GENERAL ASSEMBLY

DIMENSIONALITY REDUCTION

Brian Chung

LAST TIME:

-BAGGING (RANDOM SAMPLES FROM THE DATA)
-RANDOM FOREST (RANDOM SAMPLES + RANDOM FEATURES)
-BOOSTING (SEQUENTIAL LEARNING FROM MISTAKES)

- WHEN USE BAGGING VS RANDOM FOREST?
- HYPERPARAMETERS ALL THE SAME FOR BOOSTING?

TYPES OF ML SOLUTIONS

	Continuous	Categorical
Supervised	Regression	Classification
Unsupervised	Dimension Reduction	Clustering

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

EXERCISE:
IV. DIMENSIONALITY REDUCTION IN SCIKIT-LEARN

I. DIMENSIONALITY REDUCTION

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

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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).

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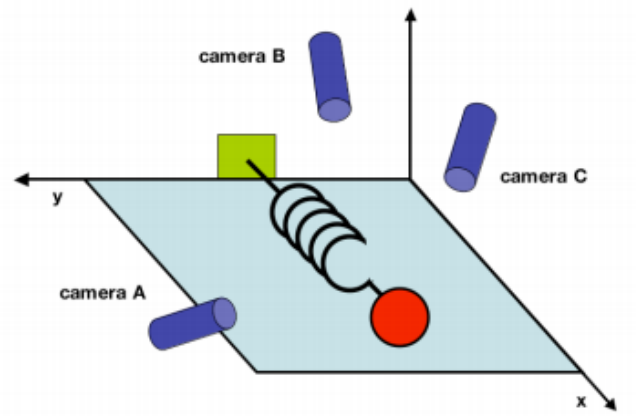
If these relationships are linear, then we can use well-established techniques like PCA/SVD.



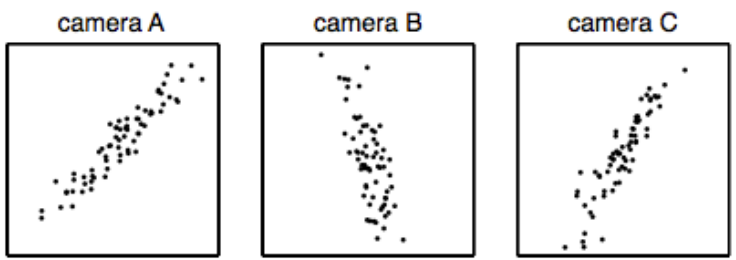
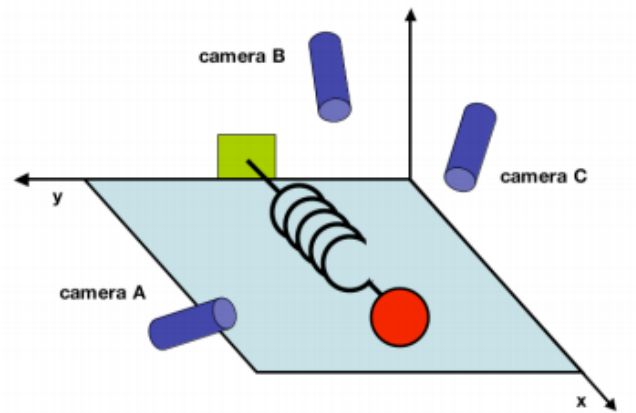
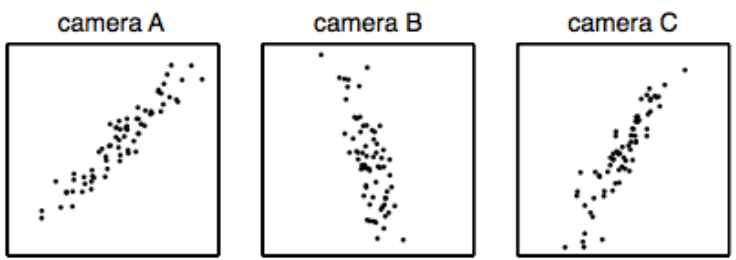


FIG. 1 A toy example. The position of a ball attached to an oscillating spring is recorded using three cameras A, B and C. The position of the ball tracked by each camera is depicted in each panel below.

