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.

	Continuous	Categorical
Supervised	???	???
Unsupervised	???	???

	Continuous	Categorical
Supervised	regression	classification
Unsupervised	dimension reduction	clustering

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 (e.g., if the relationships are actually simpler than they appear).

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Ideally, we would like to eliminate this redundancy and consolidate the number of variables we're looking at.

To say this more intuitively, we want to go from a more complex representation of our data to a less complex one (while retaining as much of the signal in our data as possible).

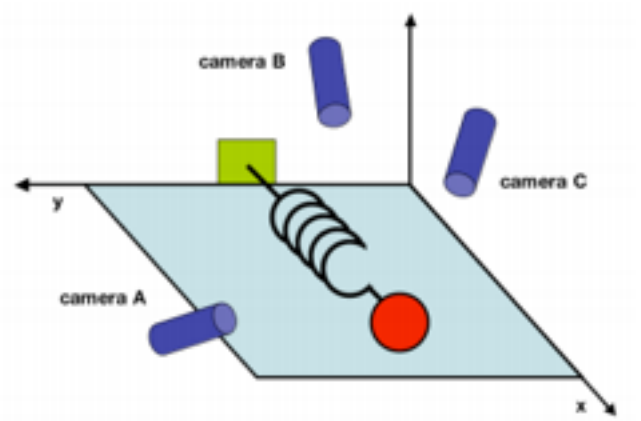
We can do this by looking at our data “from another angle”.

In doing this, we tease out the “principal components” of our data.

For example, suppose we have a dataset with some features that are related to each other.

Ideally, we would like to eliminate this redundancy and consolidate the number of variables we're looking at.
If these relationships are *linear*, then we can use well-established techniques like PCA/SVD.

EXAMPLE: 1D HARMONIC OSCILLATOR



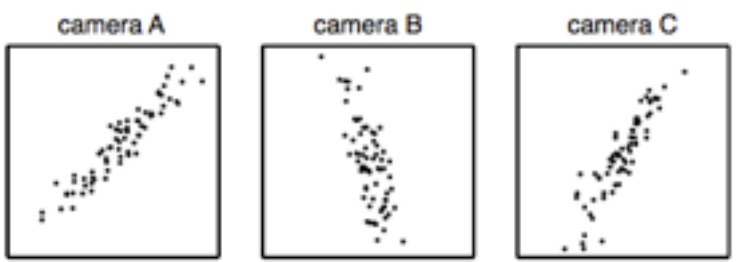


FIG. 1 A toy example. The position of a ball attached to an oscillating spring is recorded using three cameras A, B and C. The position of the ball tracked by each camera is depicted in each panel below.

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

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).

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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We'd like to analyze the data using the most meaningful basis (or coordinates) possible.

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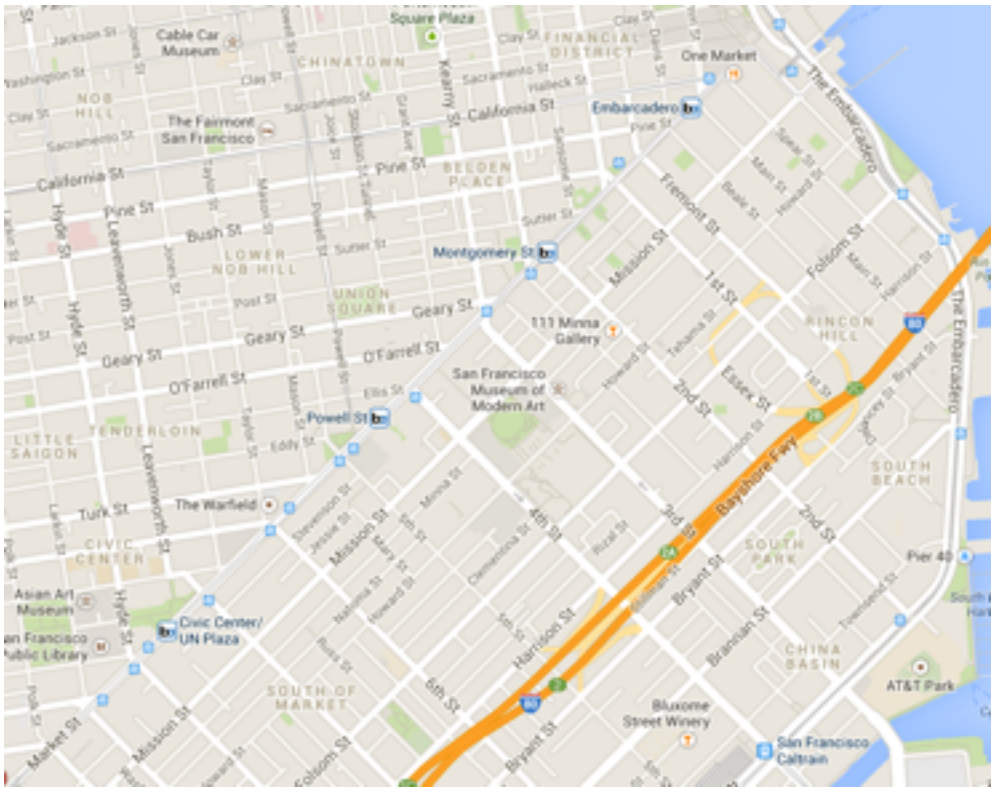
The goal of feature extraction is to create a new set of coordinates that *simplify the representation* of the data.

