

# INTRO to DATA SCIENCE

## DIMENSIONALITY REDUCTION

**I. DIMENSIONALITY REDUCTION**

**II. PRINCIPAL COMPONENTS ANALYSIS**

**III. SINGULAR VALUE DECOMPOSITION**

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**EXERCISE:**

**IV. DIMENSIONALITY REDUCTION IN SCIKIT-LEARN**

# **I. 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.

## EXAMPLE: 1D HARMONIC OSCILLATOR

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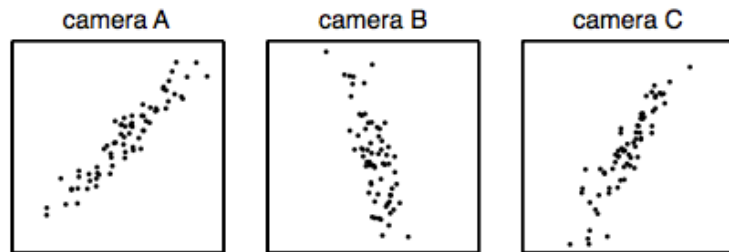
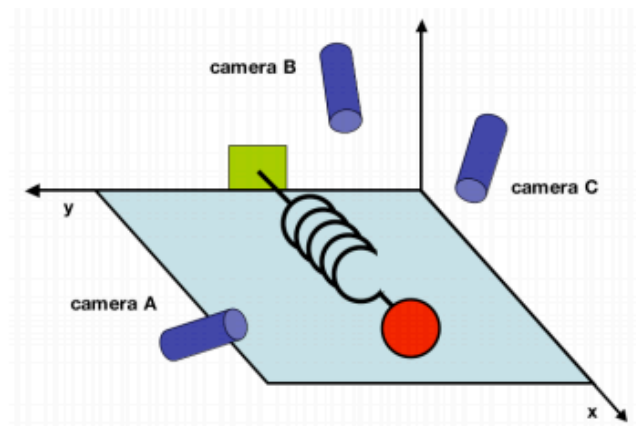
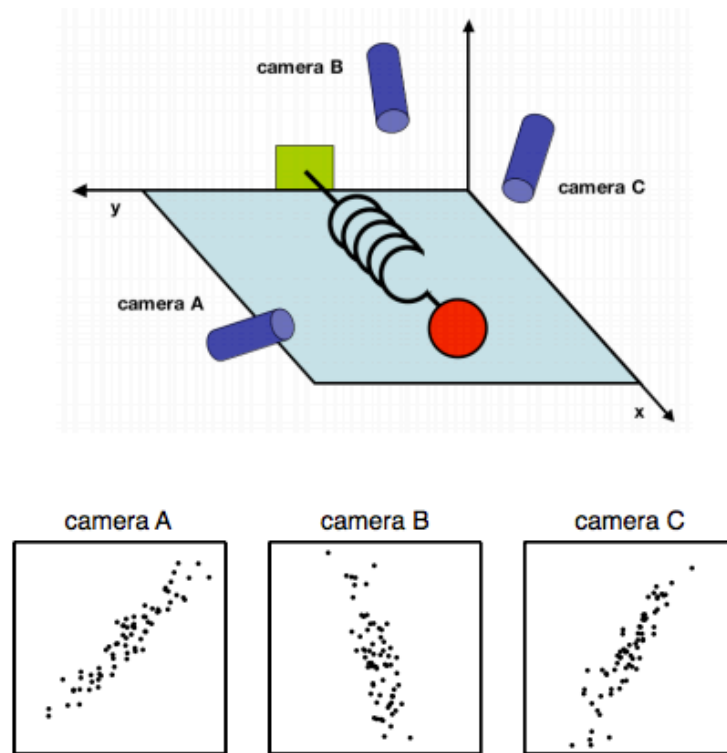


FIG. 1 A toy example. The position of a ball attached to an oscillating spring is recorded using three cameras A, B and C. The position of the ball tracked by each camera is depicted in each panel below.

## EXAMPLE: 1D HARMONIC OSCILLATOR

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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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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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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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More precisely: given an  $n \times d$  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.



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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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.

