

# Diagnostic Medical Image Processing

## Singular Value Decomposition (SVD)

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# Diagnostic Medical Image Processing



## 1 Singular Value Decomposition (SVD)

### ■ General Remarks

- On the Geometry of Linear Mappings
- Normal Form of Matrices: SVD
- Properties of SVD
- Optimization Problem I
- Optimization Problem II
- Optimization Problem III
- Optimization Problem IV
- Take Home Messages
- Further Readings



# Singular Value Decomposition

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

- Powerful normal form for matrices that allows for a simple solution of most linear problems in imaging and image processing.
- Method of numerical linear algebra
  - invented in the 19th century,
  - rediscovered and pushed for practical application by Gene Golub,
  - established in computer vision by Carlo Tomasi's famous factorization algorithm to compute structure and camera motion from image sequences
  - extremely robust, and simple to use.



# Singular Value Decomposition

SVD is a perfect tool for the

- computation of singular values
- computation of null space
- computation of (pseudo-) inverse
- solution of overdetermined linear equations
- computation of condition numbers
- enforcing rank criterion (numerical rank)
- etc.

$$A \vec{x} = \vec{0}$$
$$[\vec{q}_1, \vec{q}_2, \vec{q}_3]$$



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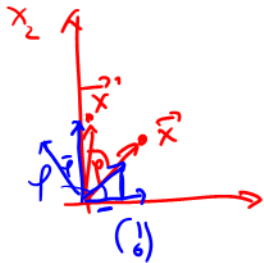
# On the Geometry of Linear Mappings

From linear algebra, we know that a matrix  $\mathbf{A}$  maps the unit vectors of the standard base to the corresponding column vector of matrix  $\mathbf{A}$ . .

## Example

$$\mathbf{A} \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \\ 0 \\ 0 \end{pmatrix} = (\mathbf{a}_1, \mathbf{a}_2, \dots, \mathbf{a}_6) \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \\ 0 \\ 0 \end{pmatrix} = \mathbf{a}_4.$$

Example:



$$R \vec{x} = \vec{x}'$$

$$R \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} \cos \varphi \\ \sin \varphi \end{pmatrix}$$

$$R \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \begin{pmatrix} -\sin \varphi \\ \cos \varphi \end{pmatrix}$$

$$R = \begin{pmatrix} \cos \varphi & -\sin \varphi \\ \sin \varphi & \cos \varphi \end{pmatrix}$$



# On the Geometry of Linear Mappings

## Example

Compute the orthogonal matrix  $\mathbf{R}$ , i.e.  $\mathbf{R}^{-1} = \mathbf{R}^T$ , that rotates points in the 2-D image plane by  $\theta$ .

**Solution:**

The base vectors are mapped as follows:

$$\begin{pmatrix} 1 \\ 0 \end{pmatrix} \mapsto \begin{pmatrix} \cos \theta \\ \sin \theta \end{pmatrix} \quad (1)$$

$$\begin{pmatrix} 0 \\ 1 \end{pmatrix} \mapsto \begin{pmatrix} -\sin \theta \\ \cos \theta \end{pmatrix} \quad (2)$$

and thus the 2-D rotation matrix is:

$$\mathbf{R} = \begin{pmatrix} \cos \theta & -\sin \theta \\ \sin \theta & \cos \theta \end{pmatrix} \quad (3)$$

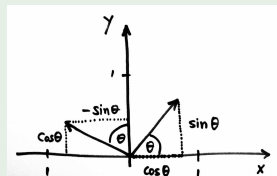


Figure 1: Rotation of 2-D unit vectors





# On the Geometry of Linear Mappings

If  $\mathbf{A}$  is a real  $(m \times n)$  matrix of rank  $r$ , then  $\mathbf{A}$  maps the unit hyper-sphere in the  $n$ -dimensional space to an  $r$ -dimensional hyper-ellipsoid in the  $m$ -dimensional space.

