Singular Value Decomposition

$$A \in M_{n \times m}(\mathbb{R}),\ n \neq m$$

Find a way to decompose A like the case if $n = m$ for orthogonal diagonalization.

Step 1: Consider $A^t A \in M_m(\mathbb{R})$, a square matrix.

A^tA

A^tA is square, and symmetric

since $(A^tA)^t = A^t(A^t)^t$

$= A^tA$ ✓

Then A^tA is orthogonally diagonalizable!

Even better: if λ is an eigenvalue of A^tA, then

$\boxed{\lambda \geq 0}$

Why is $\lambda \geq 0$?

Because if v is an eigenvector,

then if we assume $\|v\|_2 = 1$,

$$
\begin{aligned}
\lambda &= \lambda \|v\|_2^2 \\
&= \lambda v \cdot v \\
&= (A^t A v) \cdot v \\
&= (v^t A^t) A v \\
&= (Av)^t A v \\
&= Av \cdot Av \\
&\geq 0 \quad \checkmark
\end{aligned}
$$

Matrix Square Roots

If D is a diagonal matrix and the entries of D are not negative, we set $D^{1/2}$ to be the matrix

$$\left(D^{1/2}\right)_{i,j} = \left(D_{i,j}\right)^{1/2}$$

i.e. $$\begin{bmatrix} 5 & 0 \\ 0 & 36 \end{bmatrix}^{1/2} = \begin{bmatrix} \sqrt{5} & 0 \\ 0 & \sqrt{36} \end{bmatrix}$$

$$= \begin{bmatrix} \sqrt{5} & 0 \\ 0 & 6 \end{bmatrix}$$

For A^tA, orthogonally diagonalize as

$$A^tA = SDS^t.$$

Then $\boxed{(A^tA)^{1/2} = S D^{1/2} S^t}$

Note: if 0 is <u>not</u> an eigenvalue for D, then D is actually invertible!

If $D = \begin{bmatrix} d_1 & & & 0 \\ & d_2 & & \\ & & \ddots & \\ 0 & & & d_m \end{bmatrix}$

with $d_i > 0$,

$$D^{-1} = \begin{bmatrix} \frac{1}{d_1} & & & 0 \\ & \frac{1}{d_2} & & \\ & & \ddots & \\ 0 & & & \frac{1}{d_m} \end{bmatrix}$$

This will then give you that $(A^tA)^{1/2}$ is invertible, which gives you that A^tA is invertible.

Singular Value Decomposition (SVD)

(reduced)

Let A be an $n \times m$ matrix.

Then there is an $m \times m$ diagonal matrix $\hat{D}$, an $n \times m$ matrix $\hat{U}$ with orthonormal columns, and an $m \times m$ orthogonal matrix $\hat{V}$ with

$$\boxed{A = \hat{U}\hat{D}\hat{V}}$$

Idea of SVD:

Consider $A^tA \in M_n(\mathbb{R})$.

A^tA is orthogonally diagonalizable

as

$$\boxed{A^tA = U_0 D_0 U_0^t}$$

So

$$U_0^t A^t A U_0 = D_0 .$$

By multiplying on left and right by a permutation matrix (always orthogonal), we may assume

$$D_0 = \begin{bmatrix} D_1 & 0 \\ 0 & 0 \end{bmatrix}$$

where D_1 is a $k \times k$ diagonal matrix with nonzero entries.

Split $U_0 = \begin{bmatrix} U_1 & U_2 \end{bmatrix}$

where U_1 is $m \times k$ and

$$D_0 = \begin{bmatrix} D_1 & 0 \\ 0 & 0 \end{bmatrix}$$

$$= U_0^t A^t A U_0$$

$$= \begin{bmatrix} u_1^t \\ u_2^t \end{bmatrix} A^t A \begin{bmatrix} u_1 & u_2 \end{bmatrix}$$

$$= \begin{bmatrix} u_1^t A^t A u_1 & u_1^t A^t A u_2 \\ u_2^t A^t A u_1 & u_2^t A^t A u_2 \end{bmatrix}$$

with $D_1 = u_1^t A^t A u_1$

Let

$$\boxed{W = \underbrace{A}_{n\times m}\,\underbrace{U_1}_{m\times k}\,\underbrace{D_1^{-1/2}}_{k\times k}}$$

Then

$$W^t W = D_1^{-1/2}\, U_1^t A^t A U_1 D_1^{-1/2}$$

$$= D_1^{-1/2} D_1 D_1^{-1/2}$$

$$= I_k$$

So W has orthonormal columns.

Observe: $W D_1^{1/2} = A U_1$

Since $W D_1^{1/2} = A V_1$,

multiplying on the right by V_1^t,

$$W D_1^{1/2} V_1^t = A V_1 V_1^t$$

$$= A I_m$$

$$= A$$

Note: if $\dim(\mathrm{Ran}(A)) = n$,

then D_1 is $n \times n$, so we'd

be done. But in general,

this is not true!

