GENERAL ASSEMBLY

INTRO TO DATA SCIENCE

DIMENSIONALITY REDUCTION

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

EXERCISE:
IV. DIMENSIONALITY REDUCTION IN SCIKIT-LEARN

I. DIMENSIONALITY REDUCTION

	continuous	categorical
Supervised		
Unsupervised		

	continuous	categorical
Supervised	**regression**	**classification**
Unsupervised	**dimension reduction**	**clustering**

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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

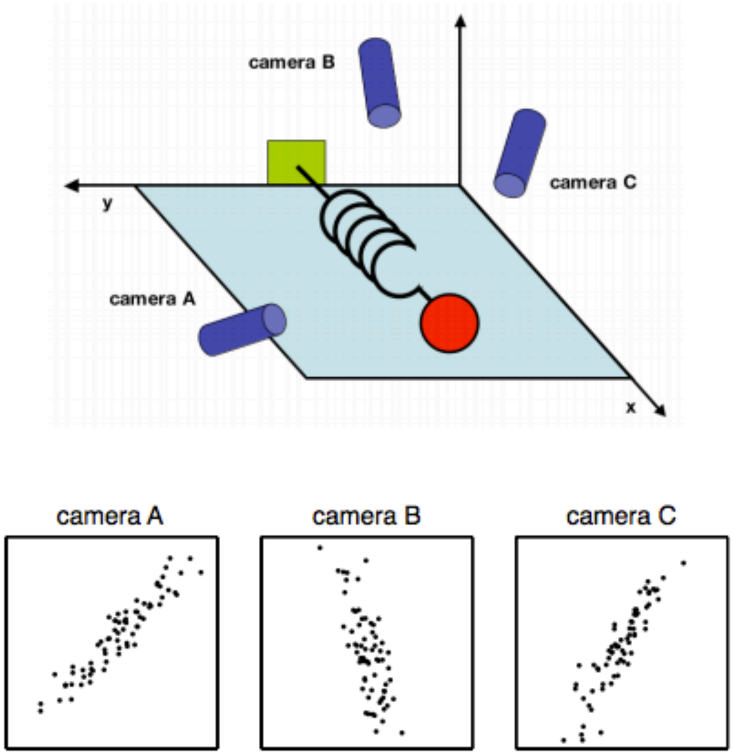

FIG. 1 A toy example. The position of a ball attached to an oscillating spring is recorded using three cameras A, B and C. The position of the ball tracked by each camera is depicted in each panel below.

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

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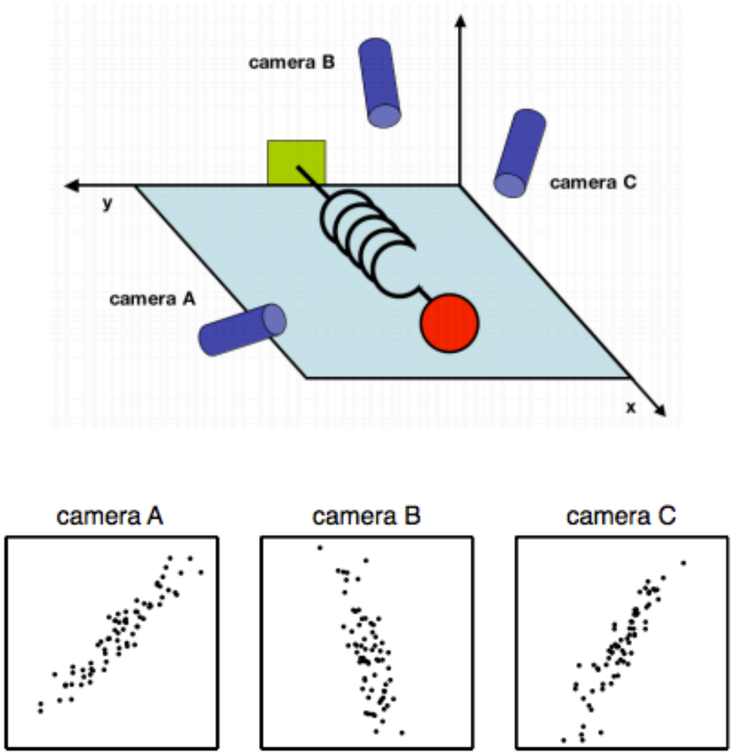

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NOTE

In this case the "truth" is (nearly) one-dimensional. We don't generally know what the "truth" is, but the same techniques can apply.

