GENERAL ASSEMBLY

INTRO TO DATA SCIENCE

LECTURE 13: DIMENSIONALITY REDUCTION

YUCHEN ZHAO / DAT-14

LAST TIME:

- SVM'S
- HARD/SOFT MARGIN CLASSIFIERS
- KERNEL METHODS FOR NONLINEAR CLASSIFICATION

I. DIMENSIONALITY REDUCTION
II. PRINCIPAL COMPONENTS ANALYSIS
III. SINGULAR VALUE DECOMPOSITION

EXERCISE:
IV. DIMENSIONALITY REDUCTION IN SCIKIT-LEARN

I. DIMENSIONALITY REDUCTION

Q: What is dimensionality reduction?

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In general, the idea is to regard the dataset is a matrix and to decompose the matrix into simpler, meaningful pieces.

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A: A set of techniques for reducing the size (in terms of features, records, and/or bytes) of the dataset under examination.

In general, the idea is to regard the dataset is a matrix and to decompose the matrix into simpler, meaningful pieces.

Dimensionality reduction is frequently performed as a pre-processing step before another learning algorithm is applied.

Q: What are the motivations for dimensionality reduction?

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The number of features in our dataset can be difficult to manage, or even misleading (eg, if the relationships are actually simpler than they appear).

For example, suppose we have a dataset with some features that are related to each other.

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If these relationships are linear, then we can use well-established techniques like PCA/SVD.

EXAMPLE: 1D HARMONIC OSCILLATOR

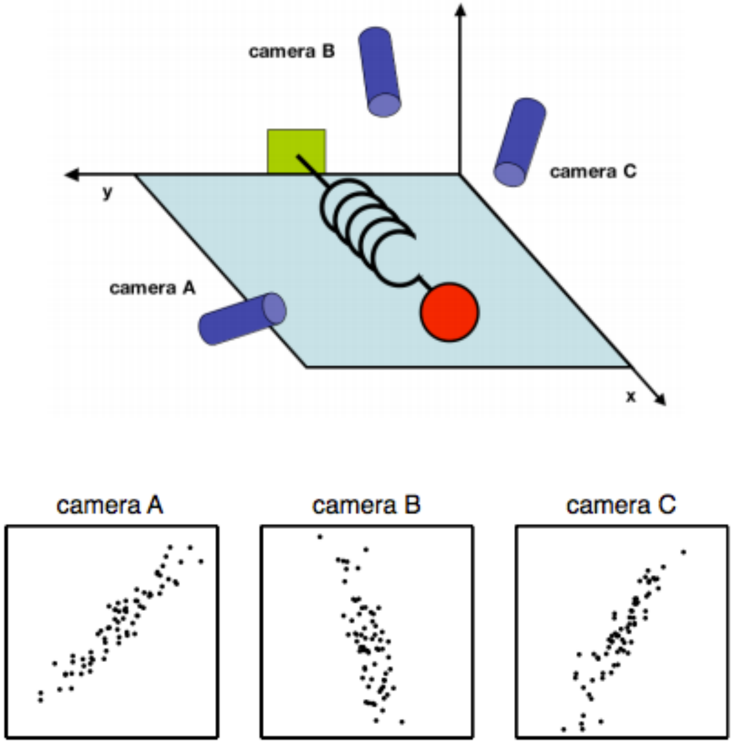

FIG. 1 A toy example. The position of a ball attached to an oscillating spring is recorded using three cameras A, B and C. The position of the ball tracked by each camera is depicted in each panel below.

source: http://www.snl.salk.edu/~shlens/pca.pdf

ASIDE: CURSE OF DIMENSIONALITY

The complexity that comes with a large number of features is due in part to the **curse of dimensionality**.

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Namely, the sample size needed to accurately estimate a random variable taking values in a d*-dimensional feature space grows exponentially with* d *(almost).*

ASIDE: CURSE OF DIMENSIONALITY

Another way of characterizing this is to say that high-dimensional spaces are inherently **sparse***.*

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This illustrates the fact that local methods will break down in these circumstances (eg, in order to collect enough neighbors for a given point, you need to expand the radius of the neighborhood so far that locality is not preserved).