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





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NOTE

Here, the "truth" is (nearly) one-dimensional. In general, we don't know what the "truth" is, but the same techniques can apply

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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).

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ex: A high-dimensional orange contains most of its volume in the rind!

ex: A high-dimensional hypercube contains most of its volume in the corners!

In either case, most of the points in the space are "far" from the center.

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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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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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We've already seen one example of feature selection for regression: *LASSO*

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

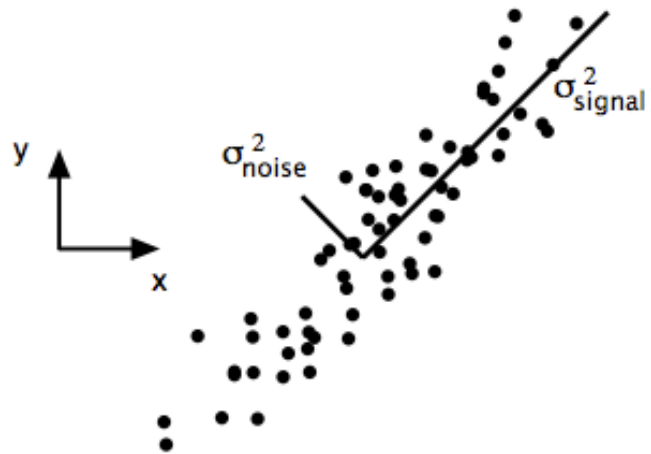

FIG. 2 Simulated data of (x, y) for camera A. The signal and noise variances σ^2_{signal} and σ^2_{noise} are graphically represented by the two lines subtending the cloud of data. Note that the largest direction of variance does not lie along the basis of the recording (x_A, y_A) but rather along the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

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

Q: What are some applications of dimensionality reduction?

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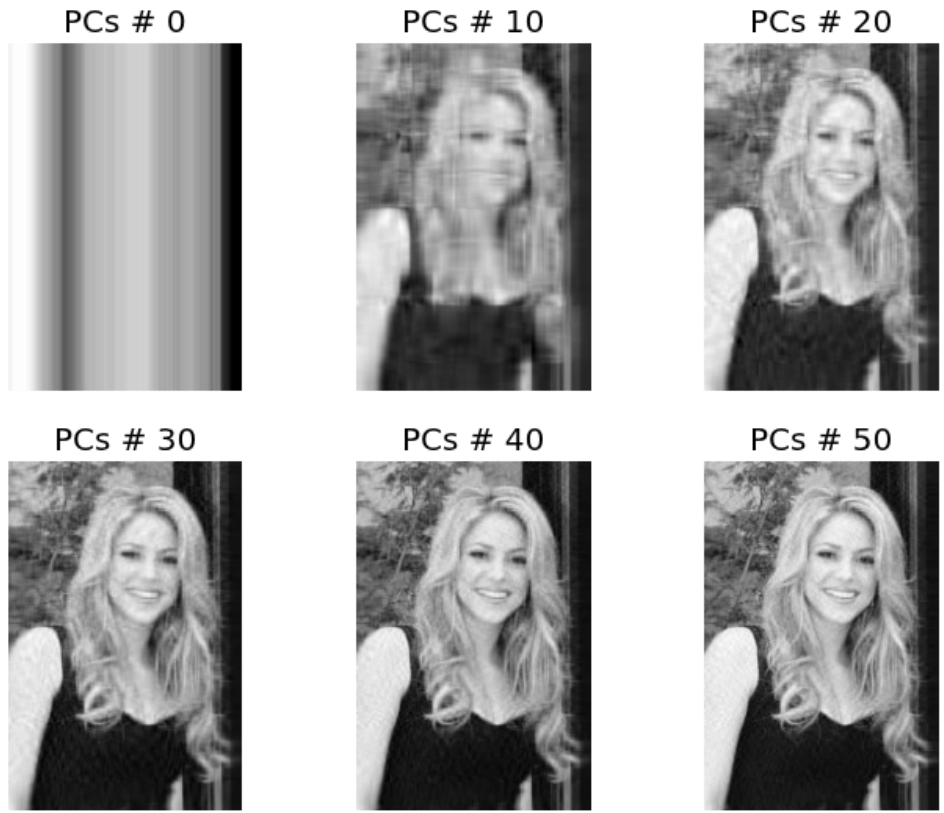
- *topic models (document clustering)*
- *image recognition/computer vision*
- *bioinformatics (microarray analysis)*
- *speech recognition*
- *astronomy (spectral data analysis)*
- *recommender systems*



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 A boils down to the* eigenvalue decomposition *of the* covariance matrix *of A.

