

INTRO to DATA SCIENCE

DIMENSIONALITY REDUCTION

I. DIMENSIONALITY REDUCTION

II. PRINCIPAL COMPONENTS ANALYSIS

III. SINGULAR VALUE DECOMPOSITION

IV. 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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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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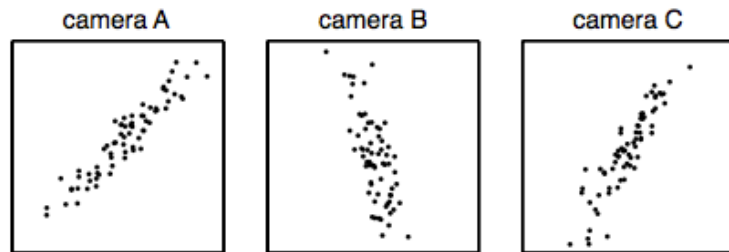
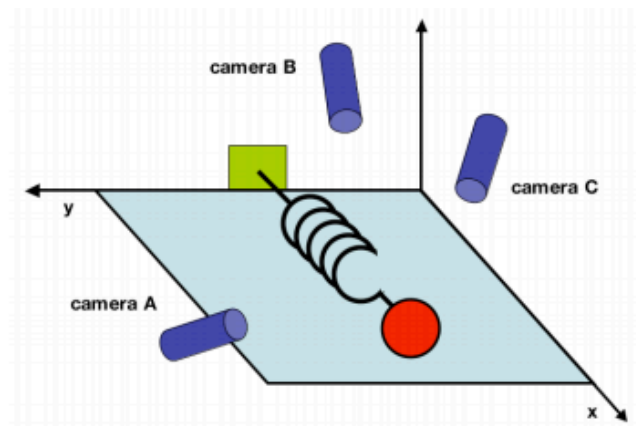
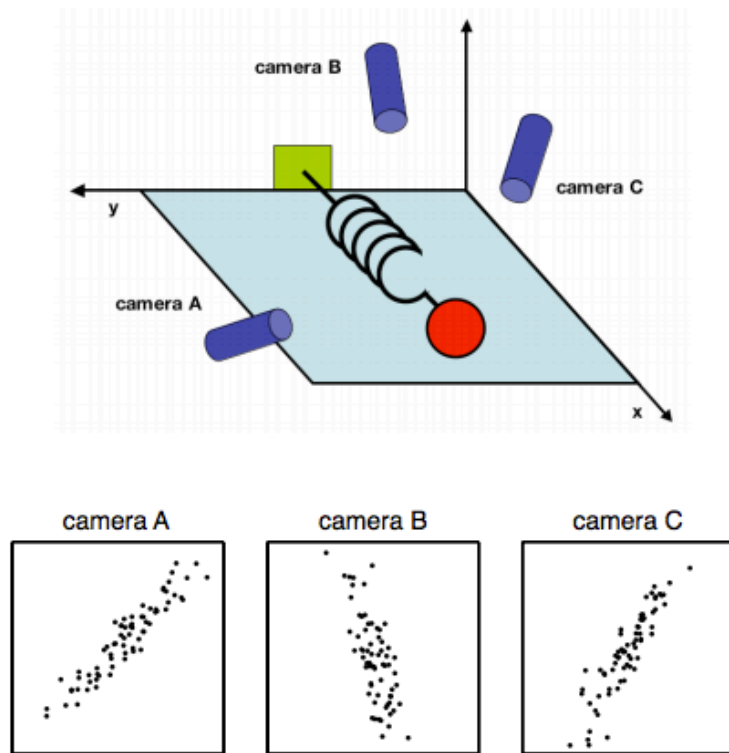


FIG. 1 A toy example. The position of a ball attached to an oscillating spring is recorded using three cameras A, B and C. The position of the ball tracked by each camera is depicted in each panel below.

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).