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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).

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

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

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

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feature selection – **selecting a subset of features using an external criterion (*filter*) or the learning algo accuracy itself (*wrapper*)**

feature extraction – **mapping the features to a lower dimensional space**

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.

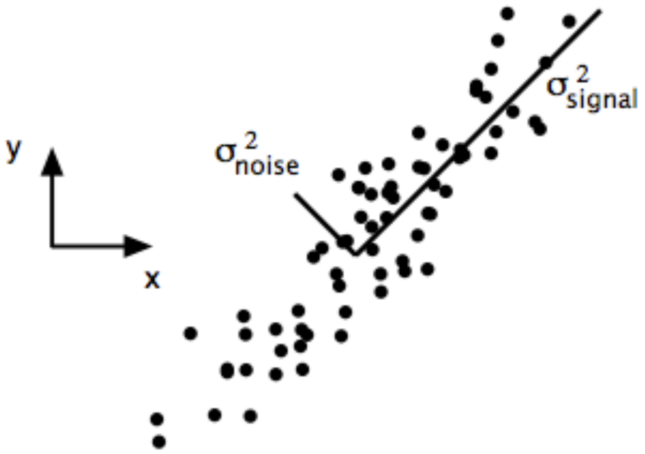

FIG. 2 Simulated data of (x, y) for camera A. The signal and noise variances σ^2_{signal} and σ^2_{noise} are graphically represented by the two lines subtending the cloud of data. Note that the largest direction of variance does not lie along the basis of the recording (x_A, y_A) but rather along the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

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

Q: What are some applications of dimensionality reduction?

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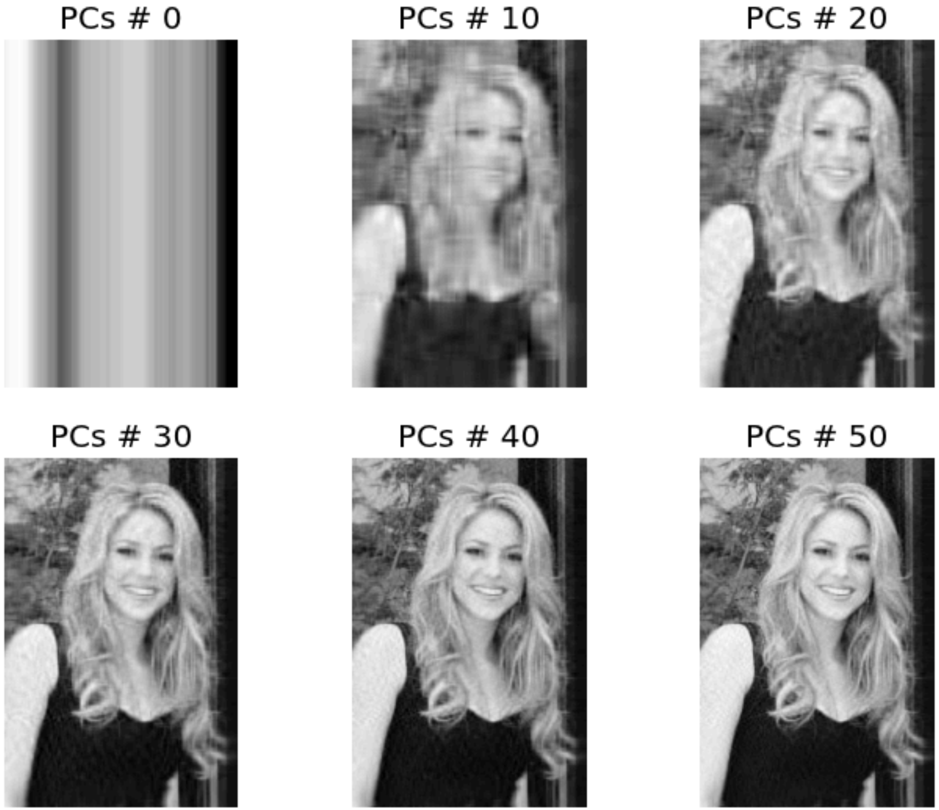
- topic models (document clustering)
- image recognition/computer vision
- bioinformatics (microarray analysis)
- speech recognition
- astronomy (spectral data analysis)
- recommender systems



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 X boils down to the eigenvalue decomposition of the covariance matrix of X.