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 C_{ij} give the covariance between X_i, X_j ($i \neq j$)

diagonal elements C_{ii} give the variance of X_i

Wait...what is a covariance?

Let's start off with variance...

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

Variance is the average squared distance from the mean of a dataset. It measures the spread of the data. The square root of the variance is the standard deviation

Variance operates only on 1 dimension. If we had multiple features we could look at the variance of each feature individually, but maybe we want to look at how much two features vary from the mean with respect to each other.

This is called covariance.

Covariance operates between two vectors. If you calculate the covariance between a vector X and itself, you will get X's variance.

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

Given some data matrix X with features along columns x_1, x_2, x_3, …, x_n,

$$\mathrm{cov}(X) = \begin{pmatrix} \mathrm{cov}(x_1, x_1) & \mathrm{cov}(x_2, x_1) & \mathrm{cov}(x_n, x_1) \\ \mathrm{cov}(x_1, x_2) & \mathrm{cov}(x_2, x_2) & \mathrm{cov}(x_n, x_2) \\ \mathrm{cov}(x_1, x_n) & \mathrm{cov}(x_2, x_n) & \mathrm{cov}(x_n, x_n) \end{pmatrix}$$

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NOTE

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

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In order to perform PCA, we perform the eigenvalue decomposition of the covariance matrix of our data matrix X

1. *Determine covariance matrix of X*
2. *Perform eigenvalue decomposition to obtain the* ***eigenvectors*** *and* ***eigenvalues*** *of the covariance matrix*

The eigenvectors form a basis of the vector space on which A acts (eg, they are orthogonal).

Furthermore the basis elements are ordered by their eigenvalues (from largest to smallest), and these eigenvalues represent the amount of variance explained by each basis element.