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This illustrates the fact that local methods will break down in these circumstances (eg, in order to collect enough neighbors for a given point, you need to expand the radius of the neighborhood so far that locality is not preserved).

The bottom line is that high-dimensional spaces can be problematic.

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More precisely: given an n *x* d *matrix* A *(encoding* n *observations of a* d*-dimensional random variable), we want to find a* k*-dimensional representation of* A *(*$k < d$*) that captures the information in the original data, according to some criterion.*

Q: What is the goal of dimensionality reduction?

- *reduce computational expense*
- *reduce susceptibility to overfitting*
- *reduce noise in the dataset*
- *enhance our intuition*

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NOTE

We've already seen one example of feature selection for regression: backward elimination.

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Feature selection is important, but typically when people say dimensionality reduction, they are referring to feature extraction.

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The goal of feature extraction is to create a new set of coordinates that simplify the representation of the data.

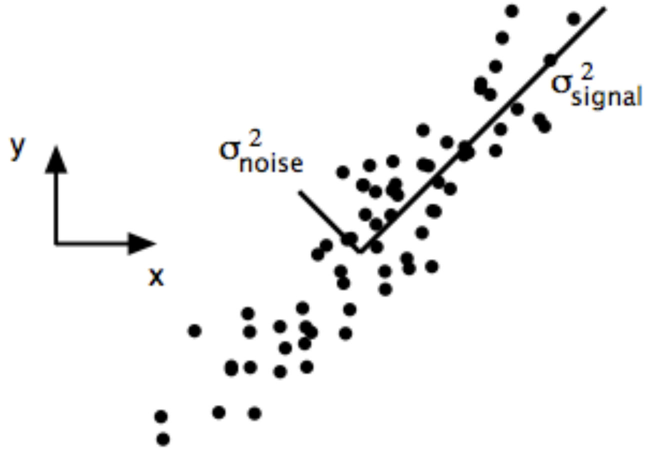

FIG. 2 Simulated data of (x, y) for camera A. The signal and noise variances σ^2_{signal} and σ^2_{noise} are graphically represented by the two lines subtending the cloud of data. Note that the largest direction of variance does not lie along the basis of the recording (x_A, y_A) but rather along the best-fit line.

source: http://www.snl.salk.edu/~shlens/pca.pdf

Q: What are some applications of dimensionality reduction?

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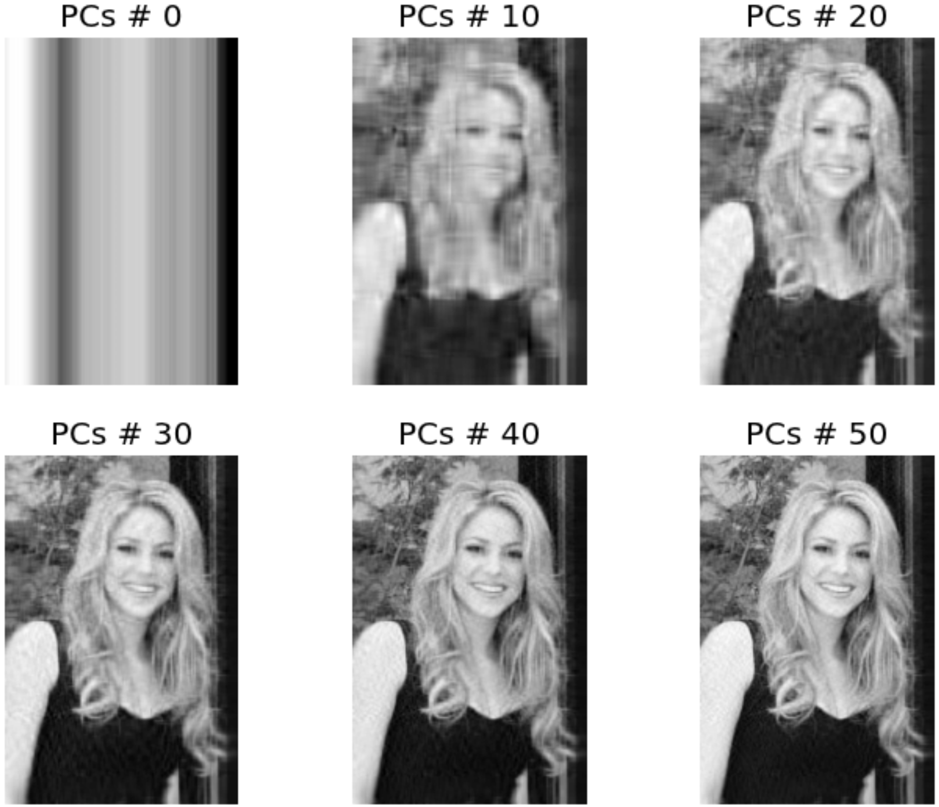
- *topic models (document clustering)*
- *image recognition/computer vision*
- *bioinformatics (microarray analysis)*
- *speech recognition*
- *astronomy (spectral data analysis)*
- *recommender systems*