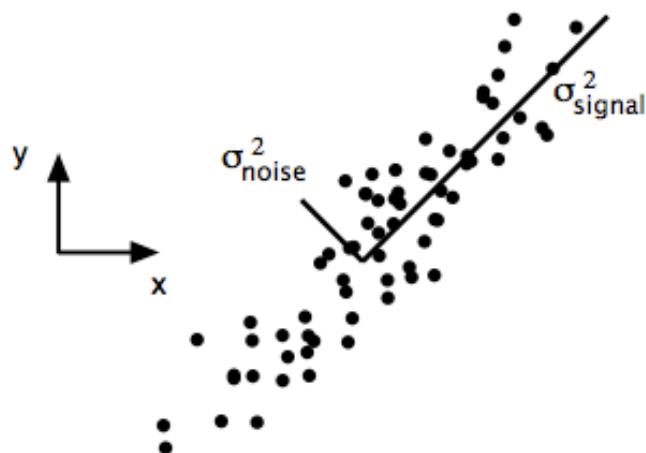


FIG. 2 Simulated data of  $(x, y)$  for camera A. The signal and noise variances  $\sigma_{signal}^2$  and  $\sigma_{noise}^2$  are graphically represented by the two lines subtending the cloud of data. Note that the largest direction of variance does not lie along the basis of the recording  $(x_A,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

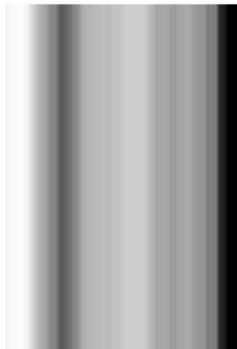
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- topic models (document clustering)
- image recognition/computer vision
- bioinformatics (microarray analysis)
- speech recognition
- astronomy (spectral data analysis)
- recommender systems

PCs # 0



PCs # 10



PCs # 20



PCs # 30



PCs # 40



PCs # 50



# **II. PRINCIPAL COMPONENT ANALYSIS**

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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:

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

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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**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).

