GENERAL ASSEMBLY

INTRO TO DATA SCIENCE

LECTURE 12: DIMENSIONALITY REDUCTION

LAST TIME:

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

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

EXERCISE:
IV. DIMENSIONALITY REDUCTION IN SCIKIT-LEARN

I. DIMENSIONALITY REDUCTION

Q: What is dimensionality reduction?

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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.

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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).

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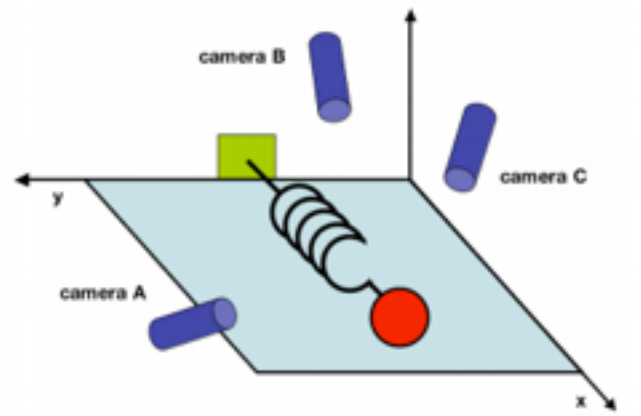
If these relationships are linear, then we can use well-established techniques like PCA/SVD.



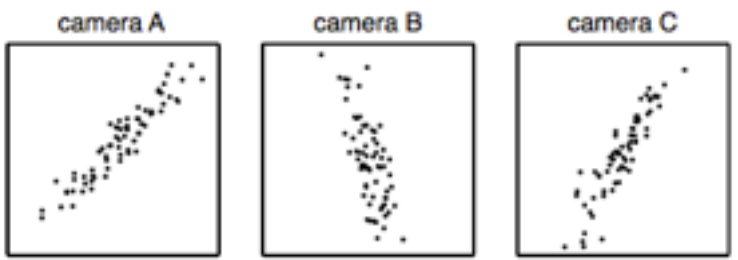


FIG. 1 A toy example. The position of a ball attached to an oscillating spring is recorded using three cameras A, B and C. The position of the ball tracked by each camera is depicted in each panel below.

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

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

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(More precisely, the sample size grows exponentially with $\mathrm{l} \leq \mathrm{d}$*, the dimension of the manifold embedded in the feature space).*

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

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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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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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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.

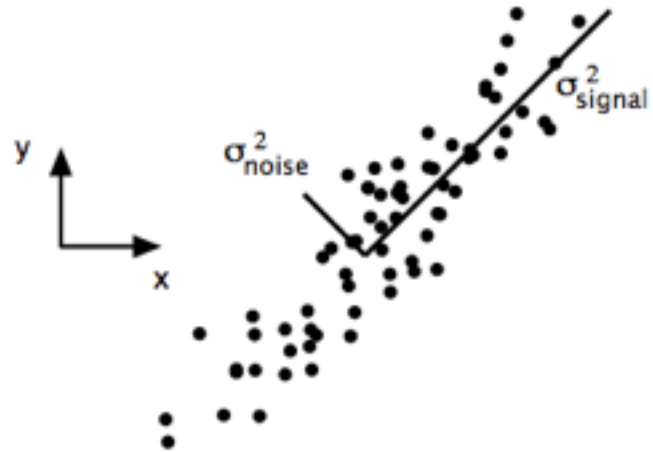

FIG. 2 Simulated data of (x,y) for camera A. The signal and noise variances σ^2_{signal} and σ^2_{noise} are graphically represented by the two lines subtending the cloud of data. Note that the largest direction of variance does not lie along the basis of the recording (x_A, y_A) but rather along the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