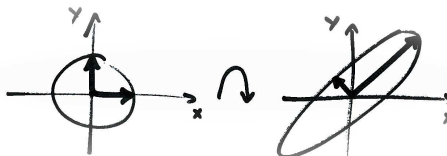


Figure 2: Rank 2 Matrix  $\mathbf{A}$  maps 2-D unit sphere to the 2-D ellipse



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# Normal Form of Matrices: SVD

## Theorem

If  $\mathbf{A}$  is a real  $(m \times n)$  matrix, then there exist orthogonal matrices  $\mathbf{U} \in \mathbb{R}^{m \times m}$  and  $\mathbf{V} \in \mathbb{R}^{n \times n}$  such that

$$\mathbf{A} = \mathbf{U}\mathbf{\Sigma}\mathbf{V}^T,$$

where

$$\mathbf{\Sigma} = \text{diag}(\sigma_1, \sigma_2, \dots, \sigma_p) \in \mathbb{R}^{m \times n} \quad (4)$$

with  $p = \min(m, n)$ ; the diagonal elements  $\sigma_i$  are the **singular values** that fulfill

$$\sigma_1 \geq \sigma_2 \geq \dots \geq \sigma_p \geq 0. \quad (5)$$



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# Properties of SVD: Rank, Norm and Eigenvectors

The Singular Value Decomposition shows many extremely useful properties that are listed here without proof:

- Rank of matrix  $\mathbf{A}$ :  $\text{rank}(\mathbf{A}) = \#\{\sigma_i > 0\} = r$
- Numerical  $\epsilon$ -rank of matrix  $\mathbf{A}$ :  $\text{rank}_\epsilon(\mathbf{A}) = \#\{\sigma_i > \epsilon\}$
- $\mathbf{A} = \sum_{i=1}^r \sigma_i \mathbf{u}_i \mathbf{v}_i^\top$
- The Frobenius norm of the matrix  $\mathbf{A}$  is given by

$$\|\mathbf{A}\|_F = \sqrt{\sum_{i=1}^m \sum_{j=1}^n a_{i,j}^2} = \sqrt{\sum_{i=1}^{\min(m,n)} \sigma_i^2}$$

- $\mathbf{A} \mathbf{v}_i = \sigma_i \mathbf{u}_i$  and  $\mathbf{A}^\top \mathbf{u}_i = \sigma_i \mathbf{v}_i$
- The column vectors of  $\mathbf{U}$  are the eigenvectors of  $\mathbf{A} \mathbf{A}^\top$ :

$$\mathbf{A} \mathbf{A}^\top \mathbf{u}_i = \sigma_i^2 \mathbf{u}_i$$

- The column vectors of  $\mathbf{V}$  are the eigenvectors of  $\mathbf{A}^\top \mathbf{A}$ :

$$\mathbf{A}^\top \mathbf{A} \mathbf{v}_i = \sigma_i^2 \mathbf{v}_i$$



# Properties of SVD

- The SVD yields orthonormal bases for the kernel (null-space) and the range of a matrix  $\mathbf{A}$ :
  - The kernel of matrix  $\mathbf{A}$  is spanned by the column vectors  $\mathbf{v}_i$  of  $\mathbf{V}$ , where the corresponding singular values fulfill  $\sigma_i = 0$ .
  - The range of matrix  $\mathbf{A}$  is spanned by the column vectors  $\mathbf{u}_i$  of  $\mathbf{U}$ , where  $\sigma_i$  are the corresponding non-zero singular values.
- For the 2-norm of matrix  $\mathbf{A}$  we get:

$$\|\mathbf{A}\|_2^2 = \max_{\|\mathbf{x}\|_2=1} \mathbf{x}^T \mathbf{A}^T \mathbf{A} \mathbf{x} = \sigma_1^2$$

and if  $\mathbf{A}$  is regular we even have:

$$\|\mathbf{A}^{-1}\|_2^2 = \frac{1}{\sigma_p^2}$$

# Example

$$\mathbf{A} = \begin{pmatrix} 11 & 10 & 14 \\ 12 & 11 & -13 \\ 14 & 13 & -66 \end{pmatrix} = \mathbf{U}\mathbf{\Sigma}\mathbf{V}^T \quad (6)$$