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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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

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

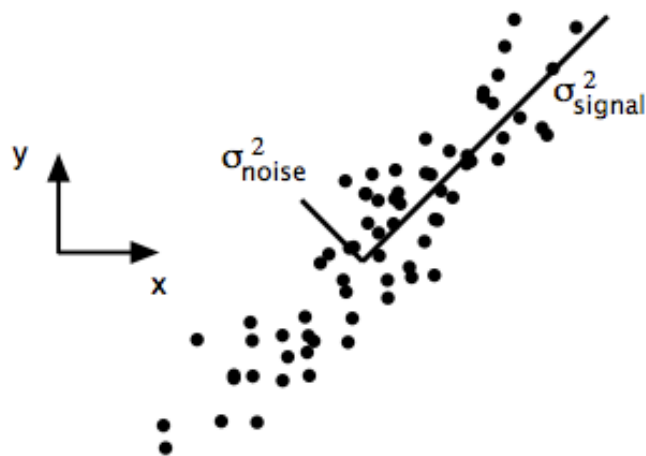


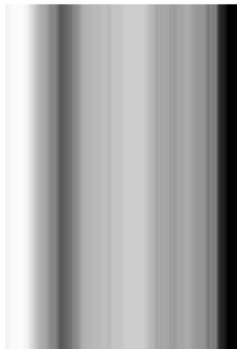
FIG. 2 Simulated data of (x, y) for camera A. The signal and noise variances σ_{signal}^2 and σ_{noise}^2 are graphically represented by the two lines subtending the cloud of data. Note that the largest direction of variance does not lie along the basis of the recording (x_A, y_A) but rather along the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

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:

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

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

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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).