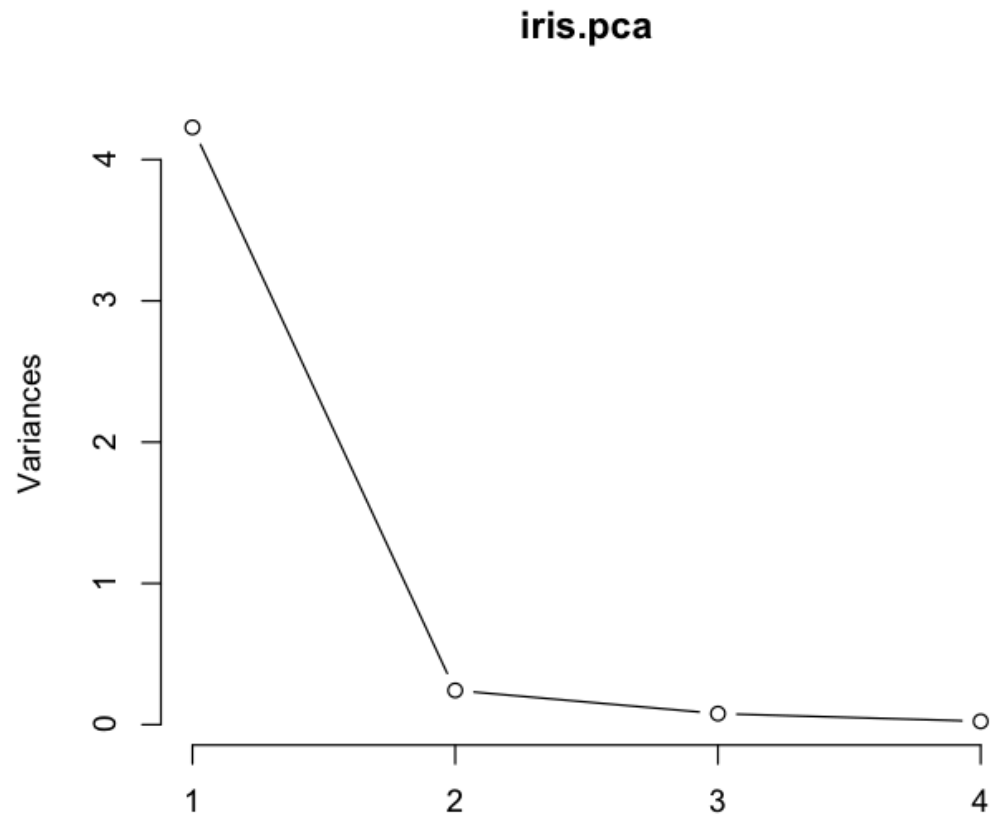
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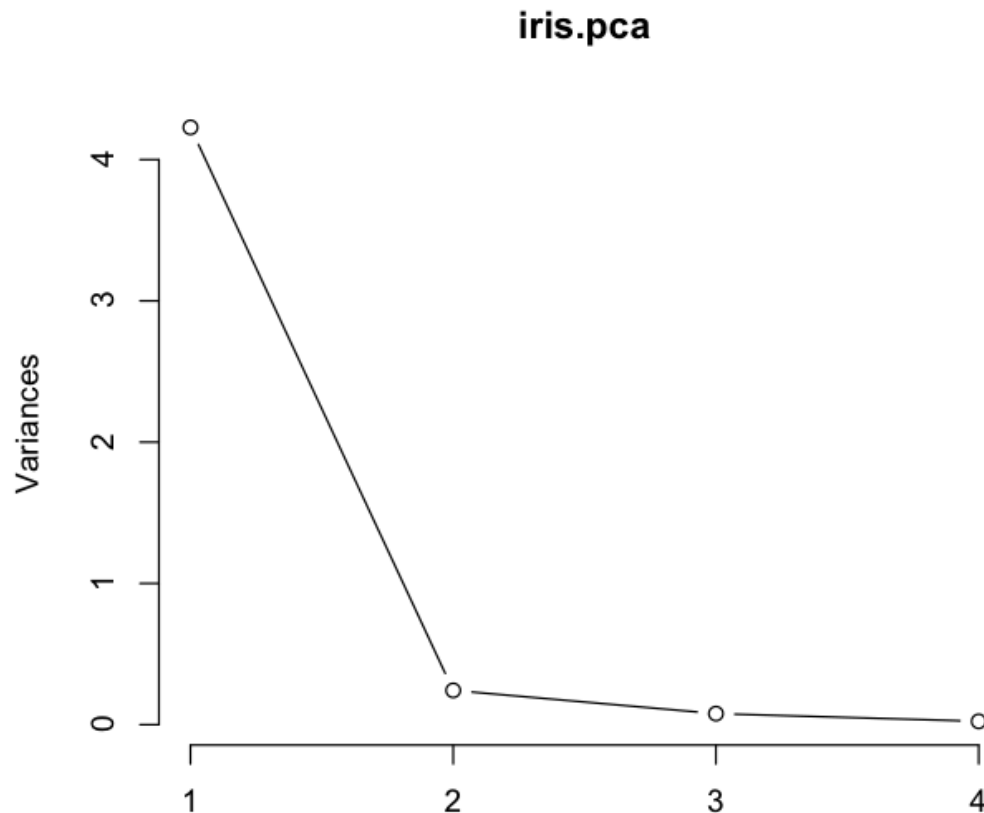
Furthermore the basis elements are ordered by their eigenvalues (from largest to smallest), and these eigenvalues represent the amount of variance explained by each basis element.

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





## 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**

Consider a matrix  $X$  with  $n$  rows and  $d$  features.

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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  $X$ .

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  $X^TX$ .

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**NOTE**

If data is centered,  
these are covariance  
matrices.

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### NOTE

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

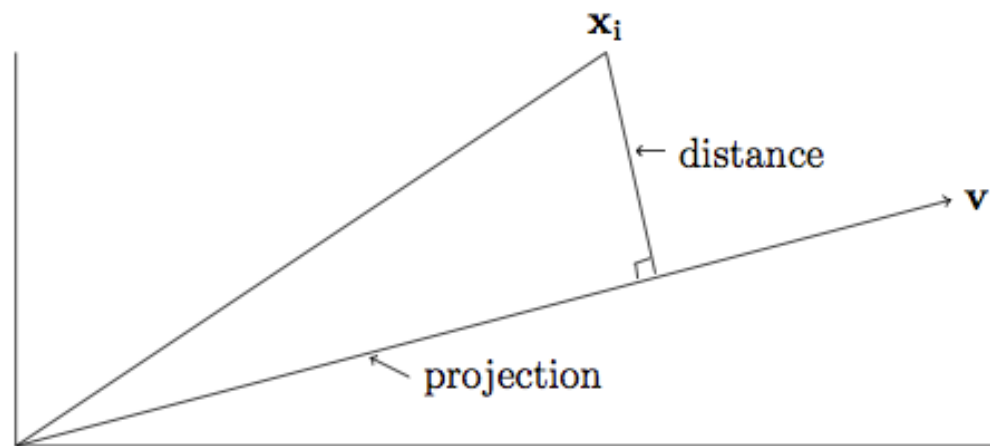


Figure 4.1: The projection of the point  $\mathbf{x}_i$  onto the line through the origin in the direction of  $\mathbf{v}$