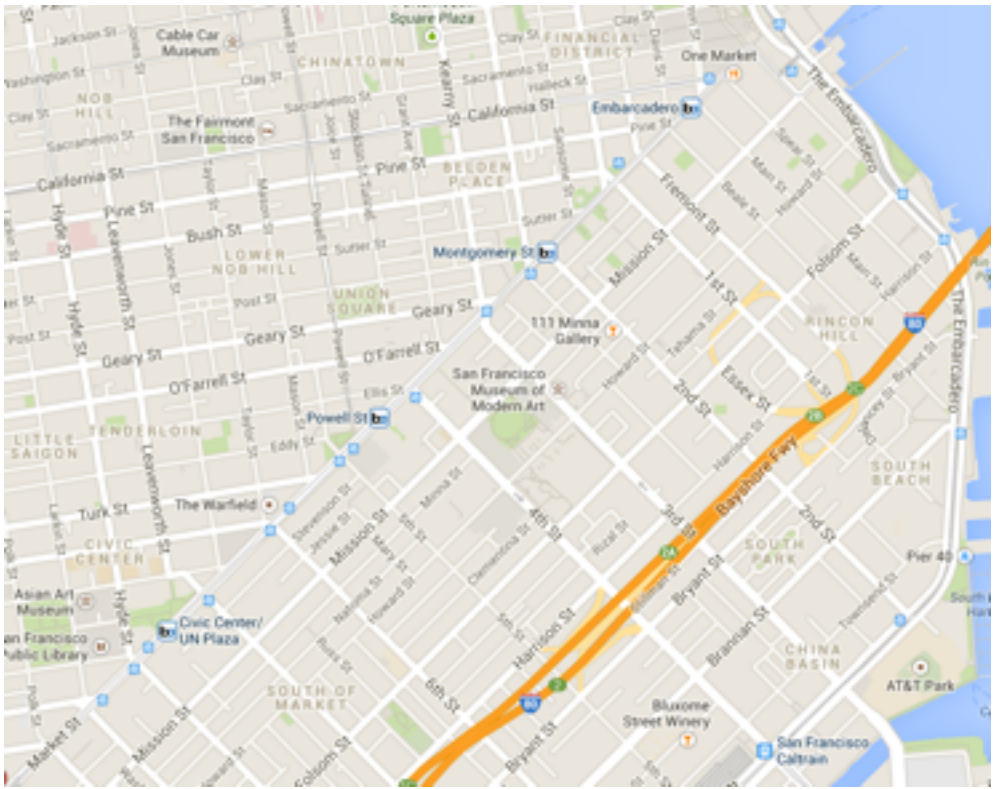
INTUITIVE EXAMPLE - BIKING DOWN MARKET STREET



W

S

INTUITIVE EXAMPLE - BIKING DOWN MARKET STREET



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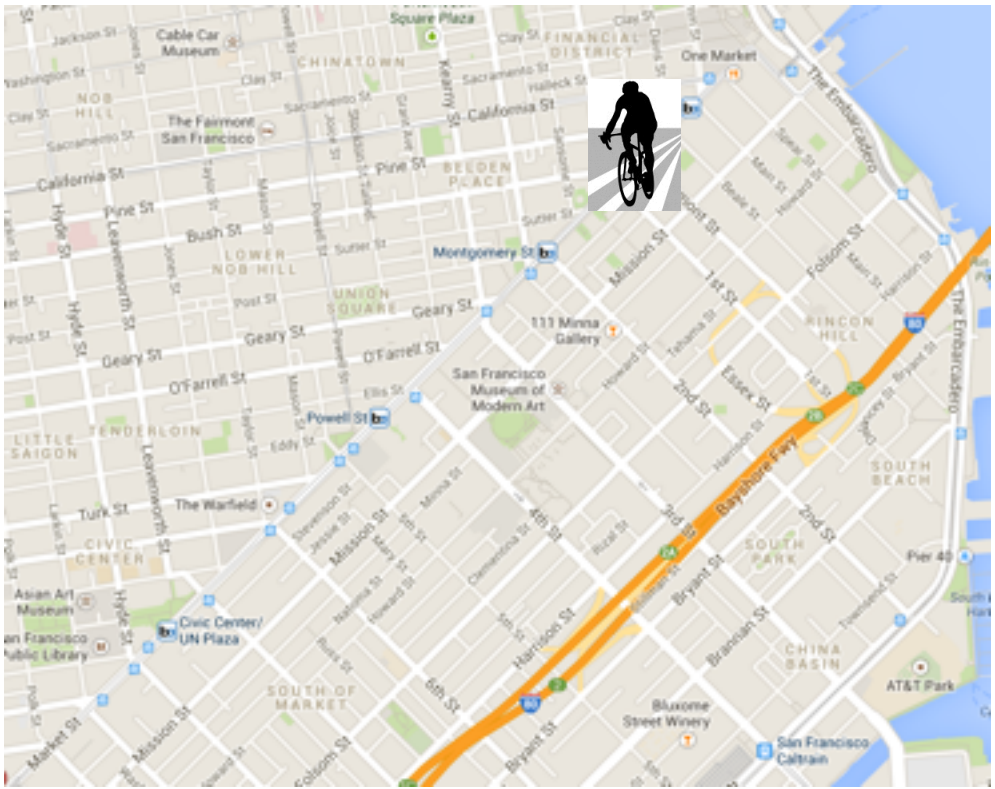
INTUITIVE EXAMPLE - BIKING DOWN MARKET STREET