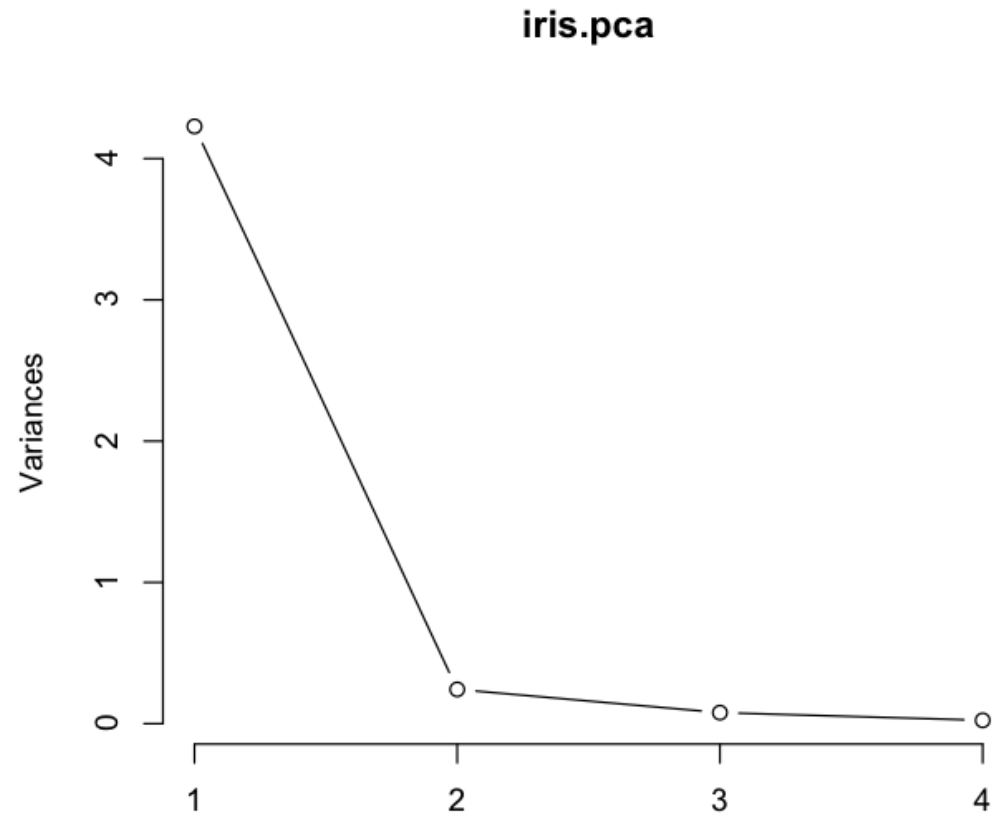
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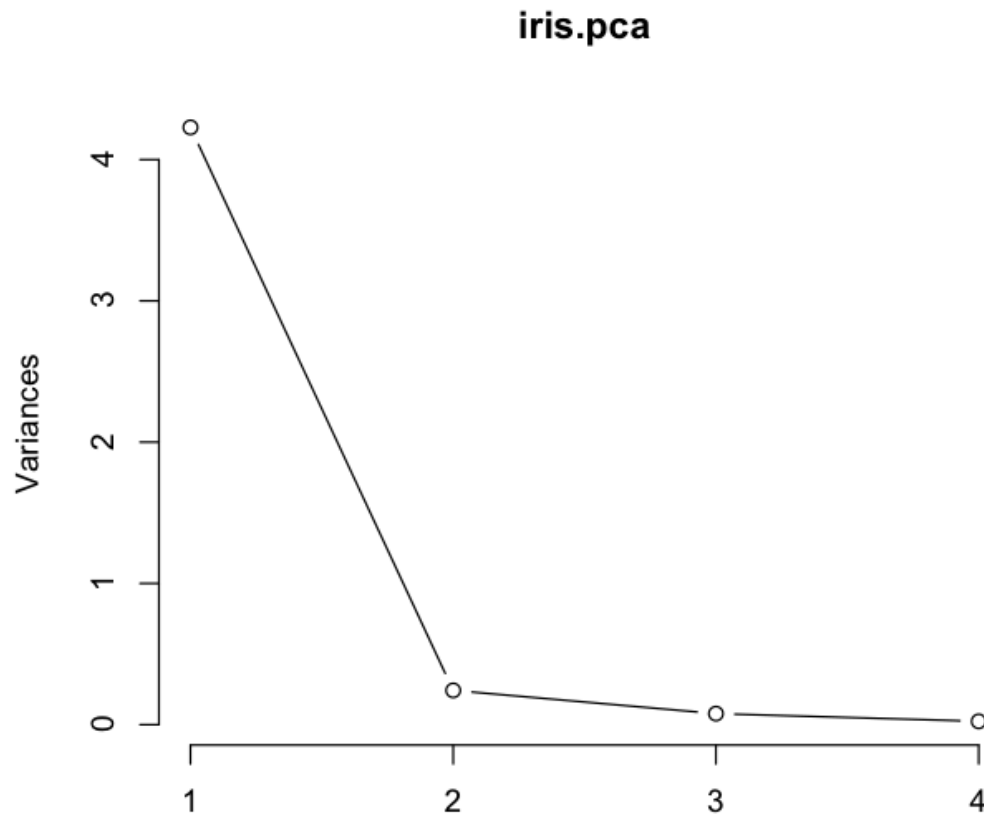
Furthermore the basis elements are ordered by their eigenvalues (from largest to smallest), and these eigenvalues represent the amount of variance explained by each basis element.

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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

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

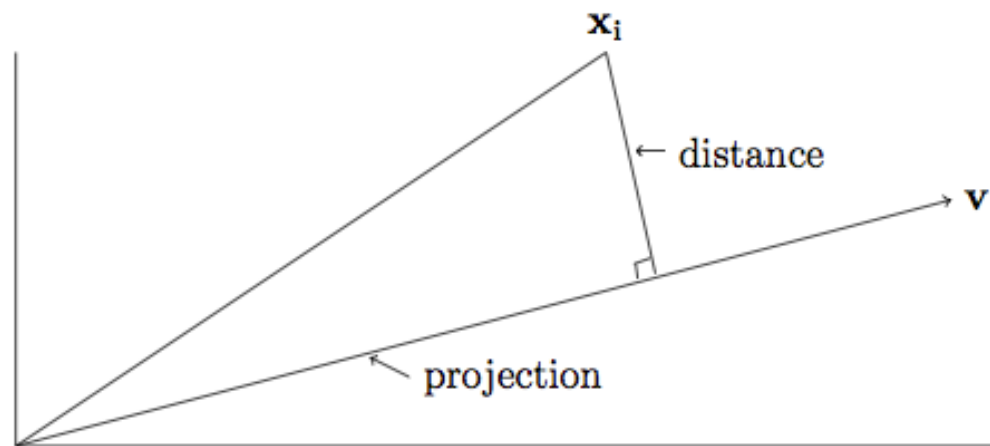


Figure 4.1: The projection of the point \mathbf{x}_i onto the line through the origin in the direction of \mathbf{v}

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 .