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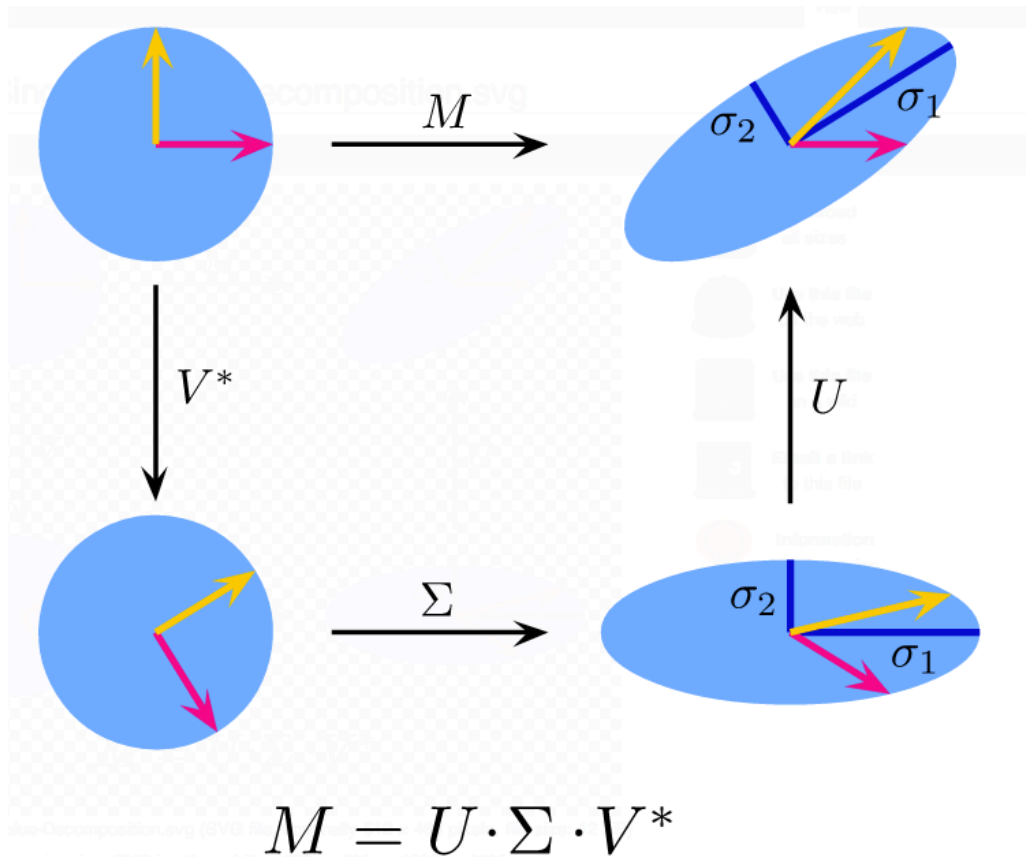
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The singular values give the magnitudes of the projection of each column of the original dataset on the elements of the new basis.



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- More numerically stable and can be more efficient to calculate (than PCA)

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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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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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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.