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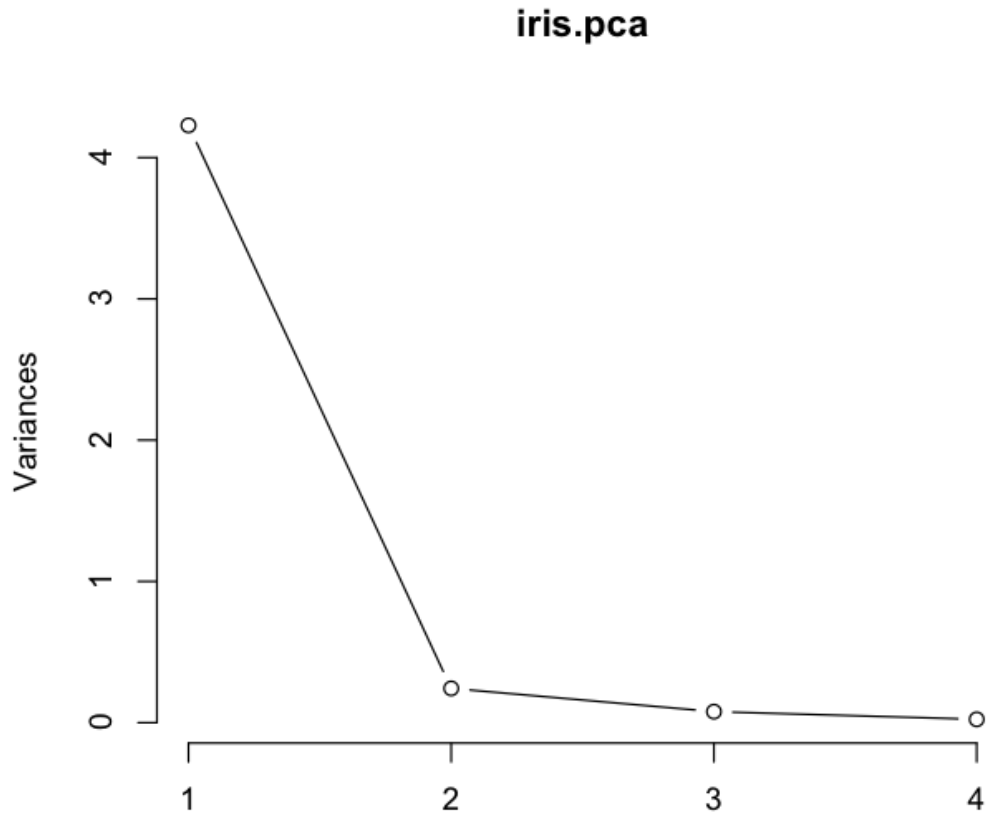
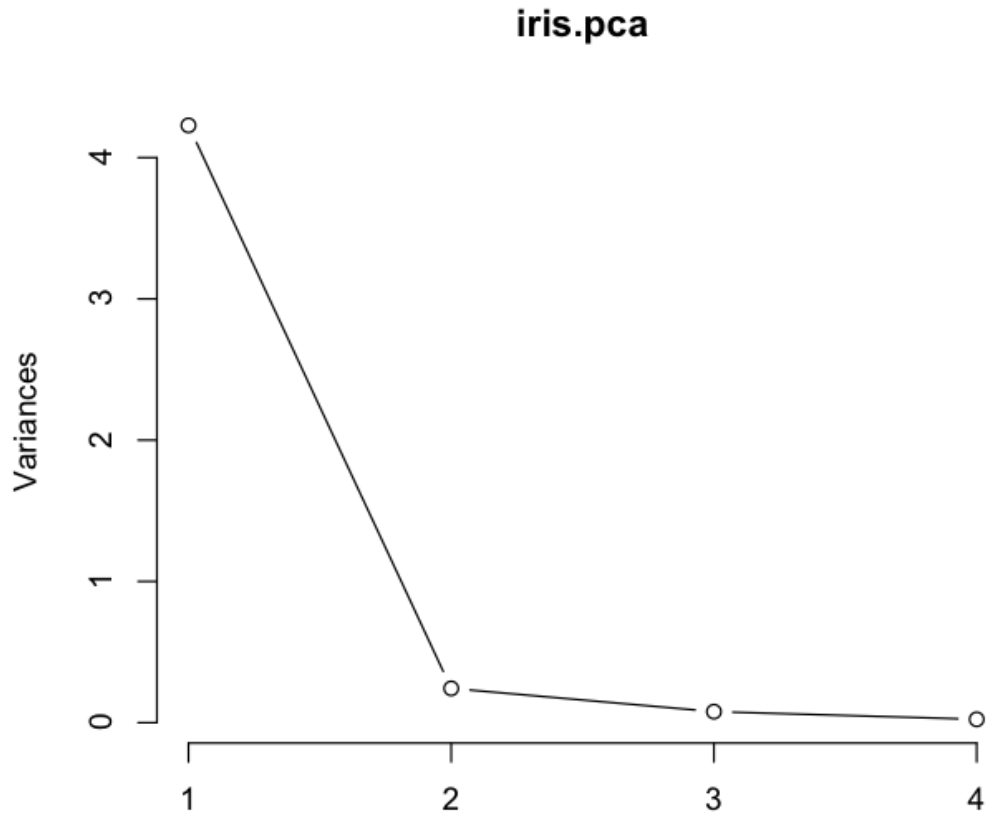
This can be visualized in a **scree plot**, *which shows the amount of variance explained by each basis vector.*


iris.pca
Variances
0
1
2
3
4
1
2
3
4



NOTE

Looking at this plot also gives you an idea of how many principal components to keep.

Apply the *elbow test*: keep only those pc's that appear to the left of the elbow in the graph.

- *PCA assumes that the change in basis is a **linear** projection (i.e. the new set of basis can be described as a linear combination of the original basis)*
- *Large variances have important structure – We assume that principal components associated with larger variances have more signal than noise (important but not always correct!)*
- *Principal components are orthogonal*

III. SINGULAR VALUE DECOMPOSITION

Lots of math ahead. If you are bewildered, don't worry.

