

# INTRO to DATA SCIENCE

## DIMENSIONALITY REDUCTION

**I. DIMENSIONALITY REDUCTION**

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**EXERCISE:**

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

# **I. DIMENSIONALITY REDUCTION**

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**In general, the idea is to regard the dataset as 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.**

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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

13

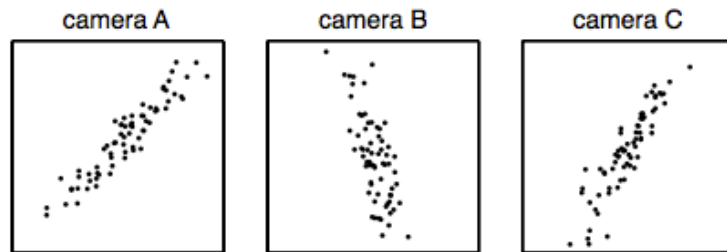
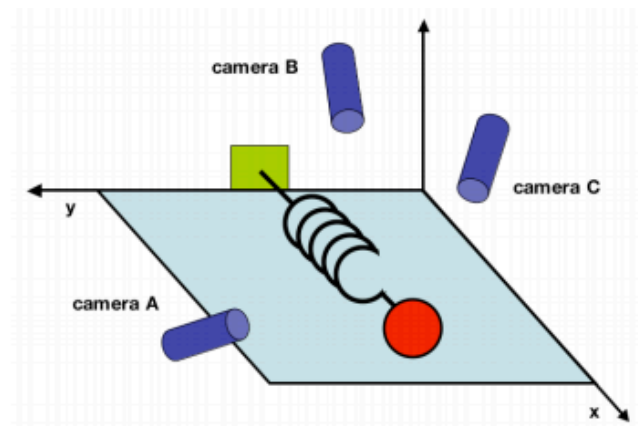
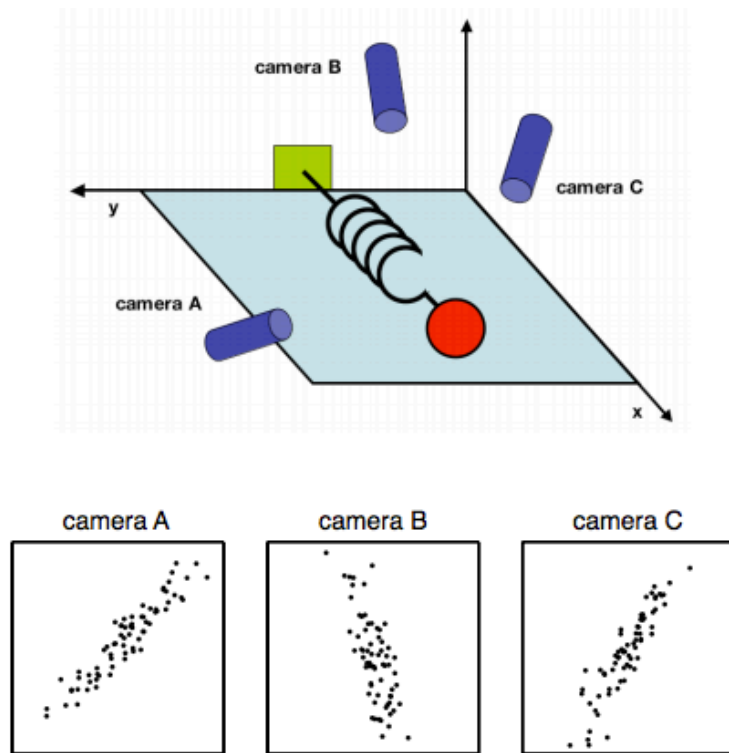


FIG. 1 A toy example. The position of a ball attached to an oscillating spring is recorded using three cameras A, B and C. The position of the ball tracked by each camera is depicted in each panel below.

## 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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(More precisely, the sample size grows exponentially with  $l \leq d$ , 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).

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

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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*)

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We've already seen examples of feature selection for regression such as *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.