DIMENSIONALITY REDUCTION



source: http://glowingpython.blogspot.it/2011/07/pca-and-image-compression-with-numpy.html

II. PRINCIPAL COMPONENT ANALYSIS

Principal Component Analysis is a dimension reduction technique that can be used on a matrix of any dimensions.

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The PCA of a matrix $\mathbf{A}$ *boils down to the* **eigenvalue decomposition** *of the* **covariance matrix** *of* $\mathbf{A}$.

what is variance?

$$s^2 = \frac{\sum_{i=1}^{n}(X_i - \bar{X})^2}{(n-1)}$$

Variance is the average distance from the mean of a data set to a point in that data set.

In other words, it is a measure of the *spread* of the data. Recall that standard deviation is the square root of variance.

what is covariance?

covariance is a measure of how much two random variables change together

Variance:

$$s^2 = \frac{\sum_{i=1}^{n}(X_i - \bar{X})^2}{(n-1)} \qquad var(X) = \frac{\sum_{i=1}^{n}(X_i - \bar{X})(X_i - \bar{X})}{(n-1)}$$

Covariance:

$$cov(X,Y) = \frac{\sum_{i=1}^{n}(X_i - \bar{X})(Y_i - \bar{Y})}{(n-1)}$$

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The covariance matrix C *of a matrix* A *is always square:*

$$\mathrm{C} = \begin{bmatrix} \mathrm{E}[(X_1-\mu_1)(X_1-\mu_1)] & \mathrm{E}[(X_1-\mu_1)(X_2-\mu_2)] & \cdots & \mathrm{E}[(X_1-\mu_1)(X_n-\mu_n)] \\ \mathrm{E}[(X_2-\mu_2)(X_1-\mu_1)] & \mathrm{E}[(X_2-\mu_2)(X_2-\mu_2)] & \cdots & \mathrm{E}[(X_2-\mu_2)(X_n-\mu_n)] \\ \vdots & \vdots & \ddots & \vdots \\ \mathrm{E}[(X_n-\mu_n)(X_1-\mu_1)] & \mathrm{E}[(X_n-\mu_n)(X_2-\mu_2)] & \cdots & \mathrm{E}[(X_n-\mu_n)(X_n-\mu_n)] \end{bmatrix}.$$

- *off-diagonal elements* $\mathrm{C_{ij}}$ *give the covariance between* $\mathrm{X_i}, \mathrm{X_j}$ $(\mathrm{i} \neq \mathrm{j})$
- *diagonal elements* $\mathrm{C_{ii}}$ *give the variance of* $\mathrm{X_i}$

