Singular Value Decomposition (SVD)

Foundations of Data Analysis

March 24, 2022

What is SVD?

Decompose a matrix A into three parts:

$$A = USV^T$$

The matrices U, S, and V have special properties

Why is SVD Useful?

Many applications in data analysis, including:

- Least squares fitting of data
- Dimensionality reduction
- Correlation analysis

Review: Data Tables

	ID	M.F	Hand	Age	Educ	SES	MMSE	CDR	eTIV	nWBV	ASF	Delay	RightHippoVol	LeftHippoVol
0	OAS1_0002_MR1	F	R	55	4	1.0	29	0.0	1147	0.810	1.531	NaN	4230	3807
1	OAS1_0003_MR1	F	R	73	4	3.0	27	0.5	1454	0.708	1.207	NaN	2896	2801
2	OAS1_0010_MR1	M	R	74	5	2.0	30	0.0	1636	0.689	1.073	NaN	2832	2578
3	OAS1_0011_MR1	F	R	52	3	2.0	30	0.0	1321	0.827	1.329	NaN	3978	4080
4	OAS1_0013_MR1	F	R	81	5	2.0	30	0.0	1664	0.679	1.055	NaN	3557	3495
5	OAS1_0015_MR1	M	R	76	2	NaN	28	0.5	1738	0.719	1.010	NaN	3052	2770
6	OAS1_0016_MR1	M	R	82	2	4.0	27	0.5	1477	0.739	1.188	NaN	3421	3119
7	OAS1_0018_MR1	M	R	39	3	4.0	28	0.0	1636	0.813	1.073	NaN	4496	4283
8	OAS1_0019_MR1	F	R	89	5	1.0	30	0.0	1536	0.715	1.142	NaN	3760	3167
9	OAS1_0020_MR1	F	R	48	5	2.0	29	0.0	1326	0.785	1.323	NaN	3557	3394
10	OAS1_0021_MR1	F	R	80	3	3.0	23	0.5	1794	0.765	0.978	NaN	3715	3019
11	OAS1_0022_MR1	F	R	69	2	4.0	23	0.5	1447	0.757	1.213	NaN	3258	3566
12	OAS1_0023_MR1	M	R	82	2	3.0	27	0.5	1420	0.710	1.236	NaN	3217	2160
13	OAS1_0026_MR1	F	R	58	5	1.0	30	0.0	1235	0.820	1.421	NaN	3783	3535
14	OAS1_0028_MR1	F	R	86	2	4.0	27	1.0	1449	0.738	1.211	NaN	3452	3100
15	OAS1_0030_MR1	F	R	65	2	3.0	29	0.0	1392	0.764	1.261	NaN	3969	3406

Row: individual data point

Column: particular dimension or feature

Review: Matrices

A matrix is an $n \times d$ array of real numbers:

$$A = \begin{pmatrix} a_{11} & a_{12} & \cdots & a_{1d} \\ a_{21} & a_{22} & \cdots & a_{2d} \\ \vdots & & & \vdots \\ a_{n1} & a_{n2} & \cdots & a_{nd} \end{pmatrix}$$

Notation: $A \in \mathbb{R}^{n \times d}$

A **data matrix** is n data points, each with d features

Review: Matrix-Vector Multiplication

We can multiply an $n \times d$ matrix A with a d-vector v:

$$Av = \begin{pmatrix} a_{11} & a_{12} & \cdots & a_{1d} \\ a_{21} & a_{22} & \cdots & a_{2d} \\ \vdots & & & \vdots \\ a_{n1} & a_{n2} & \cdots & a_{nd} \end{pmatrix} \begin{pmatrix} v_1 \\ v_2 \\ \vdots \\ v_d \end{pmatrix} = \begin{pmatrix} \sum_{j=1}^{d} a_{1j} v_j \\ \sum_{j=1}^{d} a_{2j} v_j \\ \vdots \\ \sum_{j=1}^{d} a_{nj} v_j \end{pmatrix}$$

The result is an n-vector.