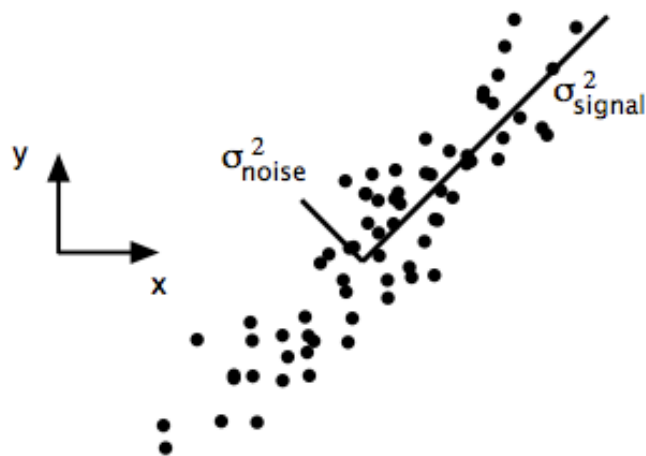


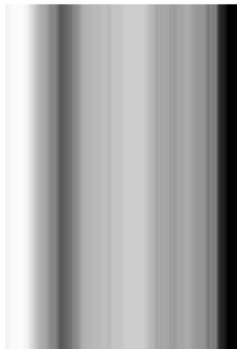
FIG. 2 Simulated data of  $(x, y)$  for camera A. The signal and noise variances  $\sigma_{signal}^2$  and  $\sigma_{noise}^2$  are graphically represented by the two lines subtending the cloud of data. Note that the largest direction of variance does not lie along the basis of the recording  $(x_A,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

**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**

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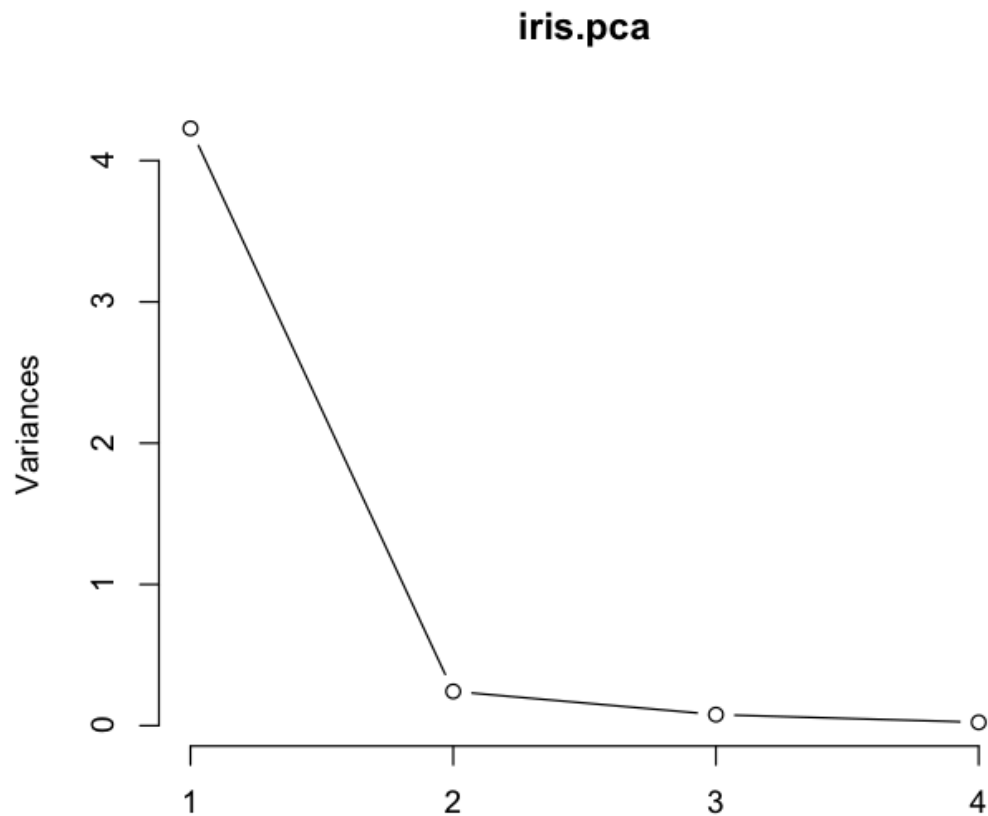
Furthermore the basis elements are ordered by their eigenvalues (from largest to smallest), and these eigenvalues represent the amount of variance explained by each basis element.