where

$$\mathbf{U} = \begin{pmatrix} 0.1285 & 0.8375 & 0.5311 \\ -0.2396 & 0.5459 & -0.8028 \\ -0.9623 & -0.0241 & 0.2708 \end{pmatrix} \quad (7)$$

$$\mathbf{\Sigma} = \begin{pmatrix} 71.3967 & 0 & 0 \\ 0 & 21.7831 & 0 \\ 0 & 0 & 0.0006 \end{pmatrix} \quad (8)$$

$$\mathbf{V} = \begin{pmatrix} -0.2092 & 0.7082 & -0.6743 \\ -0.1941 & 0.6458 & 0.7384 \\ 0.9584 & 0.2854 & 0.0024 \end{pmatrix} \quad (9)$$

## Example

- Obviously matrix  $\mathbf{A}$  has a rank deficiency, if we select  $\epsilon = 10^{-3}$ .
- The kernel of  $\mathbf{A}$  is given by:

$$\text{kernel}(\mathbf{A}) = \left\{ k \cdot \begin{pmatrix} -0.6743 \\ 0.7384 \\ 0.0024 \end{pmatrix} ; k \in \mathbb{R} \right\}$$

- The range of  $\mathbf{A}$  is:

$$\text{range}(\mathbf{A}) = \left\{ k \cdot \begin{pmatrix} 0.1285 \\ -0.2396 \\ -0.9623 \end{pmatrix} + l \cdot \begin{pmatrix} 0.8375 \\ 0.5459 \\ -0.0241 \end{pmatrix} ; k, l \in \mathbb{R} \right\}$$





# Ill-conditioned Matrix

## Definition

A matrix **A** is called **ill-conditioned** if for a given linear system

$$\mathbf{Ax} = \mathbf{b}$$

minor changes in **b** cause major changes in **x**

## Definition

The **condition number** of a regular matrix **A** with respect to a matrix norm  $||\cdot||$  is defined by

$$\kappa(\mathbf{A}) = ||\mathbf{A}^{-1}|| \cdot ||\mathbf{A}||$$

If **A** is singular,  $\kappa(\mathbf{A}) = +\infty$ .



## Ill-conditioned Matrix

### Remarks

- A matrix with a condition number close to 1 is called **well-conditioned**.
- A matrix with a condition number significantly greater than 1 is said to be **ill-conditioned**.
- The condition number is a measure of the stability or sensitivity of a matrix.
- Using the 2-norm, the condition number of the quadratic matrix  $\mathbf{A} \in \mathbb{R}^{n \times n}$  can be computed by SVD:

$$\kappa(\mathbf{A}) = \frac{\sigma_1}{\sigma_n} \quad (10)$$

where  $\sigma_1$  is the largest, and  $\sigma_n$  is the smallest singular value.

- The SVD allows for the exact computation of the condition number, but it is computationally expensive.



## Ill-conditioned Matrix

### Example

Consider the previous matrix:

$$\mathbf{A} = \begin{pmatrix} 11 & 10 & 14 \\ 12 & 11 & -13 \\ 14 & 13 & -66 \end{pmatrix}$$

where we obviously have  $\det \mathbf{A} = 1$ . The singular value decomposition of  $\mathbf{A}$  results in the singular values:

$$\sigma_1 = 71.3967, \sigma_2 = 21.7831, \text{ and } \sigma_3 = 0.0006.$$

Thus the condition number  $\kappa(\mathbf{A}) = 118994.5$ .

### Exercise problem:

Show that a variation in  $\mathbf{b}$  by 0.1% implies a change in  $\mathbf{x}$  by 240%.