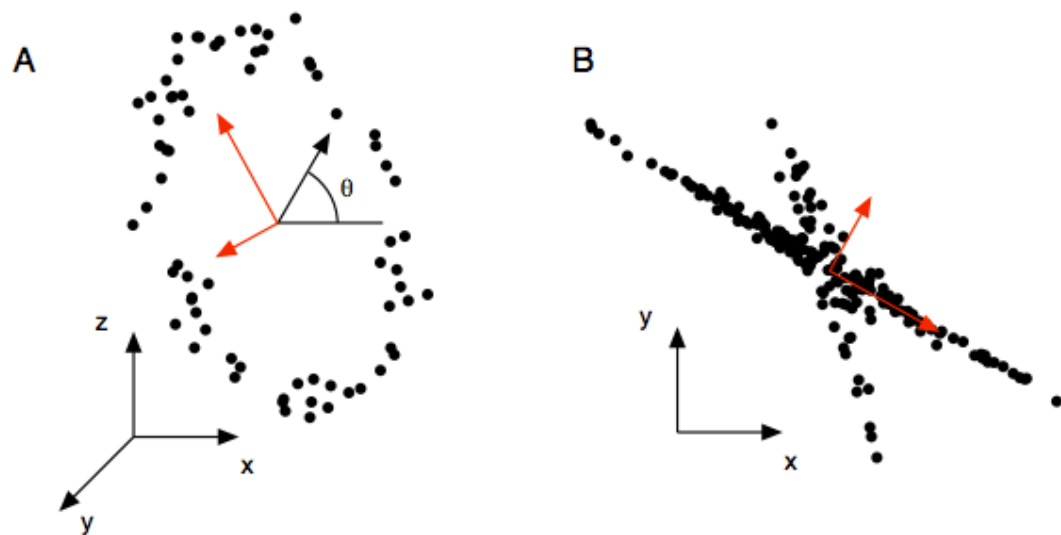
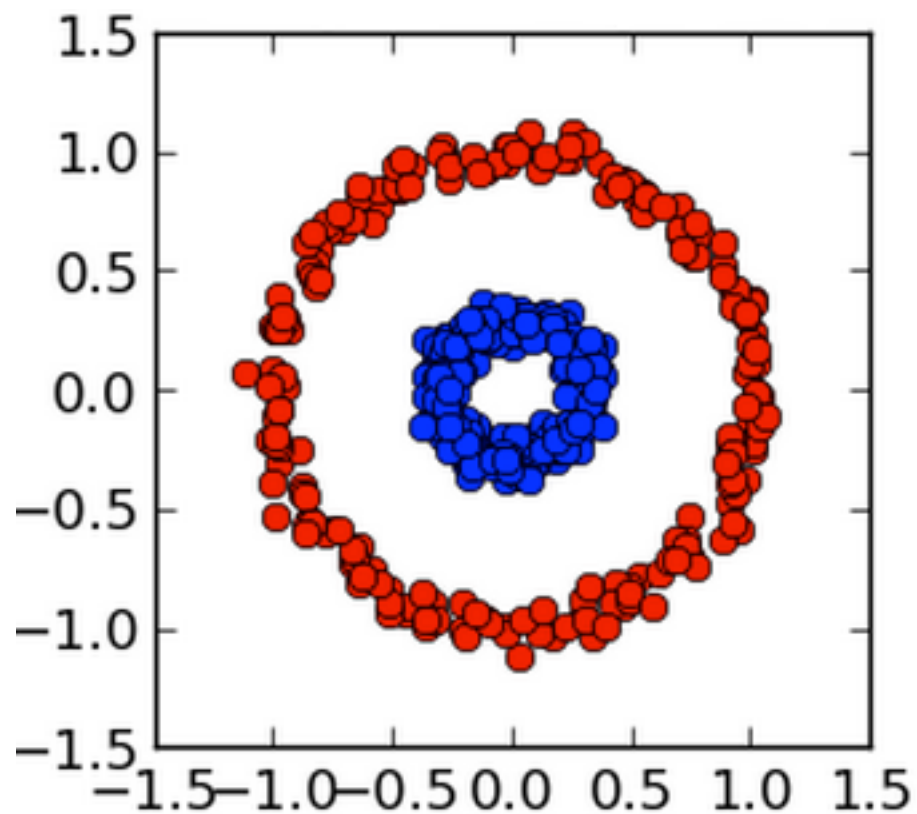


FIG. 6 Example of when PCA fails (red lines). (a) Tracking a person on a ferris wheel (black dots). All dynamics can be described by the phase of the wheel  $\theta$ , a non-linear combination of the naive basis. (b) In this example data set, non-Gaussian distributed data and non-orthogonal axes causes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





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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**NOTE**

See [sklearn.manifold](https://scikit-learn.org/stable/modules/manifold.html)

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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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**NOTE**

See  
`sklearn.decomposition`  
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kernel PCA: exploits PCA dependence product

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**NOTE**

And more!

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

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**