Fix: $\hat{D} = \begin{bmatrix} D_1^{1/2} & 0 \\ 0 & 0 \end{bmatrix}$ $(m \times m)$

By Gram Schmidt, add orthonormal rows to v_1^t to get $\hat{v}$ and orthonormal columns to w to get $\hat{u}$.

$\square$

Full SVD

Let A be an $n \times m$ matrix.

Then there is a $n \times m$ diagonal matrix D, an $n \times n$ orthogonal matrix U, and an $m \times m$ orthogonal matrix V with

$$\boxed{A = UDV}$$

Example 1:

Let $A = \begin{bmatrix} 1 & 2 & 5 & 8 \\ -9 & 3 & 1 & 0 \end{bmatrix}$

$$A \in M_{2\times 4}(\mathbb{R})$$

Want: singular value decomposition for A.

Use Wolfram Alpha!

Idea: to compress an image, given by an $n \times m$ matrix, perform the singular value decomposition, throw away "unimportant" rows from the diagonal matrix. This reduces the size of the image!

Announcements

1) HW 8 clarification - find the full SVD (this is what Wolfram Alpha does)

Singular Values

These are the eigenvalues of

$(A^tA)^{1/2}$ = the diagonal

entries of $\hat{D}$ = the diagonal

entries of D

Principal Component Analysis (PCA)

- or -

"What does the SVD do?"

We've already tried to fit polynomials to data. What if we try to fit equations that are not the graph of a function to the data?