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# Optimization Problem I

Let us consider the following problem that appears in many image processing and computer vision problems:

We computed a matrix  $\mathbf{A}$  out of sensor data like an image. By theory the matrix  $\mathbf{A}$  must have the singular values  $\sigma_1, \sigma_2, \dots, \sigma_p$ , where  $p = \min(m, n)$ . Of course, in practice  $\mathbf{A}$  does not fulfill this constraint.

**Problem:** What is the matrix  $\mathbf{A}'$  that is closest to  $\mathbf{A}$  (according to the Frobenius norm) and has the required singular values?

**Solution:** Let  $\mathbf{A} = \mathbf{U}\mathbf{\Sigma}\mathbf{V}^T$ , then

$$\mathbf{A}' = \mathbf{U} \operatorname{diag}(\sigma_1, \sigma_2, \dots, \sigma_p) \mathbf{V}^T$$



# Optimization Problem I

## Example

The measurements lead to the following matrix:

$$\mathbf{A} = \begin{pmatrix} 11 & 10 & 14 \\ 12 & 11 & -13 \\ 14 & 13 & -66 \end{pmatrix} = \mathbf{U}\mathbf{\Sigma}\mathbf{V}^T$$

Let us assume that by theoretical arguments the matrix  $\mathbf{A}$  is required to have a rank deficiency of one, and the two non-zero singular values are identical. The matrix  $\mathbf{A}'$  that is closest to  $\mathbf{A}$  according to the Frobenius norm and fulfills the above requirements is:

$$\mathbf{A}' = \mathbf{U} \operatorname{diag}((71.3967 + 21.7831)/2, (71.3967 + 21.7831)/2, 0) \mathbf{V}^T$$



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# Optimization Problem II



**Problem:** In image processing, we are often required to solve the following optimization problem:

$$\hat{\mathbf{x}} = \operatorname{argmin}_{\mathbf{x}} \mathbf{x}^T \mathbf{A}^T \mathbf{A} \mathbf{x} \quad \text{subject to} \quad \|\mathbf{x}\|_2 = 1. \quad (11)$$

or in the extreme:

$$\mathbf{A} \mathbf{x} = 0 \quad \text{subject to} \quad \|\mathbf{x}\|_2 = 1. \quad (12)$$

**Solution:** The solution can be constructed using the rightmost column of  $\mathbf{V}$  (check this!).





# Optimization Problem II

## Example

Estimate the matrix  $\mathbf{A} \in \mathbb{R}^{2 \times 2}$  such that for the following vectors

$$\mathbf{b}_1 = \begin{pmatrix} 1 \\ 1 \end{pmatrix}, \mathbf{b}_2 = \begin{pmatrix} -1 \\ 2 \end{pmatrix}, \mathbf{b}_3 = \begin{pmatrix} 1 \\ -3 \end{pmatrix}, \mathbf{b}_4 = \begin{pmatrix} -1 \\ -4 \end{pmatrix}$$

the optimization problem gets solved:

$$\sum_{i=1}^4 \mathbf{b}_i^T \mathbf{A} \mathbf{b}_i \rightarrow \min \quad \text{s.t.} \quad \|\mathbf{A}\|_F = 1$$



# Optimization Problem II

## Example

The objective function is linear in the components of  $\mathbf{A}$ , thus the whole sum can be rewritten in matrix notation:

$$\mathbf{M}\mathbf{a} = \mathbf{M} \begin{pmatrix} a_{1,1} \\ a_{1,2} \\ a_{2,1} \\ a_{2,2} \end{pmatrix} = \mathbf{0} \quad \text{s.t.} \quad \|\mathbf{a}\|_2 = 1$$

where the **measurement matrix**  $\mathbf{M}$  is built from single elements of the sum. Let us consider the  $i$ -th component:

$$\mathbf{b}_i^\top \mathbf{A} \mathbf{b}_i = \mathbf{b}_i^\top \begin{pmatrix} a_{1,1} & a_{1,2} \\ a_{2,1} & a_{2,2} \end{pmatrix} \mathbf{b}_i = (b_{i,1}^2, b_{i,1}b_{i,2}, b_{i,1}b_{i,2}, b_{i,2}^2) \begin{pmatrix} a_{1,1} \\ a_{1,2} \\ a_{2,1} \\ a_{2,2} \end{pmatrix}$$