The covariance matrix C of a matrix X 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

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$$C = Q\Lambda Q^{-1}$$

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NOTE

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

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

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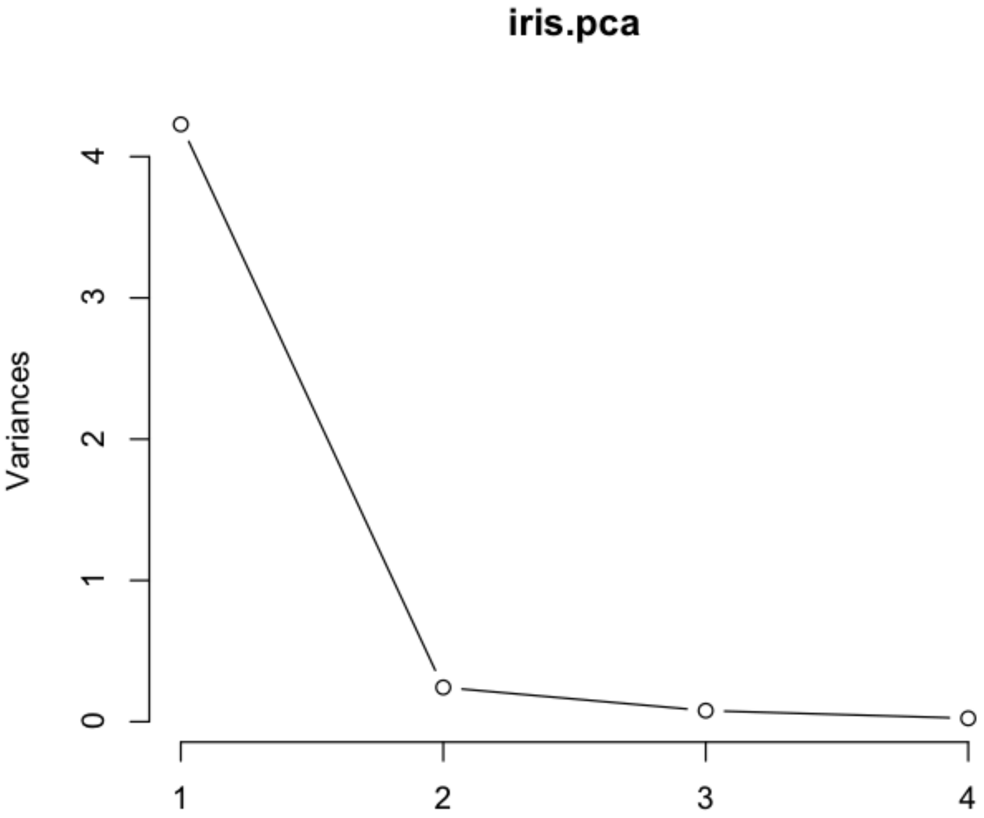
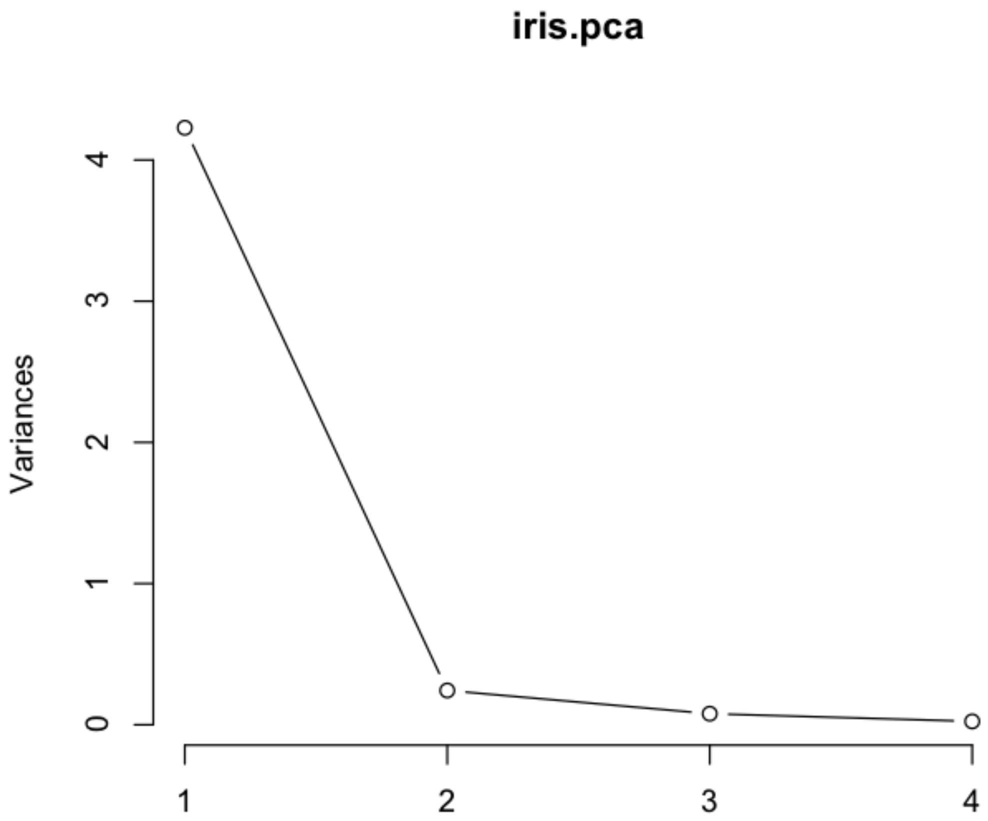
This can be visualized in a scree plot, which shows the amount of variance explained by each basis vector.