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

diagonal elements $\mathrm{C_{ii}}$ *give the variance of* $\mathrm{X_i}$

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

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

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

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

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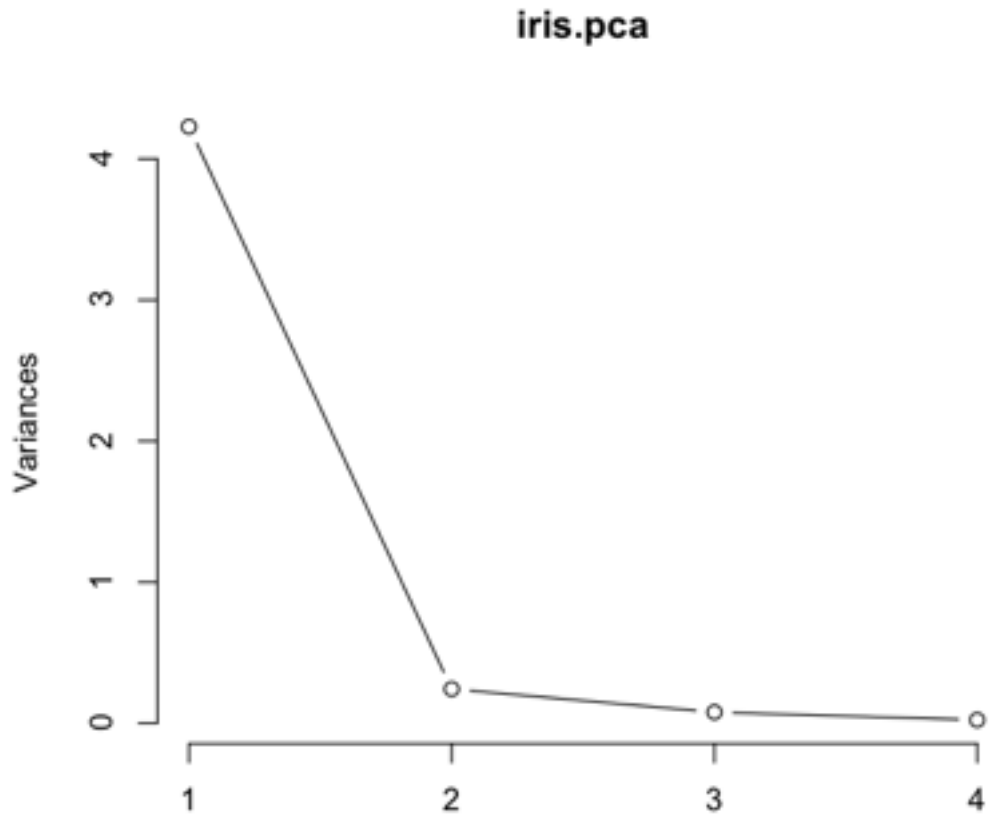
This can be visualized in a **scree plot**, *which shows the amount of variance explained by each basis vector.*