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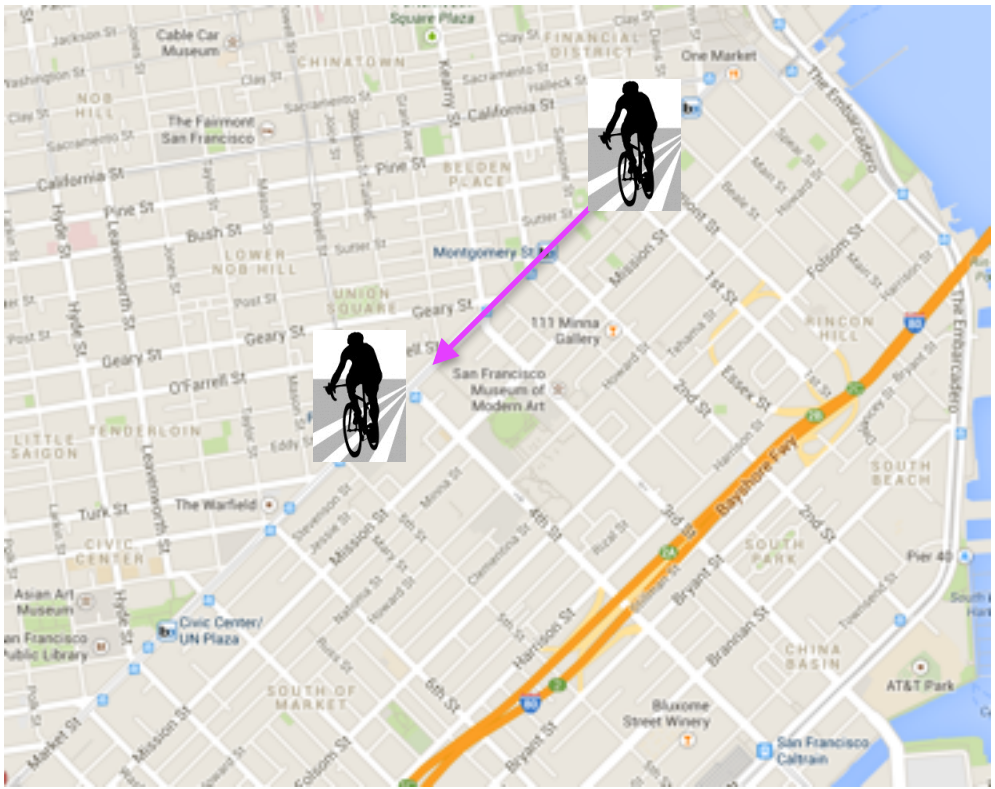
INTUITIVE EXAMPLE - BIKING DOWN MARKET STREET



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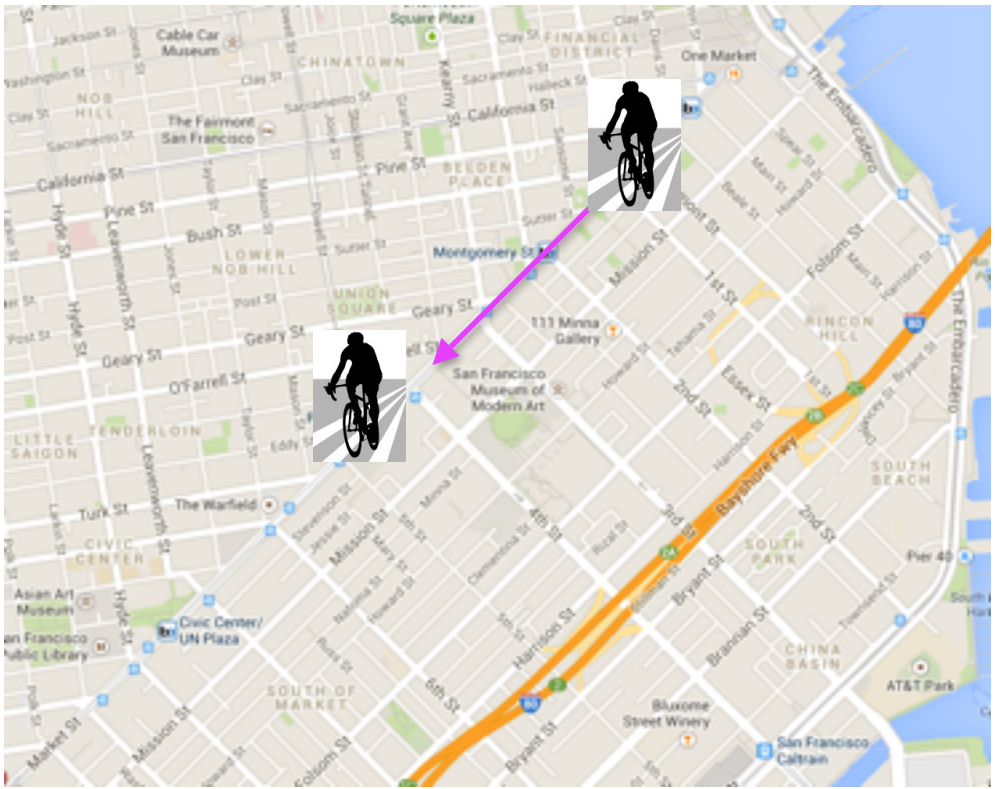
INTUITIVE EXAMPLE - BIKING DOWN MARKET STREET