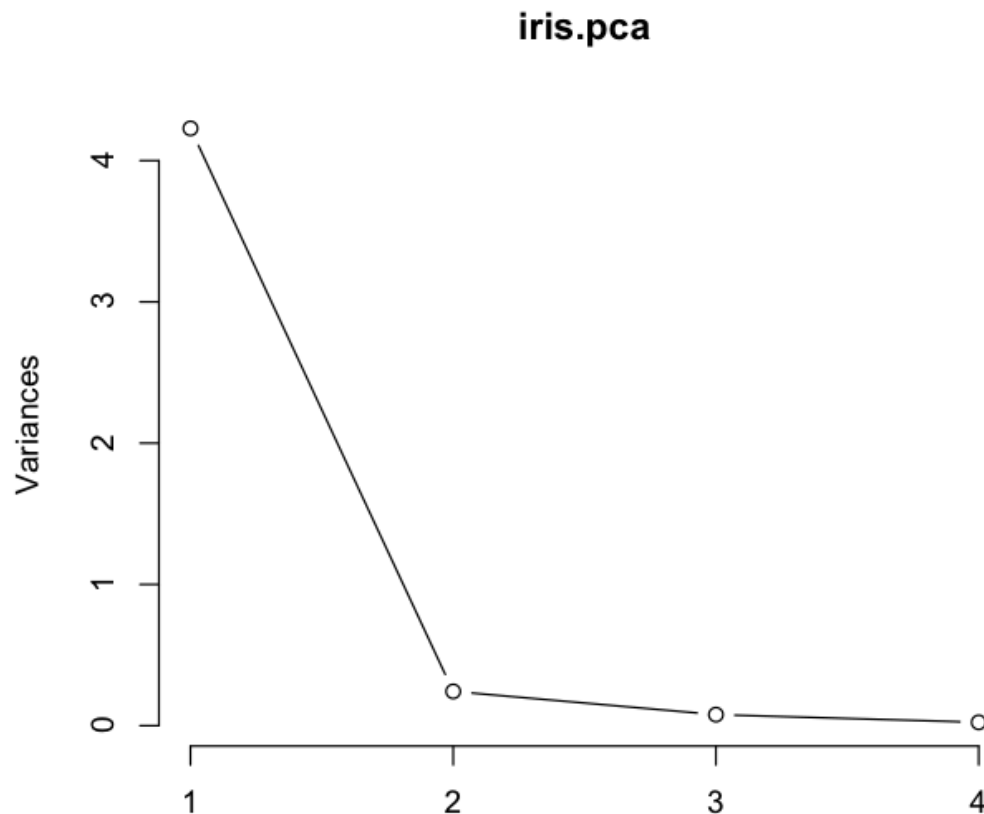
The eigenvectors form a basis of the vector space on which  $C$  acts (eg, they are orthogonal).

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







## 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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st.  $U$ ,  $V$  are **orthogonal** matrices and  $\Sigma$  is a **diagonal** matrix.

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



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

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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*.

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

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



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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  $X$ ), 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.

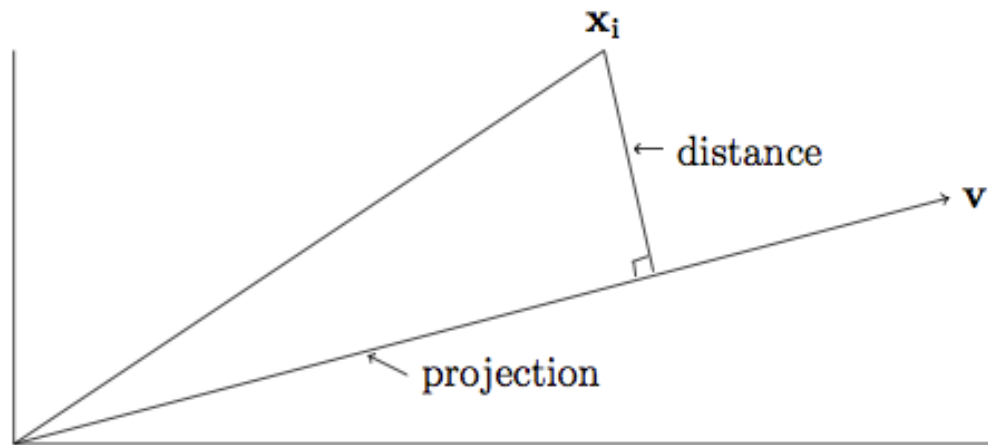


Figure 4.1: The projection of the point  $\mathbf{x}_i$  onto the line through the origin in the direction of  $\mathbf{v}$

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  $R_d$ .