ASIDE: EIGENVALUE DECOMPOSITION

The eigenvalue decomposition of a square matrix A *is given by:*

$$\mathrm{A} = \mathrm{Q}\Lambda\mathrm{Q}^{-1}$$

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The columns of Q *are the* **eigenvectors** *of* A*, and the values in* Λ *are the associated* **eigenvalues** *of* A*.*

$$\begin{aligned} A &= \begin{bmatrix} -1/2 & 3/2 \\ 3/2 & -1/2 \end{bmatrix} \\ &= \left(\frac{1}{\sqrt{2}}\begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}\right)\begin{bmatrix} 1 & 0 \\ 0 & -2 \end{bmatrix}\left(\frac{1}{\sqrt{2}}\begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}\right)^T \end{aligned}$$

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This relationship defines what it means to be an eigenvector of A.

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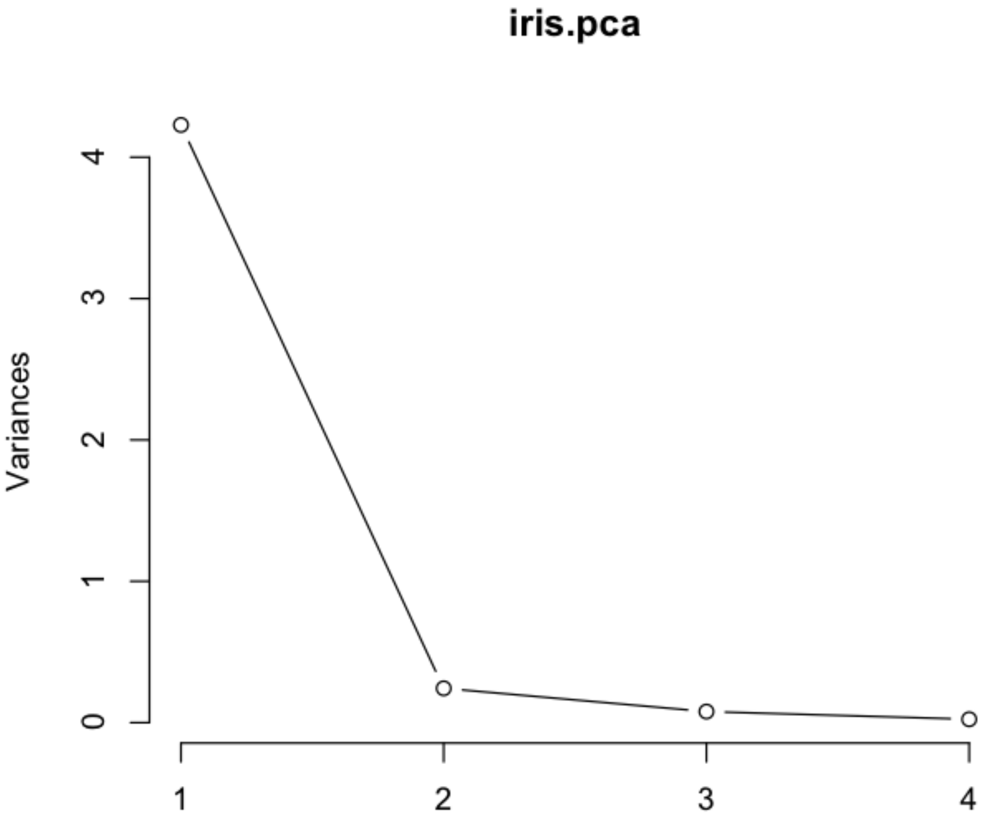
This can be visualized in a **scree plot***, which shows the amount of variance explained by each basis vector.*