iris.pca
Variances
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.

III. SINGULAR VALUE DECOMPOSITION

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(n x d) (n x n) (n x d) (d x d)

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

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 X.

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

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For a general SVD, the columns of U are the eigenvectors of XX^T, and the columns of V are the eigenvectors of X^TX.

Also, the singular values of X are the square roots of the eigenvalues of XX^T and X^TX.

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NOTE

If data is centered, these are covariance matrices.

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

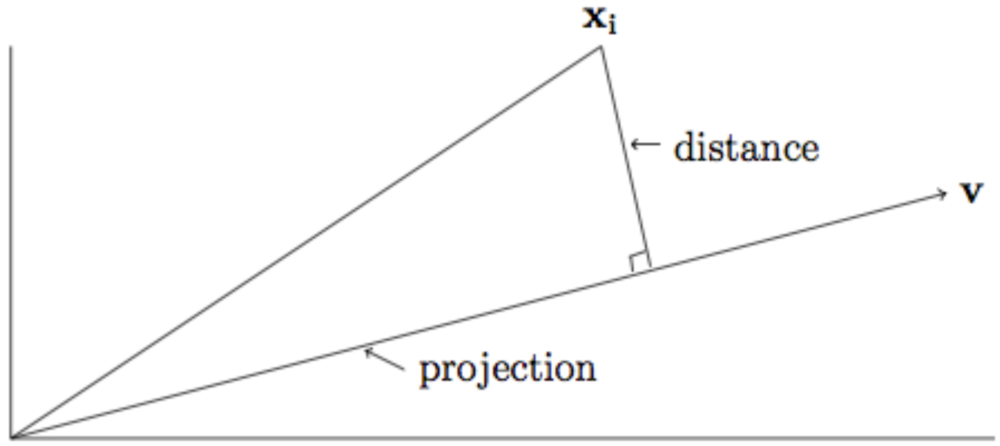

Figure 4.1: The projection of the point $\mathbf{x_i}$ onto the line through the origin in the direction of $\mathbf{v}$