# Optimization Problem II

## Example

Using this result we get for the overall measurement matrix:

$$\mathbf{M} = \begin{pmatrix} b_{1,1}^2 & b_{1,1}b_{1,2} & b_{1,1}b_{1,2} & b_{1,2}^2 \\ b_{2,1}^2 & b_{2,1}b_{2,2} & b_{2,1}b_{2,2} & b_{2,2}^2 \\ b_{3,1}^2 & b_{3,1}b_{3,2} & b_{3,1}b_{3,2} & b_{3,2}^2 \\ b_{4,1}^2 & b_{4,1}b_{4,2} & b_{4,1}b_{4,2} & b_{4,2}^2 \end{pmatrix} = \begin{pmatrix} 1 & 1 & 1 & 1 \\ 1 & -2 & -2 & 4 \\ 1 & -3 & -3 & 9 \\ 1 & 4 & 4 & 16 \end{pmatrix}$$

The nullspace of  $\mathbf{M}$  can be computed by SVD and yields the required matrix:

$$\mathbf{A} = \begin{pmatrix} 0 & -0.7071 \\ 0.7071 & 0 \end{pmatrix}$$



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## Optimization Problem III

**Problem:** Another quite important optimization problem in image processing and pattern recognition is the following:

Given a matrix  $\mathbf{A} \in \mathbb{R}^{n \times n}$ . Compute the matrix  $\hat{\mathbf{B}} \in \mathbb{R}^{n \times n}$  of rank  $k < n$  that minimizes:

$$\hat{\mathbf{B}} = \operatorname{argmin}_{\mathbf{B}} \|\mathbf{A} - \mathbf{B}\|_2 \quad \text{s.t.} \quad \operatorname{rank}(\mathbf{B}) = k \quad .$$

**Solution:** Using SVD, the solution is quite simple:

$$\hat{\mathbf{B}} = \sum_{i=1}^k \sigma_i \mathbf{u}_i \mathbf{v}_i^T \quad .$$



# Optimization Problem III

## Example

The SVD can be used to compute the image matrix of rank 1 that best approximates an image. Figure ?? shows an example of an image  $I$  and its rank-1-approximation  $I' = \sigma_1 \mathbf{u}_1 \mathbf{v}_1^T$ .

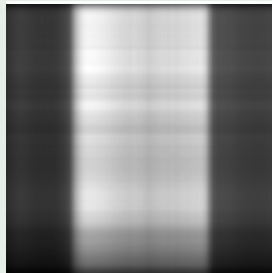
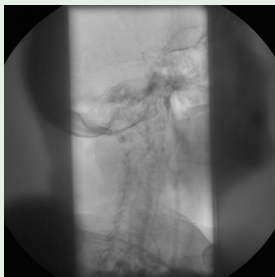


Figure 3: Original X-ray image and its rank-1-approximation



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## Optimization Problem IV

**Problem:** The **Moore-Penrose pseudo-inverse** is required to find the solution to the following optimization problem:

$$\|\mathbf{Ax} - \mathbf{b}\|_2 \rightarrow 0 \quad (13)$$

**Solution:** The least square solution of this equation is given by

$$\mathbf{x} = \mathbf{A}^\dagger \mathbf{b} \quad (14)$$

where we get based on the SVD of  $\mathbf{A}$ :

$$\mathbf{A}^\dagger = (\mathbf{A}^\top \mathbf{A})^{-1} \mathbf{A}^\top = \mathbf{V} \Sigma^\dagger \mathbf{U}^\top. \quad (15)$$





## Optimization Problem IV

The diagonal matrix in the pseudo-inverse is defined via:

$$\Sigma^\dagger = \begin{pmatrix} \frac{1}{\sigma_1} & & & & 0 & \dots & 0 \\ & \ddots & & & & & \\ & & \frac{1}{\sigma_r} & & \vdots & & \vdots \\ & & & 0 & & \ddots & \\ & & & & 0 & \dots & 0 \end{pmatrix} \in \mathbb{R}^{n \times m} \quad (16)$$

where  $\sigma_r > \epsilon$  is the smallest nonzero singular value.