Take your time to read through things later, and take it slow :)

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$\rightarrow \quad UU^T = I_n, \; VV^T = I_d \qquad \rightarrow \quad \Sigma_{ij} = 0 \;\; (i \neq j)$

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$$\underset{(n \times d)}{A} = \underset{(n \times n)}{U} \; \underset{(n \times d)}{\Sigma} \; \underset{(d \times d)}{V^T}$$

The columns of U & V are the (left- and right-) **singular vectors** *of A.*

These singular vectors provide **orthonormal bases** *for the spaces* K_n *&* K_d *(columns of U & V, respectively).*

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NOTE

The number of singular values is equal to the *rank* of A.

The rank of a matrix measures its *non-degeneracy.*

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NOTE

If the data is centered, these are proportional to covariance matrices

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Here "best" refers to the representation that minimizes the squared *orthogonal* distances from the points to the subspace.

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A: Recall that given a set of n points in d-dimensional space (eg, a matrix A), we want to find the best $k < d$ dimensional subspace to represent the data.

For $k = 1$, this subspace is a line passing through the origin.

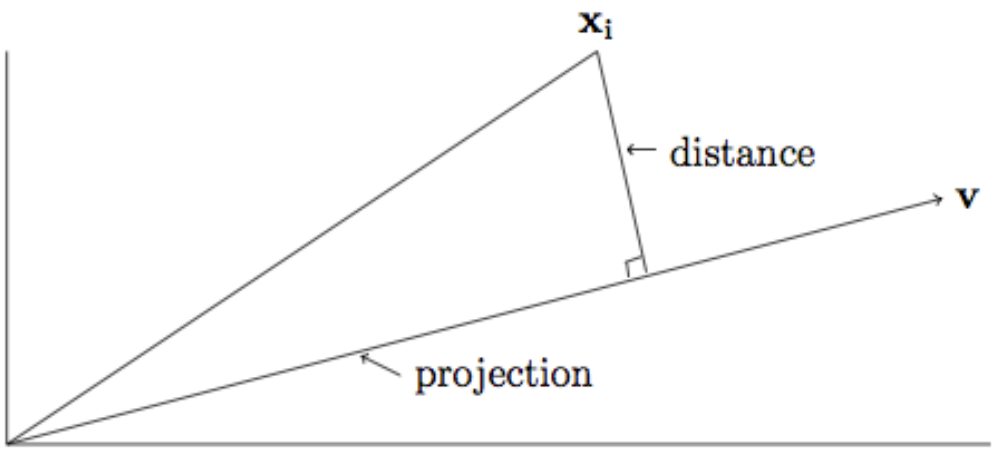

Figure 4.1: The projection of the point $\mathbf{x_i}$ onto the line through the origin in the direction of $\mathbf{v}$

source: http://www.cs.princeton.edu/courses/archive/spring12/cos598C/svdchapter.pdf

For a geometric interpretation of the singular values, consider a unit sphere in R_n and a linear map T (eg, a rotation and a stretch) that sends this sphere to an ellipsoid in R_d.