Each entry is a dot product between a row of A and v:

$$Av = \begin{pmatrix} \langle a_{1\bullet}, v \rangle \\ \langle a_{2\bullet}, v \rangle \\ \vdots \\ \langle a_{n\bullet}, v \rangle \end{pmatrix}$$

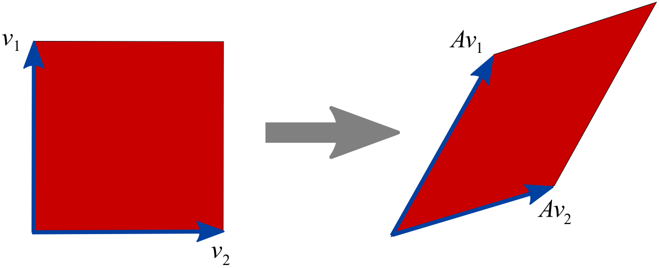
Review: Matrices as Transformations

Consider a 2D matrix and coordinate vectors in $\mathbb{R}^2$:

$$A = \begin{pmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{pmatrix}, \qquad v_1 = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad v_2 = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

Then Av_1 and Av_2 result in the columns of A:

$$Av_1 = \begin{pmatrix} a_{11} \\ a_{21} \end{pmatrix}, \qquad Av_2 = \begin{pmatrix} a_{12} \\ a_{22} \end{pmatrix}$$



Orthogonal Matrices

A matrix U is called **orthogonal** if the columns of U have unit length and are orthogonal to each other:

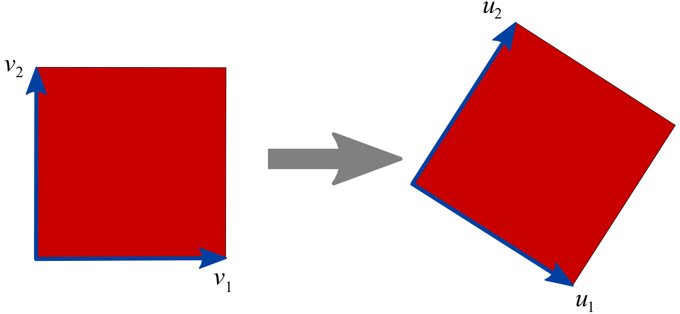
Unit length: $\|u_{\bullet i}\| = 1$
Orthogonal: $\langle u_{\bullet i}, u_{\bullet j} \rangle = 0$

Orthogonal Matrix Transformations

$$U = \begin{pmatrix} u_{11} & u_{12} \\ u_{21} & u_{22} \end{pmatrix}, \qquad v_1 = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad v_2 = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

Then Uv_1 and Uv_2 result in the columns of U:

$$Uv_1 = \begin{pmatrix} u_{11} \\ u_{21} \end{pmatrix} = u_{\bullet 1}, \qquad Uv_2 = \begin{pmatrix} u_{12} \\ u_{22} \end{pmatrix} = u_{\bullet j}$$



SVD

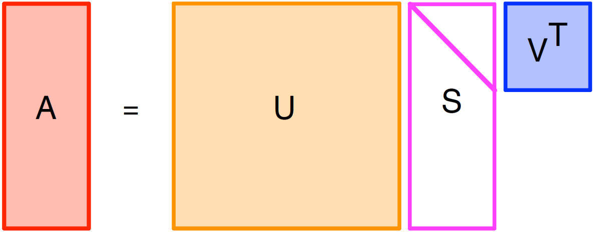


Figure from M4D

$$A = USV^T$$

U : $n \times n$ orthogonal matrix

S : $n \times d$ diagonal matrix

V : $d \times d$ orthogonal matrix

SVD

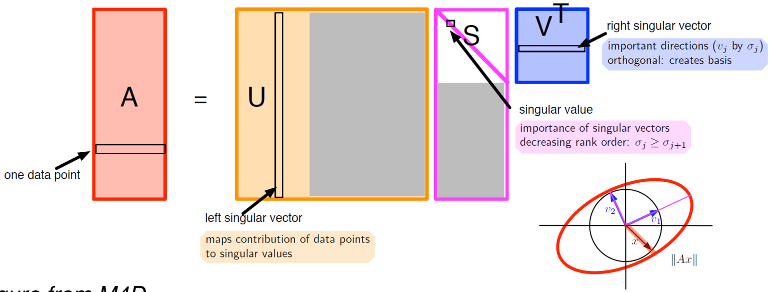


Figure from M4D

Application: Orthogonal Procrustes Analysis

Problem:

Find the rotation R^* that minimizes distance between two $d \times k$ matrices A, B:

$$R^* = \arg\min_{R \in \mathrm{SO}(d)} \|RA - B\|^2$$

Solution:

Let $U\Sigma V^T$ be the SVD of BA^T, then

$$R^* = UV^T$$