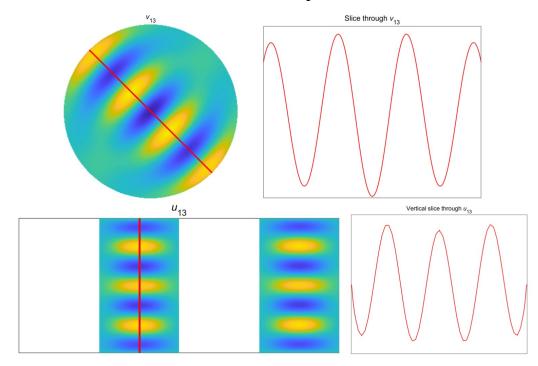
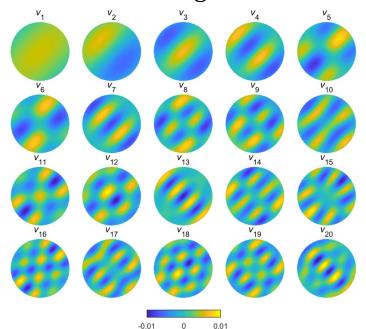


Figure 10.12. Top: Right singular vector v_{13} , shown as an image, with a black line $x_2 = -x_1$ (which has angle $\theta = 135^{\circ}$), and a graph of v_{13} along that black line. Bottom: Left singular vector u_{13} , shown as an image, with a black vertical line at $\theta = 135^{\circ}$, and a graph of that function along that black line. Note how v_{13} oscillates on the black line with angle $\theta = 135^{\circ}$ and how u_{13} oscillates on the black line at angle $\theta = 135^{\circ}$.

¹ Computed Tomography: Algorithms, Insight, and Just Enough Theory

We know from Chapter 8 that we can only expect to recover structures and edges along the projection angles. Our singular vectors are completely in accordance with this.

Since the reconstruction x is a weighted sum over the right singular vectors, it will inherit the dominating features of these vectors. In this case, features and structures at angles around 45° , around which the singular vectors are elongated.



$$x = A^{-1} b = \sum_{i=1}^{n} \frac{u_i^T b}{\sigma_i} v_i$$

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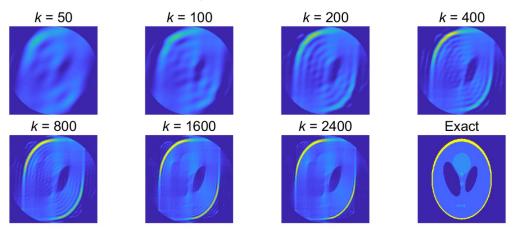


Figure 10.14. TSVD solutions to the limited-angle problem for selected values of the truncation parameter k, together with the exact solution. We use the same color axis from zero to one in all plots, and hence pixel values outside this range are truncated in the TSVD plots.

SVD Analysis of Discretized CT Problems

What is the real power of the SVD?

SVD analysis can be applied to a variety of geometries where closed-form expressions for singular values and vectors aren't available or hard to derive. Such as problems...

- with a square domain,
- with measurement geometries other than parallel beam,
- with limited projection angles

It can also be used to study the influence of practical issues such as the number and the choice of projection angles, the size of the detector array and the resolution of the image.

The Role of the Null Space

The Null Space Null(A) is the linear subspace of all vectors mapped to zero:

$$Null(A) = \{x \in \mathbb{R}^n \mid Ax = 0\}$$

- As discussed earlier, the reconstruction x is a weighted sum over the right singular vectors that can be obtained from the SVD of A. They represent the basis vectors of the column space of A.
- The right singular vectors corresponding to the Null Space represent features that cannot be reconstructed from the data at hand.
- Overall, the singular vectors outside the null space represent structures that we can reconstruct, whereas the ones in the null space represent structures we cannot reconstruct.

Summary

The Singular Value Decomposition

Intuitive Interpretations of the SVD

Matrix 2-Norm and Condition Number

What SVD looks like

Similarities to Singular Functions of the Radon Transform

Image Reconstruction using SVD

Picard plot and what Picard plot looks like

Ill-Conditioned Problems and Noisy Data

Spectral Filtering and TSVD

SVD Analysis for a limited-angle problem

The Role of the Null Space

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Thank you