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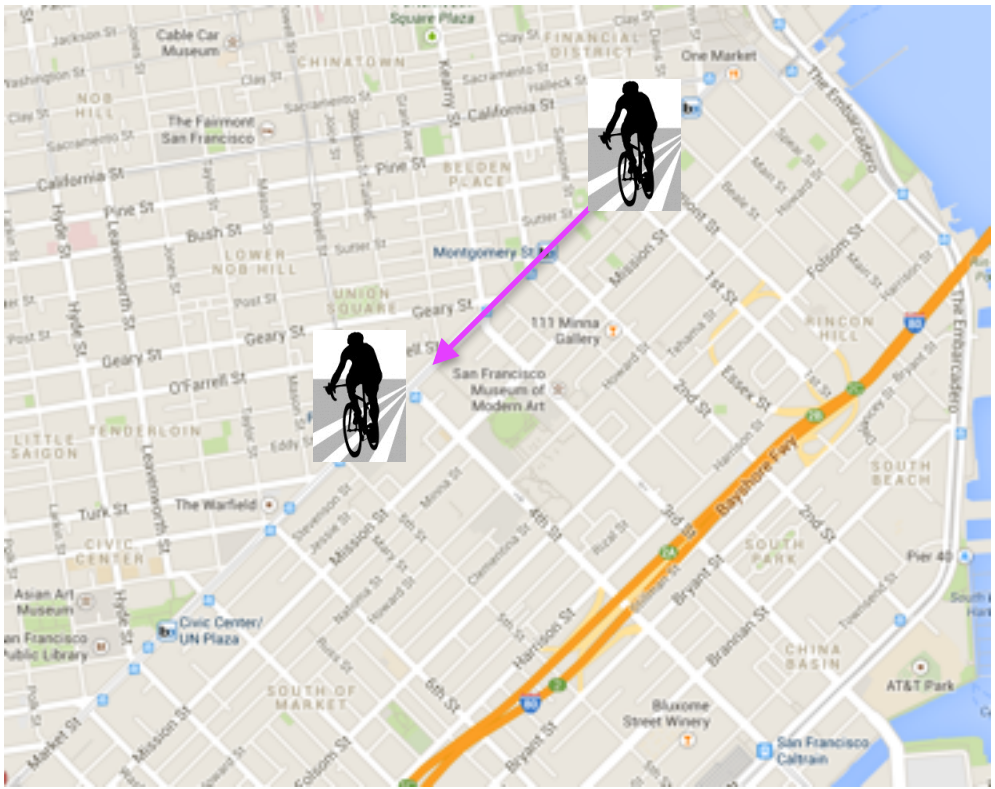
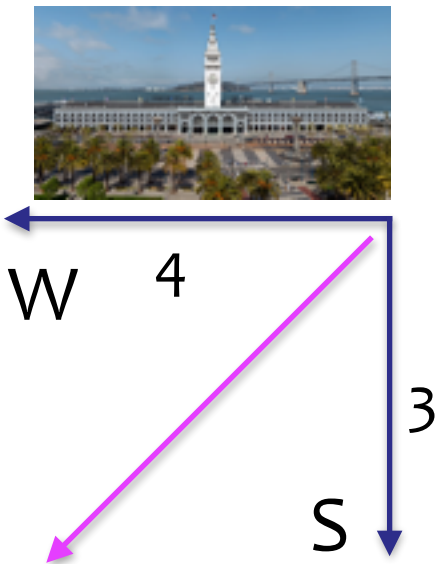
S

How many dimensions do we need to specify the position of this bike?