Easiest example: circle

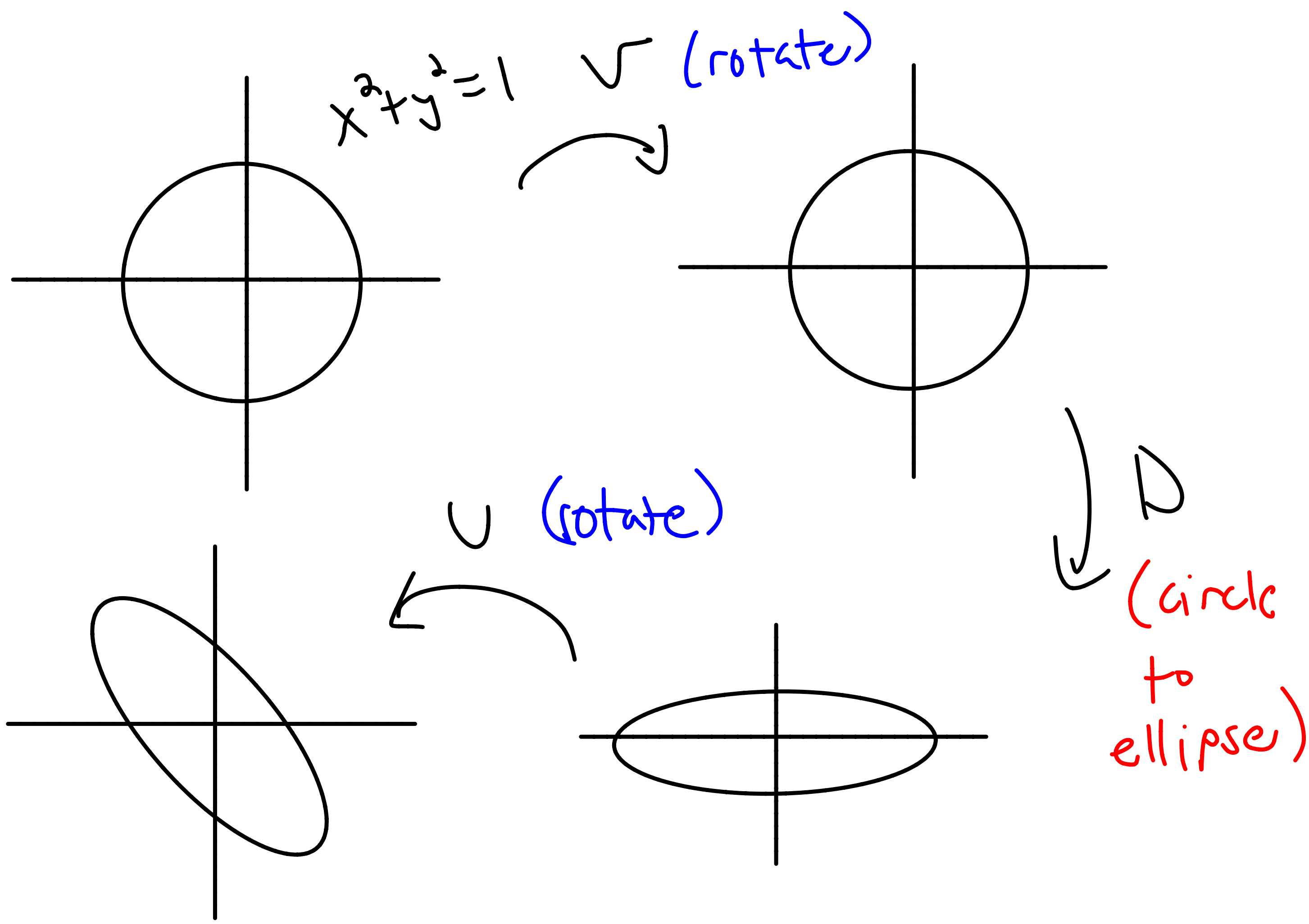
Picture - full SVD

A is 2×2,

$A = U D V$

V, U orthogonal, D diagonal

If A is invertible, so is D.



Ellipsoids

ellipse: $$\frac{x^2}{a^2} + \frac{y^2}{b^2} = 1$$

major & minor axes associated to $x=0$ and $y=0$

In higher dimensions, we have

ellipsoids:

$$\boxed{\frac{x_1^2}{a_1^2} + \frac{x_2^2}{a_2^2} + \cdots + \frac{x_k^2}{a_k^2} = 1}$$

axes associated to all but one coordinate equalling zero.

Idea: (PCA) picks out the axes of the ellipse.

1^{st} principal component = longest axis

2^{nd} " " = next-longest axis

and so on

From SVD

$A = UDV^T$ (full SVD)

Score matrix $T = UD$

1^{st} principal component $= 1^{st}$ column of T

2^{nd} " " $= 2^{nd}$ column of T

and so on

The first column is sometimes called <u>the</u> principal component.

Example 1:

$$A = \begin{bmatrix} 1 & 1 & 0 \\ 0 & 1 & 1 \end{bmatrix}$$

Find the principal component of A.

Singular Value Decomposition of A:

$$A = UDV^T \quad \text{(full SVD)}$$

where

$$U = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & -1 \\ 1 & 1 \end{bmatrix}$$

$$D = \begin{bmatrix} \sqrt{3} & 0 & 0 \\ 0 & 1 & 0 \end{bmatrix}, \quad V = \begin{bmatrix} \frac{1}{\sqrt{6}} & \sqrt{\frac{2}{3}} & \frac{1}{\sqrt{6}} \\ -\frac{1}{\sqrt{2}} & 0 & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{3}} & -\frac{1}{\sqrt{3}} & \frac{1}{\sqrt{3}} \end{bmatrix}$$

Score matrix:

$$T = UD$$

$$= \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & -1 \\ 1 & 1 \end{bmatrix} \cdot \begin{bmatrix} \sqrt{3} & 0 & 0 \\ 0 & 1 & 0 \end{bmatrix}$$

$$= \frac{1}{\sqrt{2}} \begin{bmatrix} \sqrt{3} & -1 & 0 \\ \sqrt{3} & 1 & 0 \end{bmatrix}$$

$$= \begin{bmatrix} \sqrt{3/2} & -\frac{1}{\sqrt{2}} & 0 \\ \sqrt{3/2} & \frac{1}{\sqrt{2}} & 0 \end{bmatrix}$$

$$\boxed{\text{Principal component: } \begin{bmatrix} \sqrt{3/2} \\ \sqrt{3/2} \end{bmatrix}}$$

Permutation Matrices

These are orthogonal matrices that can change the order of components in a vector while preserving the value of the components.

Convention: I_n is a permutation matrix

Example 2: (low dimensions)

$n=2$ There are two permutation matrices,

$$\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}, \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$$

$n=3$ There are six permutation matrices,

$$\begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}, \begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix}, \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{bmatrix}$$

$$\begin{bmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{bmatrix}, \begin{bmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{bmatrix}, \begin{bmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{bmatrix}$$

In general, there are $n!$ permutation matrices in $M_n(\mathbb{R})$.

These are matrices with a single nonzero entry in every row and column, and the nonzero entry is always 1.

If you want to, say, make the 4^{th} coordinate move to the 2^{nd} coordinate, the entry 1 will occur in the (second row, fourth column) of the matrix.

Any such matrix is always orthogonal since: the columns are orthonormal.

To change the order of the diagonal entries on a diagonal $n \times n$ matrix D: multiply

$$U D U^t$$ where U is a permutation matrix, chosen to effect the order you desire.

Example 3:

$$D = \begin{bmatrix} 1 & 0 \\ 0 & 2 \end{bmatrix},$$

we can rearrange the diagonal by

$$\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \begin{bmatrix} 1 & 0 \\ 0 & 2 \end{bmatrix} \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$$

$$= \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \begin{bmatrix} 0 & 1 \\ 2 & 0 \end{bmatrix}$$

$$= \begin{bmatrix} 2 & 0 \\ 0 & 1 \end{bmatrix} \quad \checkmark$$