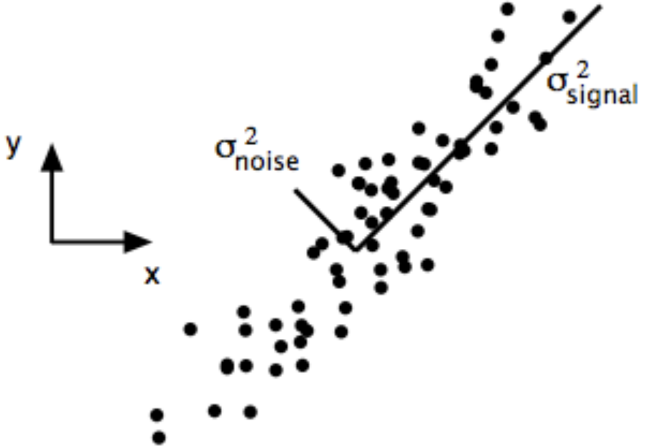
PRINCIPAL COMPONENT ANALYSIS



1. Linearity *– The change in basis is a linear projection*

2. Large variances have important structure

we assume that principal components with larger associated variances are signal, while those with lower variances represent noise.



*3. The principal components are **orthogonal***

III. SINGULAR VALUE DECOMPOSITION

Consider a matrix M *with* m *rows and* n *features.*

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st. U, V *are* **orthogonal** *matrices and* Σ *is a* **diagonal** *matrix.*

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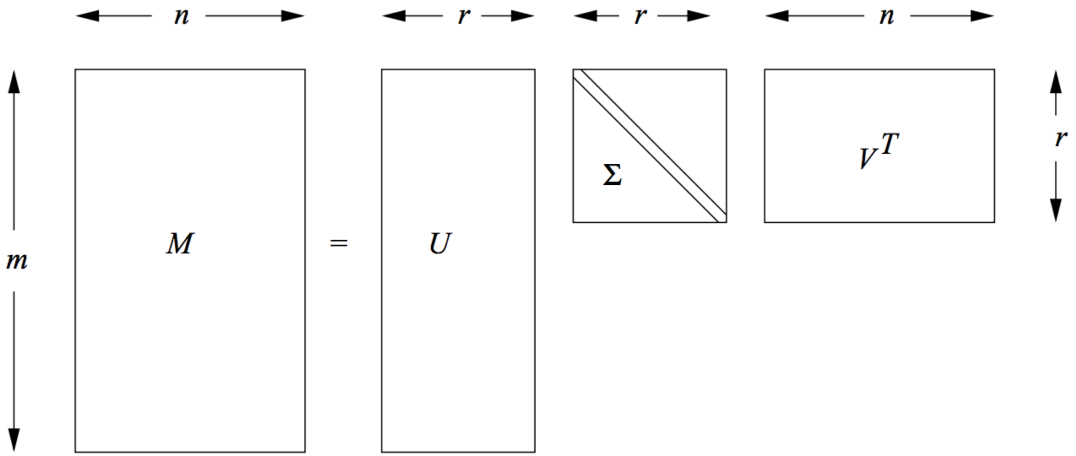
(m x n) (m x r) (r x r) (r x n)



source: http://infolab.stanford.edu/~ullman/mmds/ch11.pdf

SINGULAR VALUE DECOMPOSITION – EXAMPLE

Ratings of movies by users:

	Matrix	Alien	Star Wars	Casablanca	Titanic
Joe	1	1	1	0	0
Jim	3	3	3	0	0
John	4	4	4	0	0
Jack	5	5	5	0	0
Jill	0	0	0	4	4
Jenny	0	0	0	5	5
Jane	0	0	0	2	2

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there are two "concepts" underlying the movies:

science-fiction and romance

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All the boys rate only science-fiction