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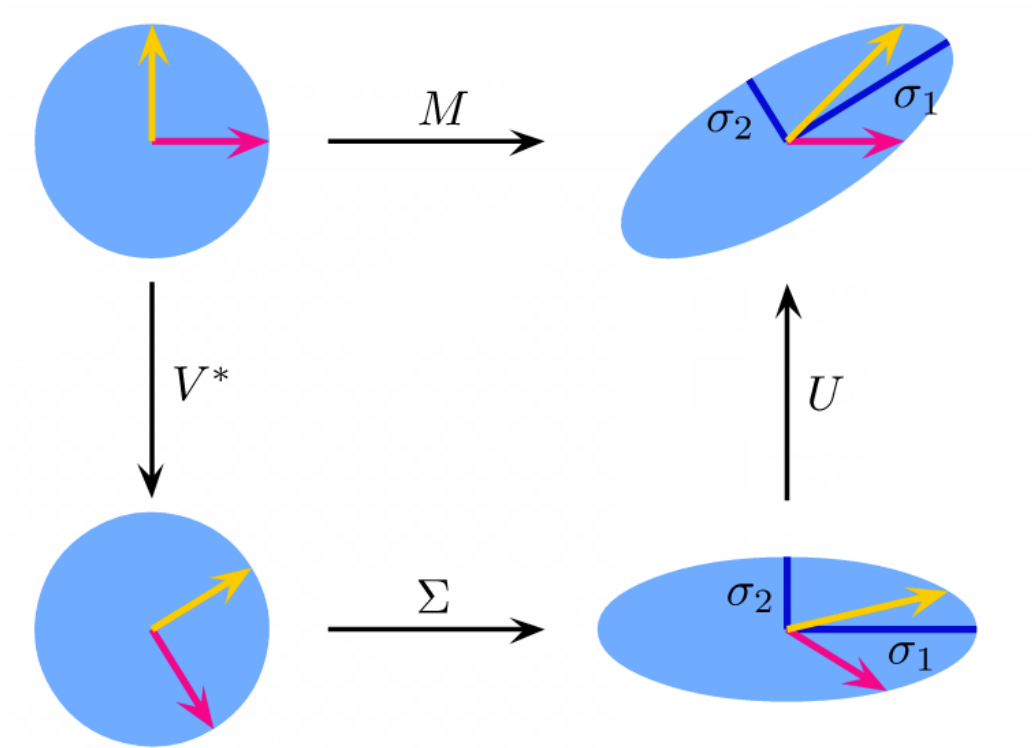
The singular vectors of T correspond to the lengths of the axes of the d-dimensional ellipsoid.

The singular values give the magnitudes of the projection of each column of the original dataset on the elements of the new basis.



$$M = U \cdot \Sigma \cdot V^*$$

source: http://en.wikipedia.org/wiki/Singular_value_decomposition

- *More numerically stable and efficient to calculate than PCA*
- *Can be used in Latent semantic analysis and recommendation systems*

III. OTHER METHODS

Whereas PCA and SVD create new coordinates by transform the old coordinates, **factor analysis** *requires new coordinates to be specified externally.*

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These new coordinates are associated with hidden or latent features that we think our data depends on.

The old coordinates are then modeled as linear combinations of the latent features.

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Though this dataset contains 10 features X_i, we may be interested in modeling these features as functions of latent variables such as the speed and strength of the participants:

$$X_i = \lambda_1 f_1 + \lambda_2 f_2 + \varepsilon$$

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$$X_i = \lambda_1 f_1 + \lambda_2 f_2 + \varepsilon$$

This would allow us to analyze the data in a more fundamental way.

SVD, PCA, and factor analysis are all linear techniques (eg, we use a linear transformation to embed the data in a lower-dimensional space).

But as we saw with SVM's, sometimes linear techniques are not sufficient.