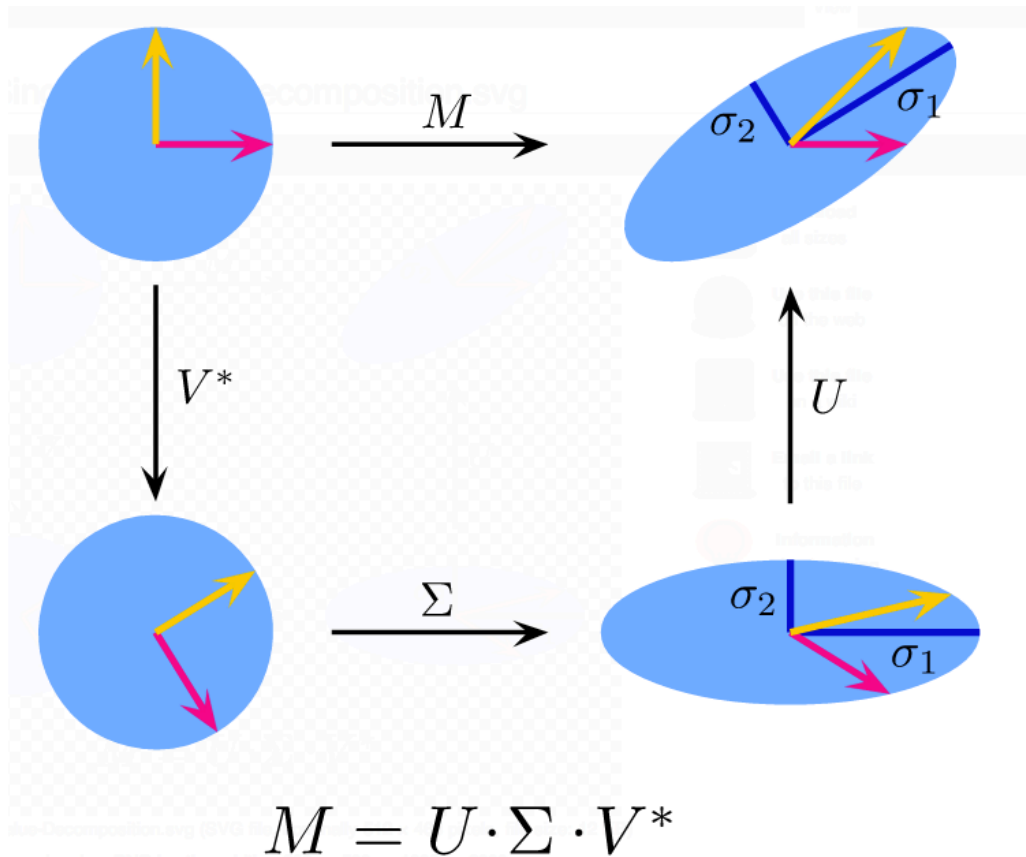
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The singular values give the magnitudes of the projection of each column of the original dataset on the elements of the new basis.



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- Latent semantic analysis, etc.

# **III. OTHER METHODS**

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

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 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.