All the girls rate only romance

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Ratings of movies by users:

$$\underset{M}{\begin{bmatrix} 1 & 1 & 1 & 0 & 0 \\ 3 & 3 & 3 & 0 & 0 \\ 4 & 4 & 4 & 0 & 0 \\ 5 & 5 & 5 & 0 & 0 \\ 0 & 0 & 0 & 4 & 4 \\ 0 & 0 & 0 & 5 & 5 \\ 0 & 0 & 0 & 2 & 2 \end{bmatrix}} = \underset{U}{\begin{bmatrix} .14 & 0 \\ .42 & 0 \\ .56 & 0 \\ .70 & 0 \\ 0 & .60 \\ 0 & .75 \\ 0 & .30 \end{bmatrix}} \underset{\Sigma}{\begin{bmatrix} 12.4 & 0 \\ 0 & 9.5 \end{bmatrix}} \underset{V^{\mathrm{T}}}{\begin{bmatrix} .58 & .58 & .58 & 0 & 0 \\ 0 & 0 & 0 & .71 & .71 \end{bmatrix}}$$

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$$\underbrace{\begin{bmatrix} 1 & 1 & 1 & 0 & 0 \\ 3 & 3 & 3 & 0 & 0 \\ 4 & 4 & 4 & 0 & 0 \\ 5 & 5 & 5 & 0 & 0 \\ 0 & 0 & 0 & 4 & 4 \\ 0 & 0 & 0 & 5 & 5 \\ 0 & 0 & 0 & 2 & 2 \end{bmatrix}}_{M} = \underbrace{\begin{bmatrix} .14 & 0 \\ .42 & 0 \\ .56 & 0 \\ .70 & 0 \\ 0 & .60 \\ 0 & .75 \\ 0 & .30 \end{bmatrix}}_{U} \underbrace{\begin{bmatrix} 12.4 & 0 \\ 0 & 9.5 \end{bmatrix}}_{\Sigma} \underbrace{\begin{bmatrix} .58 & .58 & .58 & 0 & 0 \\ 0 & 0 & 0 & .71 & .71 \end{bmatrix}}_{V^{\mathrm{T}}}$$

M: people -> movies

U: people -> concepts

V: concepts -> movies

Σ: the strength of each of the concepts

source: http://infolab.stanford.edu/~ullman/mmds/ch11.pdf

SINGULAR VALUE DECOMPOSITION – A MORE REALISTIC EXAMPLE

$$
\begin{array}{r|ccccc|}
 & \text{Matrix} & \text{Alien} & \text{Star Wars} & \text{Casablanca} & \text{Titanic} \\
\hline
\text{Joe} & 1 & 1 & 1 & 0 & 0 \\
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\text{Jill} & 0 & 0 & 0 & 4 & 4 \\
\text{Jenny} & 0 & 0 & 0 & 5 & 5 \\
\text{Jane} & 0 & 0 & 0 & 2 & 2 \\
\hline
\end{array}
$$

$$
\underbrace{\begin{bmatrix}
1 & 1 & 1 & 0 & 0 \\
3 & 3 & 3 & 0 & 0 \\
4 & 4 & 4 & 0 & 0 \\
5 & 5 & 5 & 0 & 0 \\
0 & 2 & 0 & 4 & 4 \\
0 & 0 & 0 & 5 & 5 \\
0 & 1 & 0 & 2 & 2
\end{bmatrix}}_{M'} =
$$

$$
\underbrace{\begin{bmatrix}
.13 & .02 & -.01 \\
.41 & .07 & -.03 \\
.55 & .09 & -.04 \\
.68 & .11 & -.05 \\
.15 & -.59 & .65 \\
.07 & -.73 & -.67 \\
.07 & -.29 & .32
\end{bmatrix}}_{U}
\underbrace{\begin{bmatrix}
12.4 & 0 & 0 \\
0 & 9.5 & 0 \\
0 & 0 & 1.3
\end{bmatrix}}_{\Sigma}
\underbrace{\begin{bmatrix}
.56 & .59 & .56 & .09 & .09 \\
.12 & -.02 & .12 & -.69 & -.69 \\
.40 & -.80 & .40 & .09 & .09
\end{bmatrix}}_{V^{\mathrm{T}}}
$$

source: http://infolab.stanford.edu/~ullman/mmds/ch11.pdf

SINGULAR VALUE DECOMPOSITION - EXAMPLE

How to reduce dimensions?