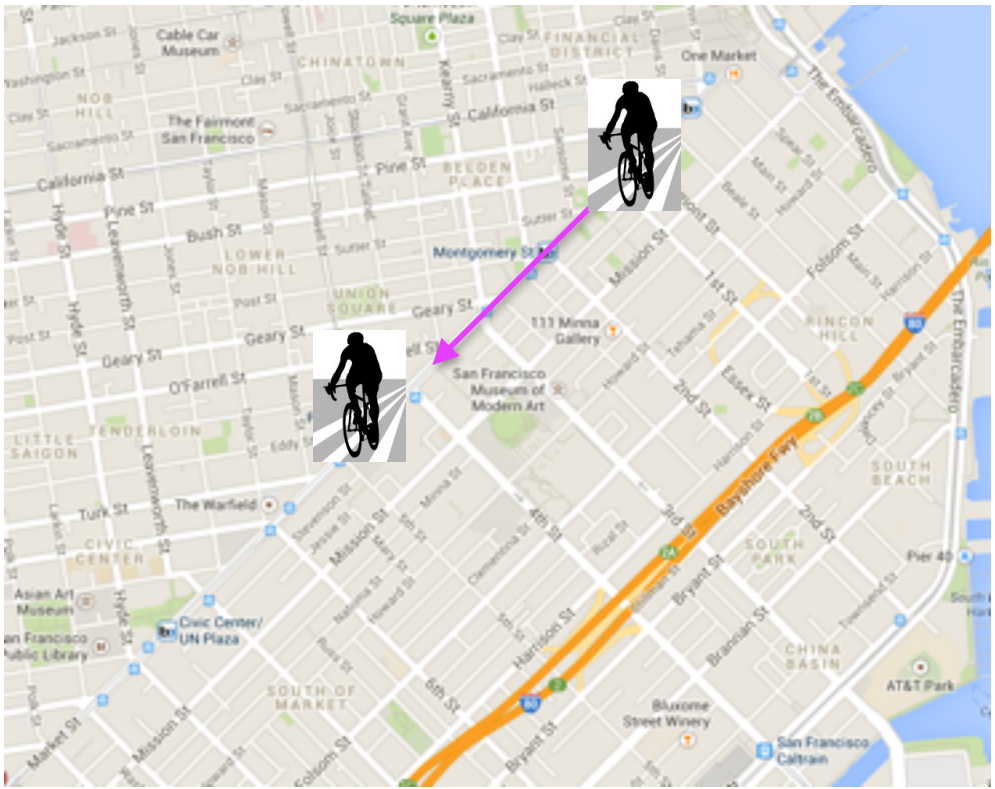
INTUITIVE EXAMPLE - BIKING DOWN MARKET STREET





Yep, two. But could we represent the biker's position with fewer dimensions? How?

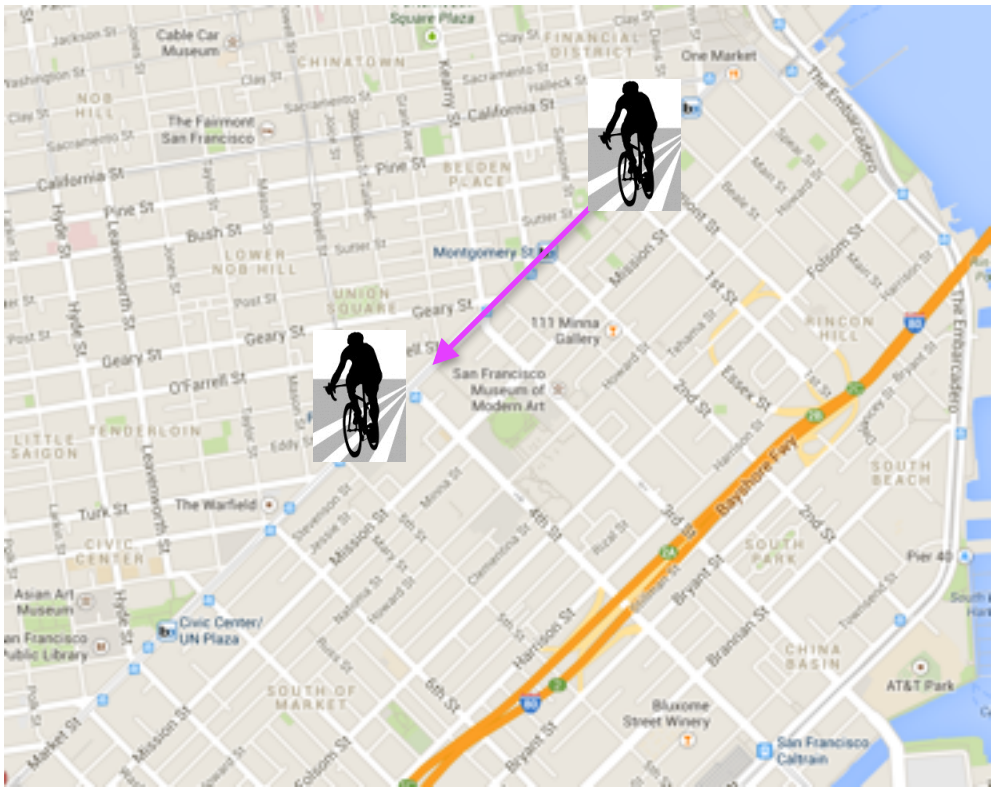
INTUITIVE EXAMPLE - BIKING DOWN MARKET STREET