iris.pca
Variances
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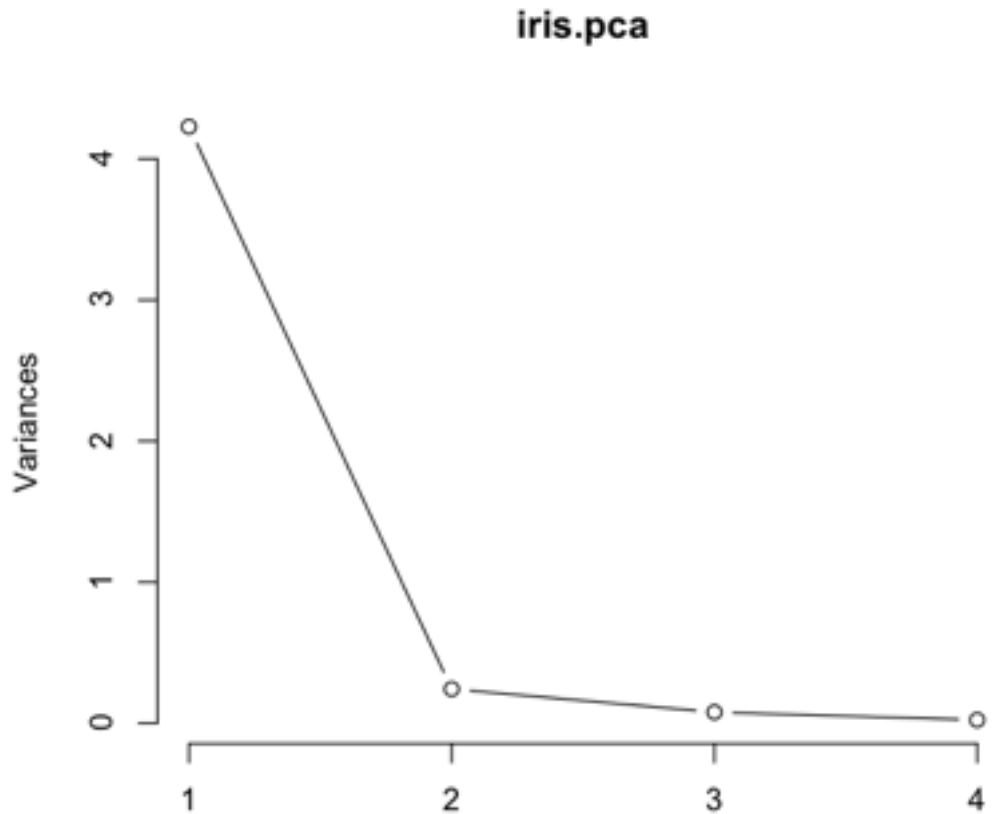

NOTE

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.

III. SINGULAR VALUE DECOMPOSITION

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

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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.

The nonzero entries of Σ *are the* **singular values** *of* A*. These are real, nonnegative, and rank-ordered (decreasing from left to right).*

For a general SVD, the columns of $\mathbf{U}$ *are the eigenvectors of* $\mathbf{A}\mathbf{A}^{\mathrm{T}}$*, and the columns of* $\mathbf{V}$ *are the eigenvectors of* $\mathbf{A}^{\mathrm{T}}\mathbf{A}$*.*

Also, the singular values of $\mathbf{A}$ *are the square roots of the eigenvalues of* $\mathbf{A}\mathbf{A}^{\mathrm{T}}$ *and* $\mathbf{A}^{\mathrm{T}}\mathbf{A}$*.*

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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* $\mathrm{k} < \mathrm{d}$ *dimensional subspace to represent the data.*

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NOTE

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* $\mathrm{k} < \mathrm{d}$ *dimensional subspace to represent the data.*

For $\mathrm{k} = 1$*, this subspace is a line passing through the origin.*

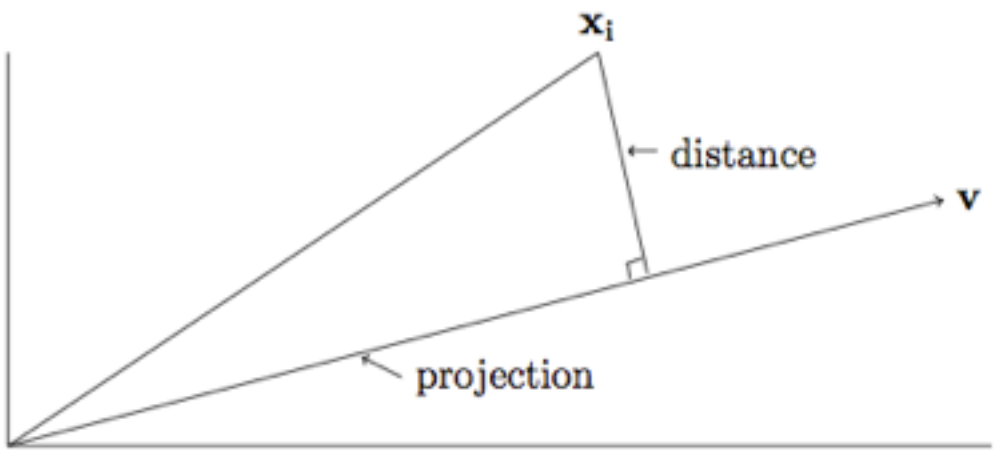

Figure 4.1: The projection of the point $\mathbf{x_i}$ onto the line through the origin in the direction of $\mathbf{v}$