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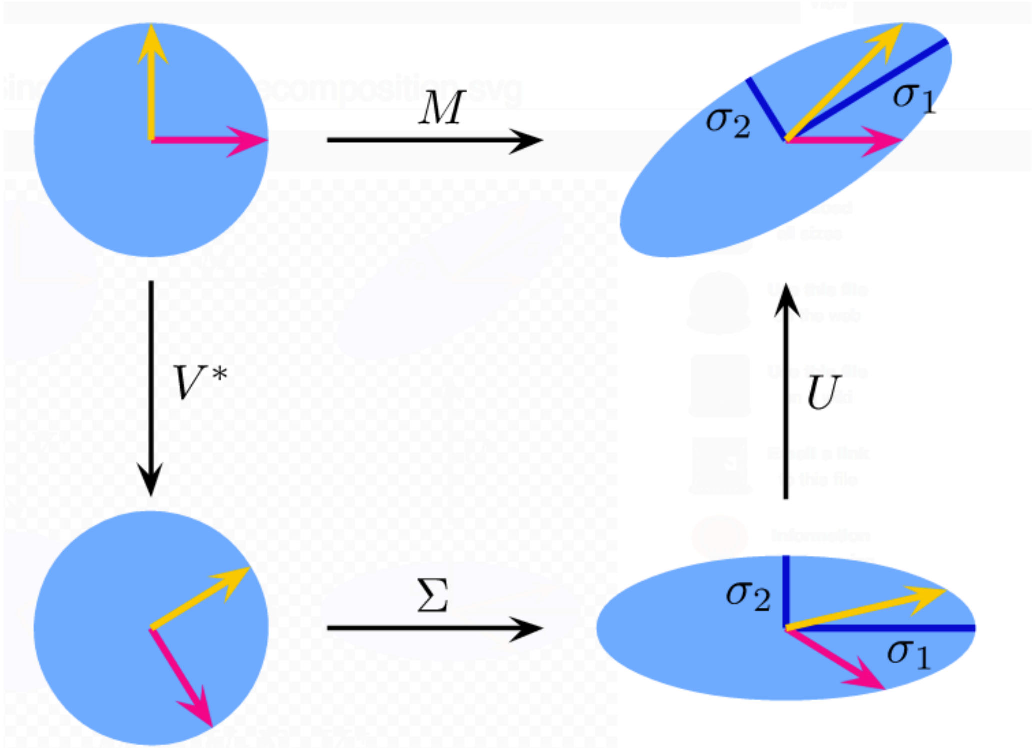
The singular vectors of T correspond to the lengths of the axes of the d-dimensional ellipsoid.

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

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- Latent semantic analysis, etc.

III. OTHER METHODS

Whereas PCA and SVD create new coordinates by transforming the old coordinates without any accompanying theory of what anything means, factor analysis **refers to a broader array of techniques.**

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In factor analysis, which may be exploratory or confirmatory, we hypothesize that our data depends on some *hidden* or *latent* features.

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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 is a new model with an error term!

In practice, PCA is often used for factor analysis, after modifying the covariance matrix somewhat. But it can also allow for non-isotropic errors, and there are other methods for fitting as well, and different theoretical concerns.

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 sometimes linear techniques are not sufficient.