<u>Drop Low Singular Values</u> -> eliminate corresponding rows of U and V

$$\underset{M'}{\begin{bmatrix} 1 & 1 & 1 & 0 & 0 \\ 3 & 3 & 3 & 0 & 0 \\ 4 & 4 & 4 & 0 & 0 \\ 5 & 5 & 5 & 0 & 0 \\ 0 & 2 & 0 & 4 & 4 \\ 0 & 0 & 0 & 5 & 5 \\ 0 & 1 & 0 & 2 & 2 \end{bmatrix}} =$$

$$\underset{U}{\begin{bmatrix} .13 & .02 & -.01 \\ .41 & .07 & -.03 \\ .55 & .09 & -.04 \\ .68 & .11 & -.05 \\ .15 & -.59 & .65 \\ .07 & -.73 & -.67 \\ .07 & -.29 & .32 \end{bmatrix}} \underset{\Sigma}{\begin{bmatrix} 12.4 & 0 & 0 \\ 0 & 9.5 & 0 \\ 0 & 0 & 1.3 \end{bmatrix}} \underset{V^{\mathrm{T}}}{\begin{bmatrix} .56 & .59 & .56 & .09 & .09 \\ .12 & -.02 & .12 & -.69 & -.69 \\ .40 & -.80 & .40 & .09 & .09 \end{bmatrix}}$$

$$\underset{\Sigma}{\begin{bmatrix} 12.4 & 0 \\ 0 & 9.5 \end{bmatrix}}$$

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$$\begin{bmatrix} 1 & 1 & 1 & 0 & 0 \\ 3 & 3 & 3 & 0 & 0 \\ 4 & 4 & 4 & 0 & 0 \\ 5 & 5 & 5 & 0 & 0 \\ 0 & 2 & 0 & 4 & 4 \\ 0 & 0 & 0 & 5 & 5 \\ 0 & 1 & 0 & 2 & 2 \end{bmatrix} =$$

$$M'$$

$$\begin{bmatrix} .13 & .02 & -.01 \\ .41 & .07 & -.03 \\ .55 & .09 & -.04 \\ .68 & .11 & -.05 \\ .15 & -.59 & .65 \\ .07 & -.73 & -.67 \\ .07 & -.29 & .32 \end{bmatrix} \begin{bmatrix} 12.4 & 0 & 0 \\ 0 & 9.5 & 0 \\ 0 & 0 & 1.3 \end{bmatrix} \begin{bmatrix} .56 & .59 & .56 & .09 & .09 \\ .12 & -.02 & .12 & -.69 & -.69 \\ .40 & -.80 & .40 & .09 & .09 \end{bmatrix}$$

$$U \qquad \Sigma \qquad V^{\mathrm{T}}$$

$$\begin{bmatrix} .13 & .02 \\ .41 & .07 \\ .55 & .09 \\ .68 & .11 \\ .15 & -.59 \\ .07 & -.73 \\ .07 & -.29 \end{bmatrix} \begin{bmatrix} 12.4 & 0 \\ 0 & 9.5 \end{bmatrix} \begin{bmatrix} .56 & .59 & .56 & .09 & .09 \\ .12 & -.02 & .12 & -.69 & -.69 \end{bmatrix}$$

$$= \begin{bmatrix} 0.93 & 0.95 & 0.93 & .014 & .014 \\ 2.93 & 2.99 & 2.93 & .000 & .000 \\ 3.92 & 4.01 & 3.92 & .026 & .026 \\ 4.84 & 4.96 & 4.84 & .040 & .040 \\ 0.37 & 1.21 & 0.37 & 4.04 & 4.04 \\ 0.35 & 0.65 & 0.35 & 4.87 & 4.87 \\ 0.16 & 0.57 & 0.16 & 1.98 & 1.98 \end{bmatrix}$$

source: http://infolab.stanford.edu/~ullman/mmds/ch11.pdf

IV. LAB