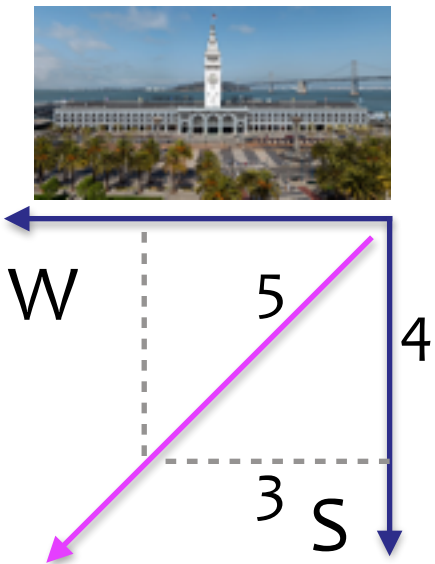


dist = 5

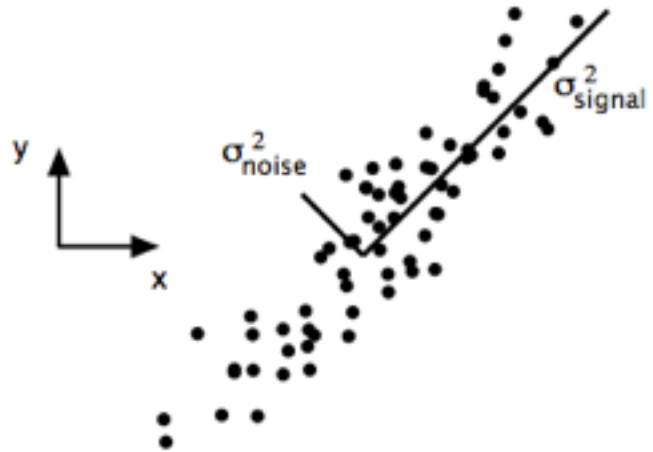
What if we just used distance down Market St.?

INTUITIVE EXAMPLE - BIKING DOWN MARKET STREET





Of course, we can always map back to the original coordinate system!



$$SNR = \frac{\sigma^2_{signal}}{\sigma^2_{noise}}.$$

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

II. PRINCIPAL COMPONENT ANALYSIS

DIMENSIONALITY REDUCTION: PCA

A technique useful for the compression and classification of data. The purpose is to reduce the dimensionality of a dataset by finding a new set of variables, smaller than the original set, that still retains most of the information of the original set.

The ***principal component*** is the one that maximizes the variance of the projected data.

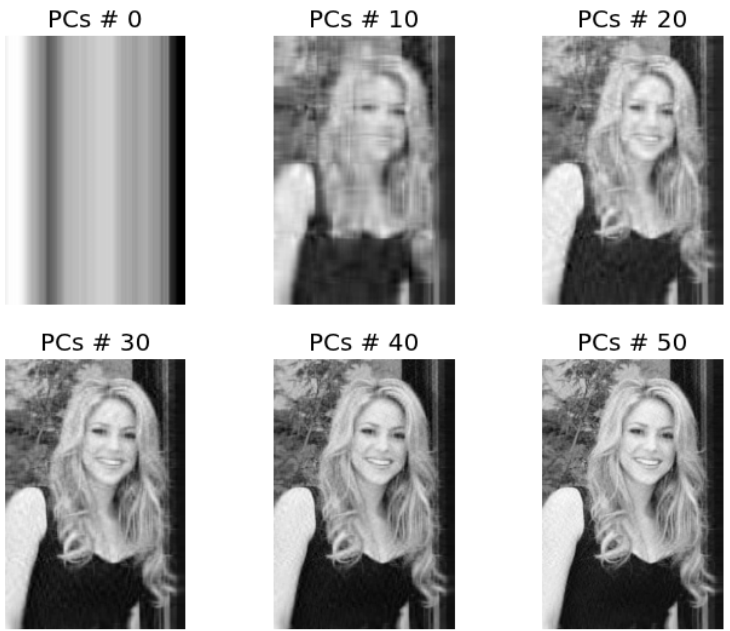
DIMENSIONALITY REDUCTION: PCA

A TECHNIQUE USEFUL FOR THE COMPRESSION AND CLASSIFICATION OF DATA. THE PURPOSE IS TO REDUCE THE DIMENSIONALITY OF A DATA SET BY FINDING A NEW SET OF VARIABLES, SMALLER THAN THE ORIGINAL VARIABLES, THAT NONETHELESS RETAINS MOST OF THE SAMPLE'S INFORMATION.

INFORMATION = VARIANCE

ADVANTAGES OF PCA

- **ALLOWS US TO COMPRESS DATA WHILE LOSING AS LITTLE OF THE VARIANCE AS POSSIBLE**



DISADVANTAGES OF PCA

- Covariance of 0 does not mean your data is independent

- Better methods for nonlinear data
- Not the best method for parsing hidden or latent factors

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

Wait a minute, what's a covariance matrix?

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For that matter, what is covariance?

Remember variance?

Remember variance?

$$s^2 = \frac{\sum_{i=1}^{n}(X_i - \bar{X})^2}{(n-1)}$$

Variance is the average distance from the mean of a data set to a point in that data set.
In other words, it is a measure of the *spread* of the data.
Recall that standard deviation is the square root of variance.

Standard deviation and variance only operate on 1 dimension, so that you could only calculate the standard deviation for each dimension of the data set *independently* of the other dimensions. However, it is useful to have a similar measure to find out how much the dimensions vary from the mean *with respect to each other*.

This is called covariance.

Variance:

$$s^2 = \frac{\sum_{i=1}^{n}(X_i - \bar{X})^2}{(n-1)} \qquad var(X) = \frac{\sum_{i=1}^{n}(X_i - \bar{X})(X_i - \bar{X})}{(n-1)}$$

Covariance:

$$cov(X,Y) = \frac{\sum_{i=1}^{n}(X_i - \bar{X})(Y_i - \bar{Y})}{(n-1)}$$

Covariance is always measured between two dimensions. If you calculate the covariance between a dimension and itself, you get the variance.