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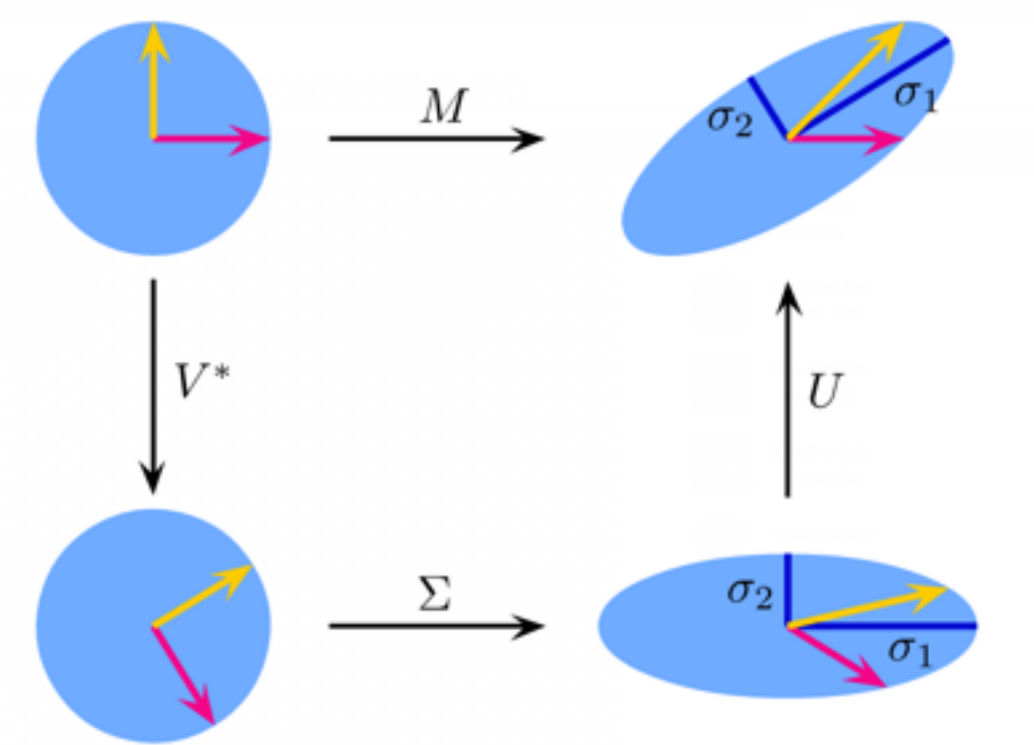
The singular values give the magnitudes of the projection of each column of the original dataset on the elements of the new basis.



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

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

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.

For example, consider a dataset that represents the results of a decathalon (rows = participants, columns = events, entries = times).

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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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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 in a lower-dimensional space).