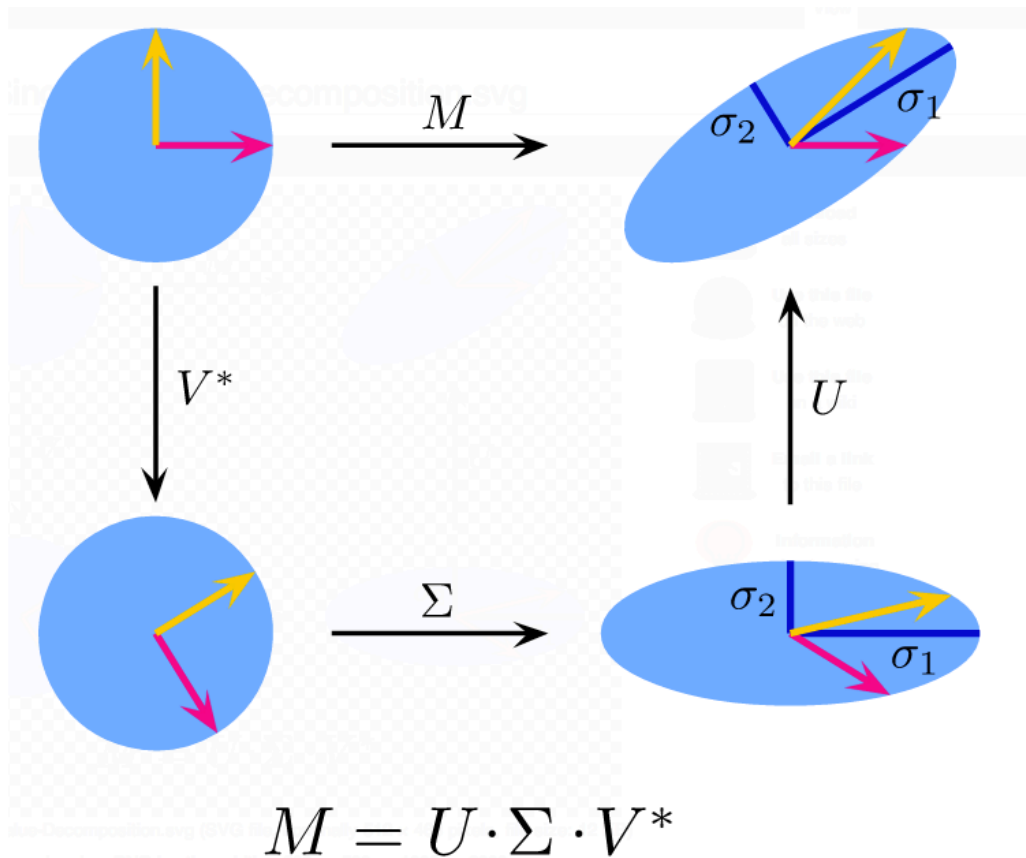
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The singular values give the magnitudes of the projection of each column of the original dataset on the elements of the new basis.



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- Latent semantic analysis, etc.

III. OTHER METHODS

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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.