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

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

The covariance matrix *C* of a matrix *A* is always square:

$$C = \begin{pmatrix} cov(x,x) & cov(x,y) & cov(x,z) \\ cov(y,x) & cov(y,y) & cov(y,z) \\ cov(z,x) & cov(z,y) & cov(z,z) \end{pmatrix}$$

off-diagonal elements C_{ij} give the *covariance* between X_i, X_j *(*$i \neq j$*)*

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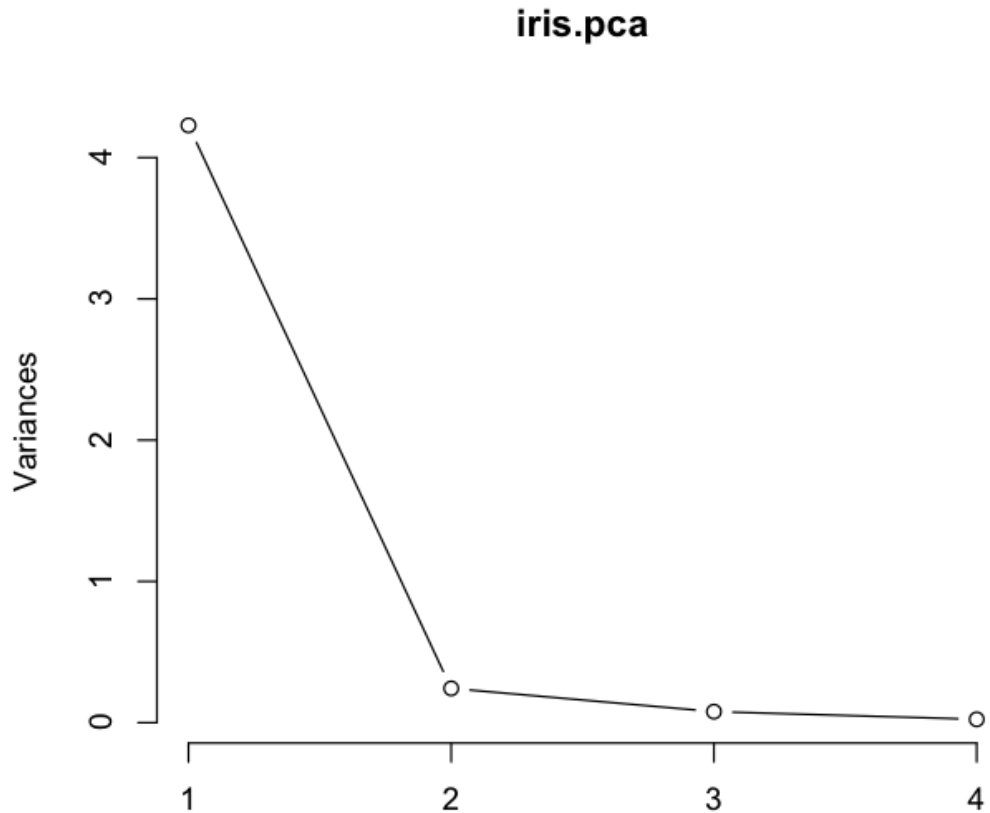
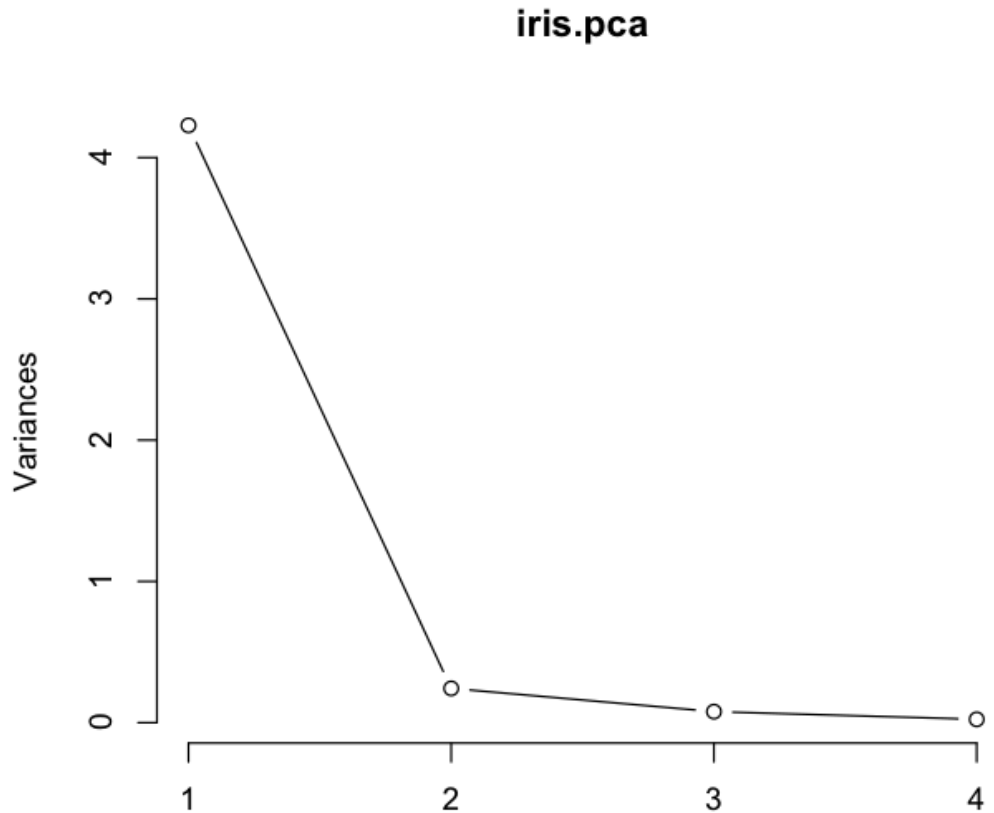
This can be visualized in a **scree plot**, which shows the amount of variance explained by each basis vector.