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

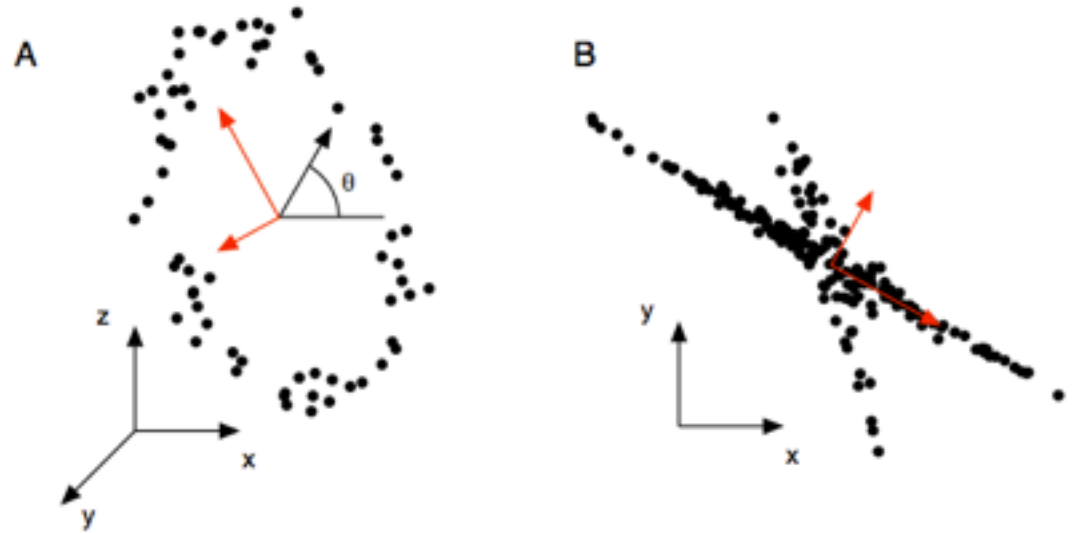
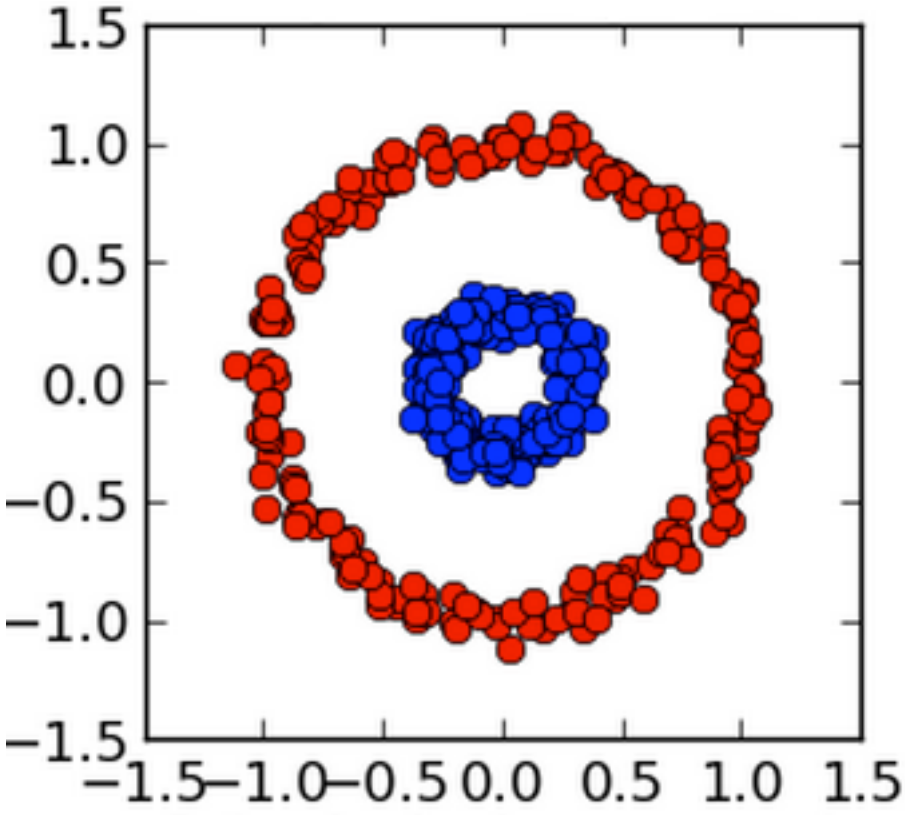


FIG. 6 Example of when PCA fails (red lines). (a) Tracking a person on a ferris wheel (black dots). All dynamics can be described by the phase of the wheel θ, a non-linear combination of the naive basis. (b) In this example data set, non-Gaussian distributed data and non-orthogonal axes causes PCA to fail. The axes with the largest variance do not correspond to the appropriate answer.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1.0
1.5

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

multidimensional scaling: *low-dim embedding that preserves pairwise distances*

locally linear embedding: *approximates local structure of data (nbd preserving embedding)*

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.