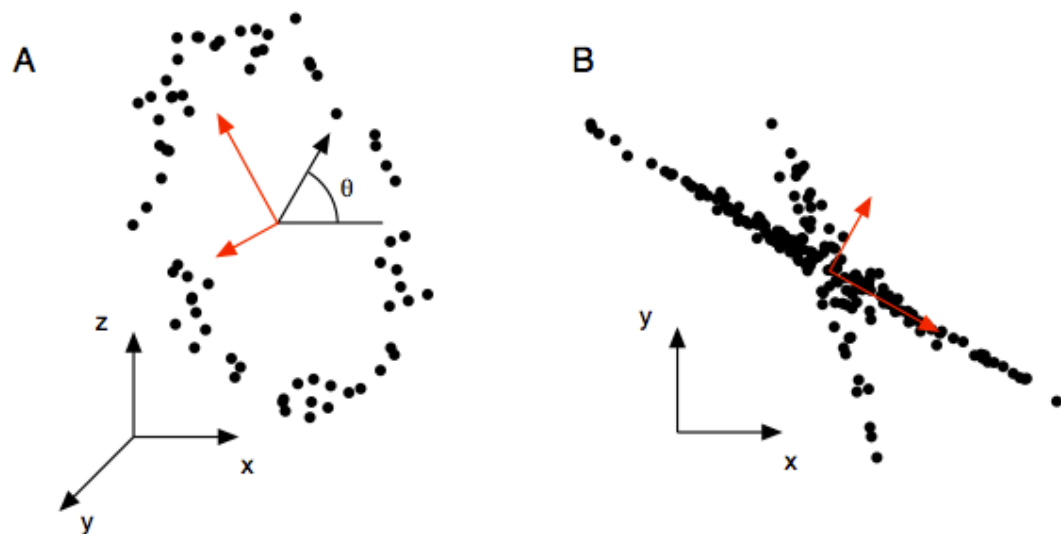
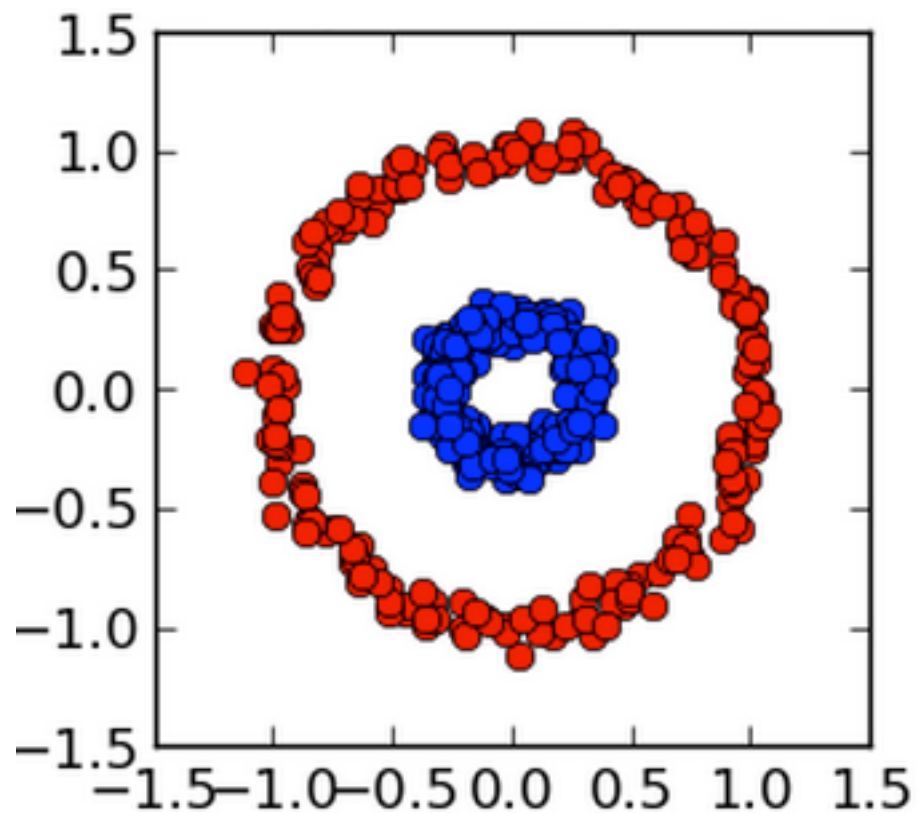


FIG. 6 Example of when PCA fails (red lines). (a) Tracking a person on a ferris wheel (black dots). All dynamics can be described by the phase of the wheel θ , a non-linear combination of the naive basis. (b) In this example data set, non-Gaussian distributed data and non-orthogonal axes causes PCA to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



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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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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See
`sklearn.decomposition`
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NOTE

And more!

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

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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