# Optimization Problem IV

## Example

Compute the regression line through the following 2-D points:

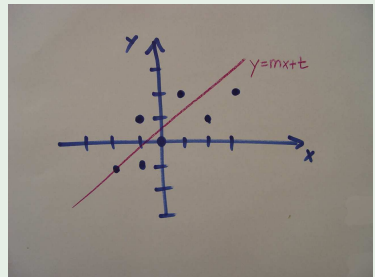
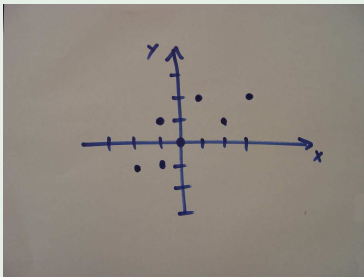


Figure 4: Regression line through 2-D points



## Optimization Problem IV

All points  $(x_i, y_i)$ ,  $i = 1, \dots, 7$ , have to fulfill the line equation:

$$y_i = mx_i + t, \quad \text{for } i = 1, \dots, 7$$

Thus we get the system of linear equations:

$$\begin{pmatrix} 3 & 1 \\ 2 & 1 \\ 1 & 1 \\ 0 & 1 \\ -1 & 1 \\ -1 & 1 \\ -2 & 1 \end{pmatrix} \begin{pmatrix} m \\ t \end{pmatrix} = \begin{pmatrix} 2 \\ 1 \\ 2 \\ 0 \\ 1 \\ -1 \\ -1 \end{pmatrix}$$

# Optimization Problem IV



The Moore-Penrose pseudo-inverse for this particular problem is:

$$\mathbf{A}^\dagger = \begin{pmatrix} 0.14 & 0.09 & 0.04 & -0.01 & -0.07 & -0.07 & -0.12 \\ 0.11 & 0.12 & 0.13 & 0.15 & 0.16 & 0.16 & 0.18 \end{pmatrix}$$

The resulting line equation thus is:

$$y = 0.56x + 0.41$$



# Remarks on SVD Computation

- For us SVD is a black box; we do not consider algorithms to compute the SVD numerically.
- SVD can be computed for any matrix
- SVD is numerically robust
- Time complexity to decompose  $\mathbf{A} \in \mathbb{R}^{m \times n}$ :

$$4m^2n + 8mn^2 + 9n^3$$

- In most practical situations we have more rows than columns, i.e.  $m \gg n$ .



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# Take Home Messages

- SVD is *the* tool for linear equations — it cannot fail (but in many special cases there may exist better solutions).
- SVD is provided by all standard libraries.
- SVD is always our first choice.
- SVD is most probably the right answer to any question in the oral exam. **Give it a try and check its limitations!**



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## Further Readings

- Read the original:  
Gene H. Golub, Charles F. Van Loan: Matrix Computations, Johns Hopkins Studies in Mathematical Sciences, 3rd edition, The Johns Hopkins University Press, Baltimore, 1996 (amazon the book right [here](#)).
- A very detailed and easy to follow introduction of the SVD can be found in Carlo Tomasi's class notes ([download pdf](#), chapter 3) ... a **must-read**.
- The theory is described in an easy to read format (one of my favorite books!):  
Lloyd N. Trefethen, David Bau: Numerical Linear Algebra, Cambridge University Press, Cambridge, 1997 (amazon the book right [here](#)).



## Further Readings

- For numerical computation of SVD see:  
William H. Press, Saul A. Teukolsky, William T. Vetterling:  
Numerical Recipes in C The Art of Scientific Computing,  
Cambridge University Press, Cambridge, 1993 (c.f.  
[NR Web Page](#)).