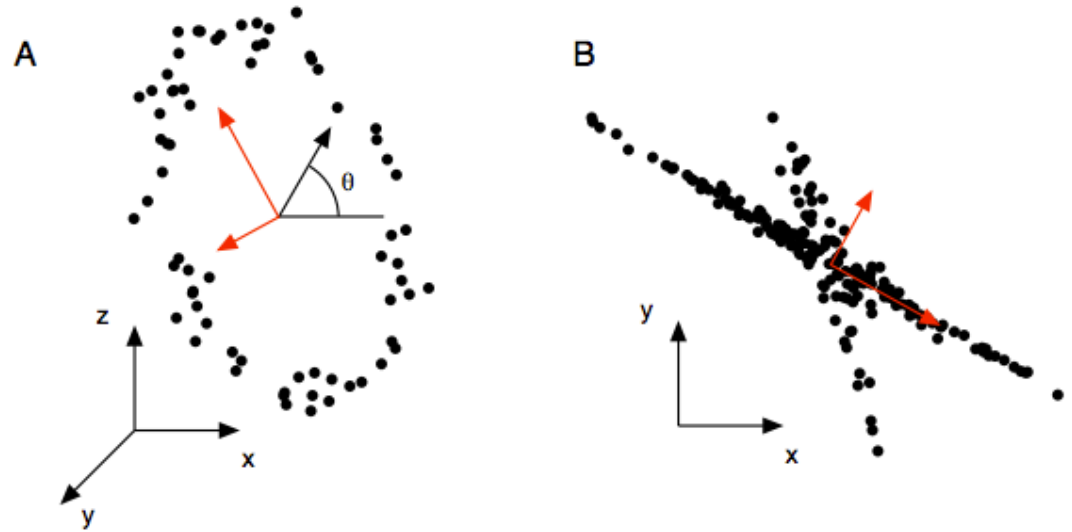
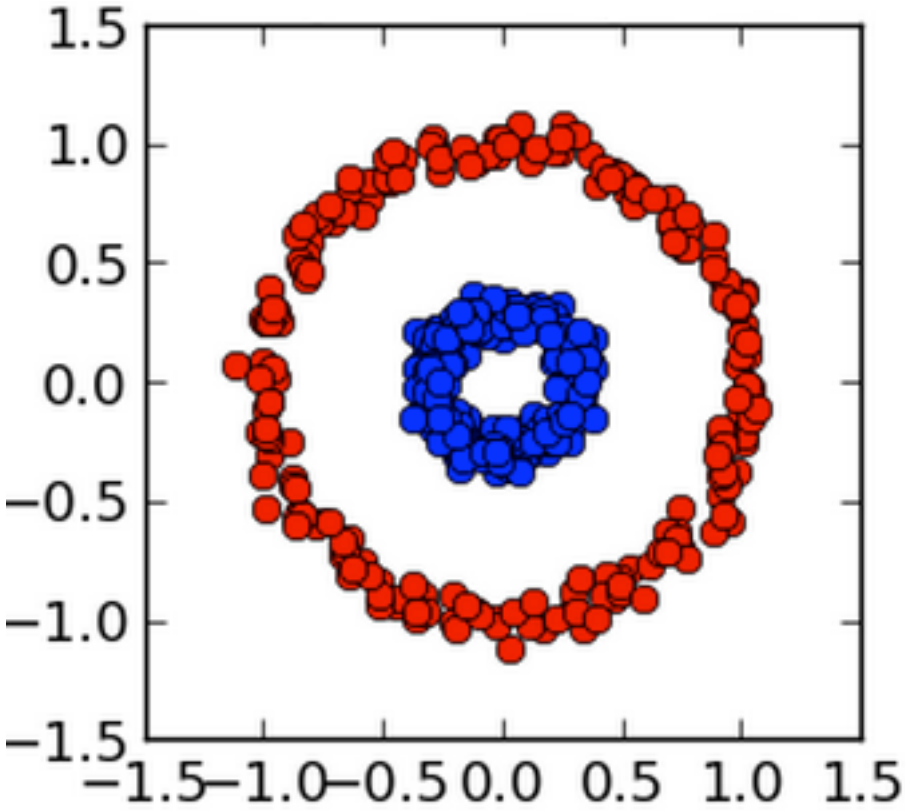


FIG. 6 Example of when PCA fails (red lines). (a) Tracking a person on a ferris wheel (black dots). All dynamics can be described by the phase of the wheel θ, a non-linear combination of the naive basis. (b) In this example data set, non-Gaussian distributed data and non-orthogonal axes causes PCA to fail. The axes with the largest variance do not correspond to the appropriate answer.


1.5
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1.0
1.5

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locally linear embedding*: approximates local structure of data*

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multidimensional scaling: *low-dim embedding that pres*
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locally linear embedding: *approximates local structure of data*

NOTE
See sklearn.manifold

Some methods for nonlinear dimensional reduction (or manifold learning) include:

kernel PCA*: exploits PCA dependence on inner product (same logic as SVM)*

isomap*: nonlinear dim reduction via MDS using geodesic (surface-bound) distances*

In any case, the key difficulties with dimensionality reduction are time/space complexity, randomness (eg different results for different runs), and selecting the number of dimensions in the lower-dim subspace.

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Furthermore, there's an obvious (bias/variance) tradeoff between the number of subspace dimensions and the size of approximation error.

THAT'S IT!

- Exit Tickets: DAT1 - Lesson 14 - Dimensionality Reduction
- More DR resources:
- PCA https://www.cs.princeton.edu/picasso/mats/PCA-Tutorial-Intuition_jp.pdf
- PCA http://ufldl.stanford.edu/wiki/index.php/PCA
- SVD vs PCA http://math.stackexchange.com/questions/3869/what-is-the-intuitive-relationship-between-svd-and-pca
- How are projects coming?