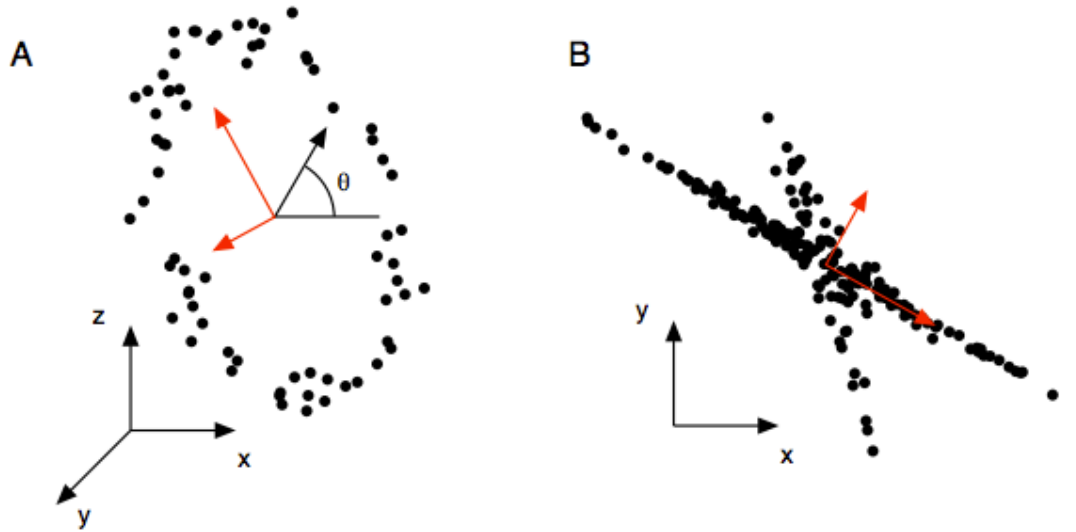
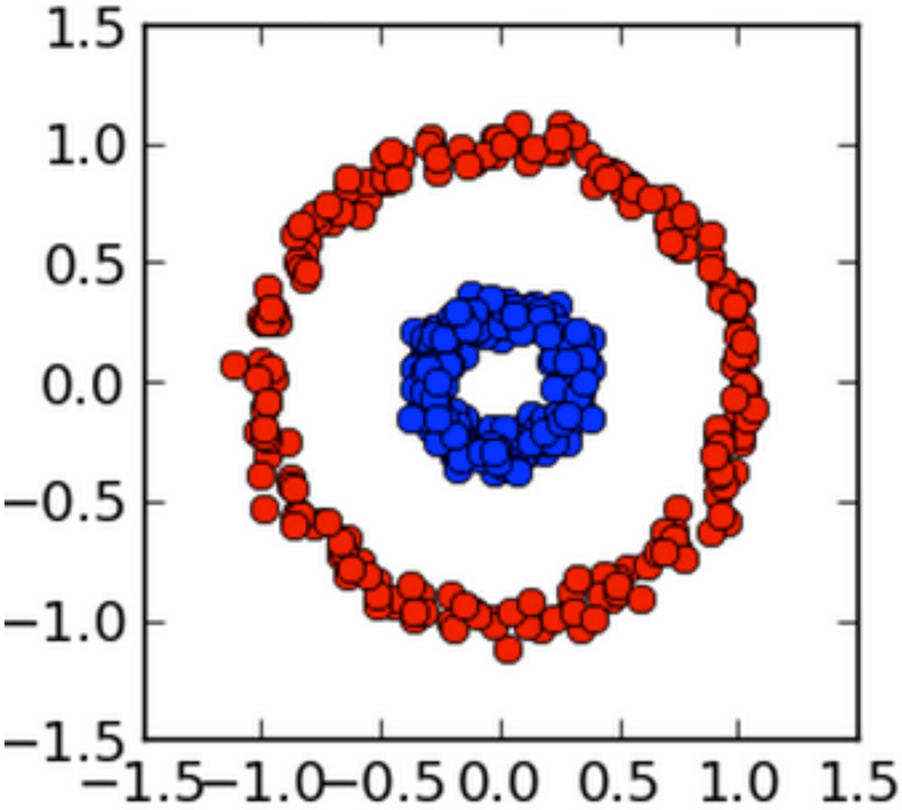


FIG. 6 Example of when PCA fails (red lines). (a) Tracking a person on a ferris wheel (black dots). All dynamics can be described by the phase of the wheel θ, a non-linear combination of the naive basis. (b) In this example data set, non-Gaussian distributed data and non-orthogonal axes causes PCA to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


1.5
1.0
0.5
0.0
−0.5
−1.0
−1.5
−1.5 −1.0 −0.5 0.0 0.5 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 (neighborhood preserving embedding)**

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See sklearn.manifold

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

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

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

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

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

isomap: **nonlinear dimension reduction via N geodesic (surface-bound) distances**

NOTE

See sklearn.decomposition and sklearn.manifold

NOTE

And more!

In any case, 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 involved with the number of subspace dimensions and the size of approximation error.

IV. EXERCISE