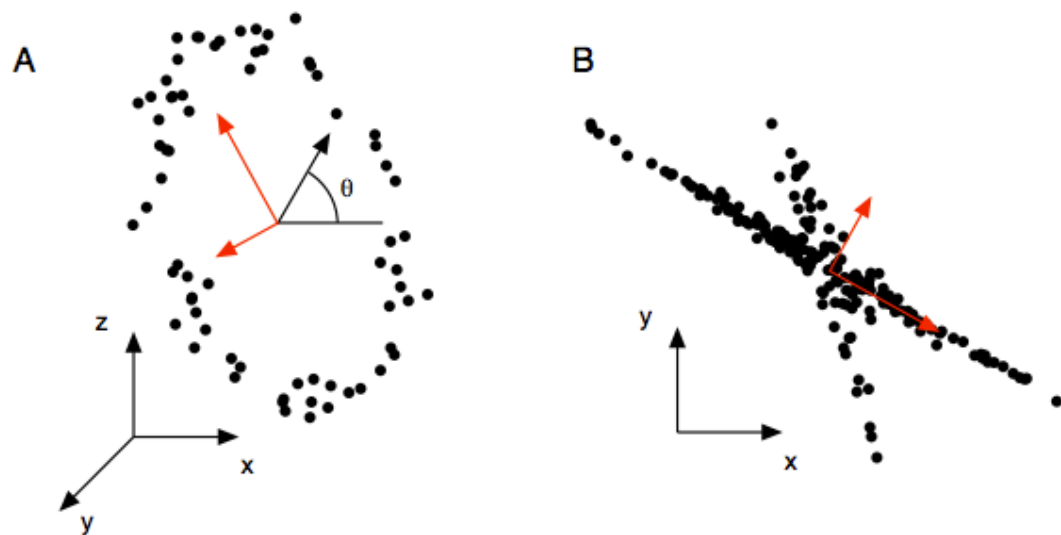
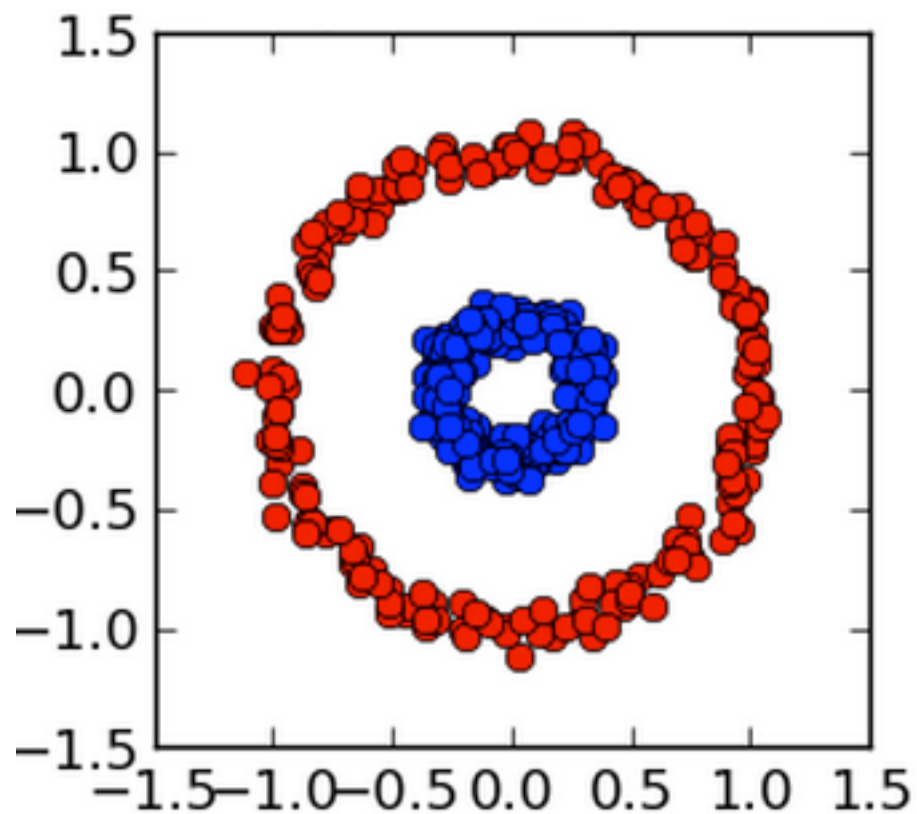


FIG. 6 Example of when PCA fails (red lines). (a) Tracking a person on a ferris wheel (black dots). All dynamics can be described by the phase of the wheel  $\theta$ , a non-linear combination of the naive basis. (b) In this example data set, non-Gaussian distributed data and non-orthogonal axes causes 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:

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NOTE

And more!

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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**