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. 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.

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.

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 now 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.

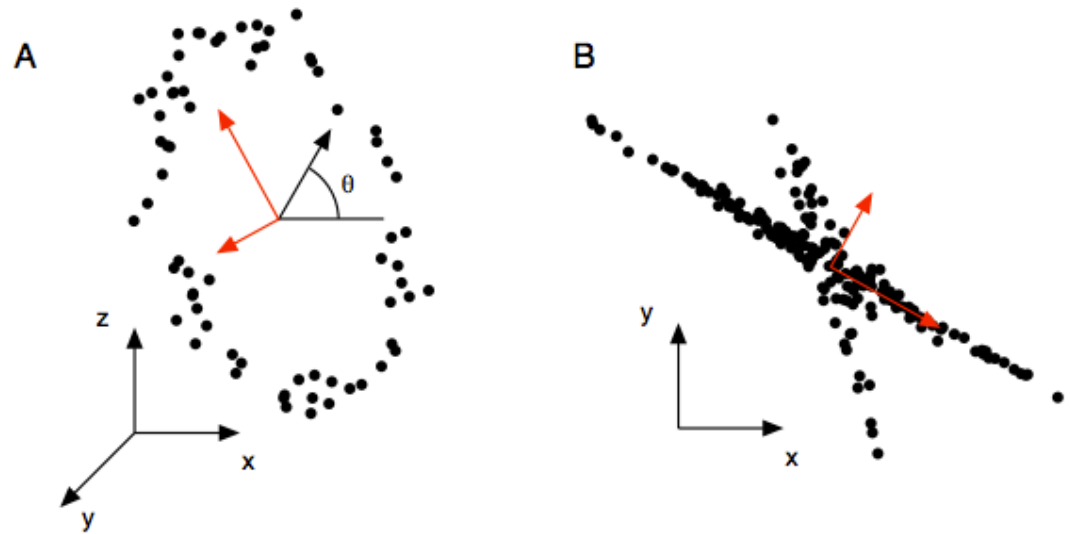
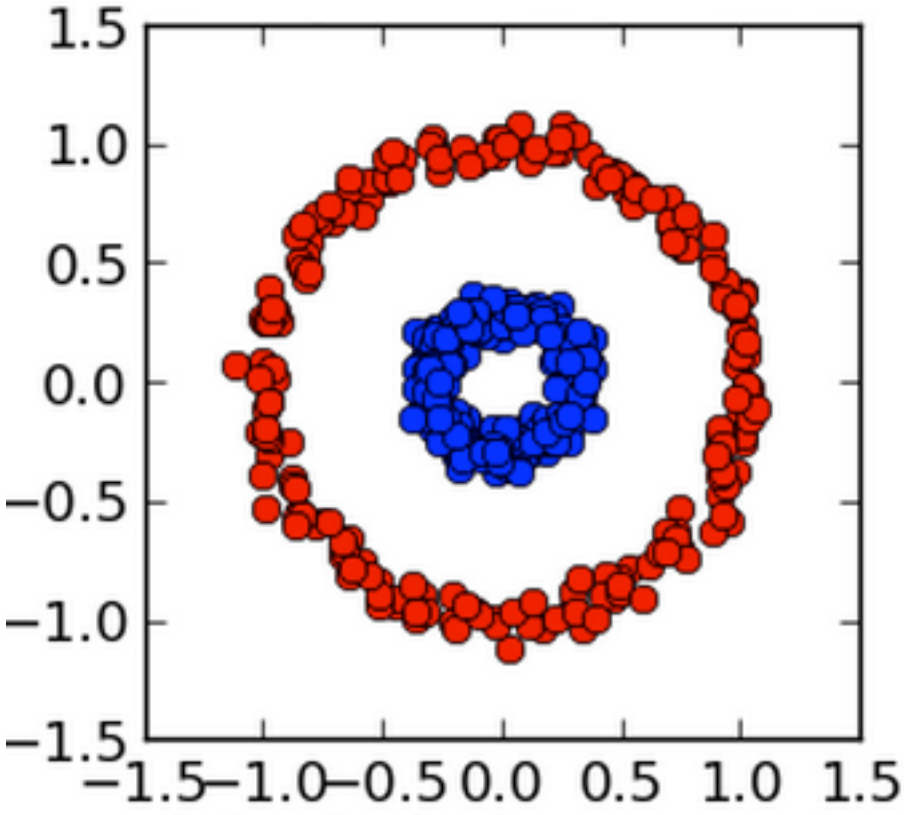


FIG. 6 Example of when PCA fails (red lines). (a) Tracking a person on a ferris wheel (black dots). All dynamics can be described by the phase of the wheel θ, a non-linear combination of the naive basis. (b) In this example data set, non-Gaussian distributed data and non-orthogonal axes causes PCA to 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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kernel PCA: exploits PCA dependence on inner product
(same logic as SVM)

isomap: nonlinear dimension reduction via MDS using geodesic
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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.