GENERAL ASSEMBLY

INTRO TO DATA SCIENCE
LECTURE 6: DIMENSIONALITY REDUCTION

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March 26, 2014

LAST TIME:

- LINEAR & MULTIPLE REGRESSION
- POLYNOMIAL REGRESSION
- REGRESSION IN PYTHON USING STATSMODEL

QUESTIONS?

AGENDA

I. DIMENSIONALITY REDUCTION
II. PRINCIPAL COMPONENTS ANALYSIS
III. SINGULAR VALUE DECOMPOSITION

EXERCISE:
IV. DIMENSIONALITY REDUCTION USING SCIKIT-LEARN

I. DIMENSIONALITY REDUCTION

Q: What is dimensionality reduction?

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DIMENSIONALITY REDUCTION

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A: A set of techniques for reducing the size (in terms of features, records, and/or bytes) of the dataset under examination.

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).

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

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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).

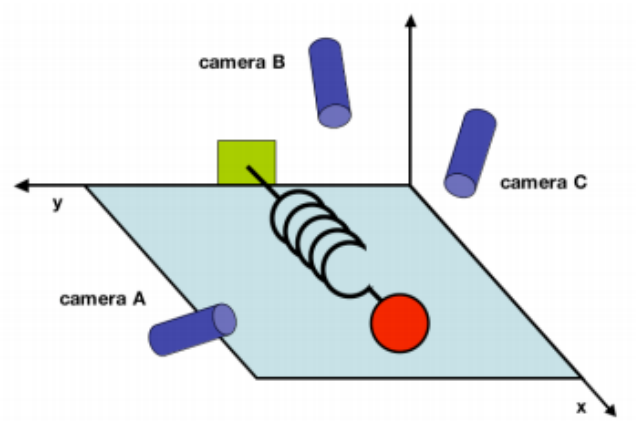
We can do this by looking at our data “from another angle”.

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



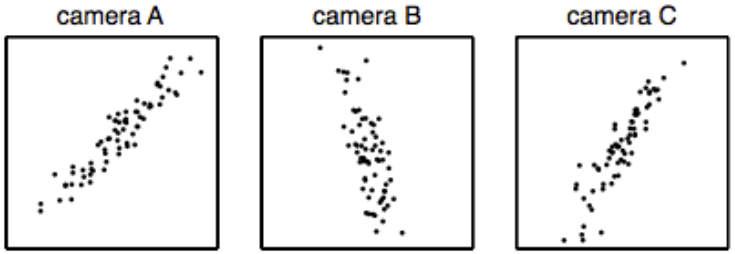


FIG. 1 A toy example. The position of a ball attached to an oscillating spring is recorded using three cameras A, B and C. The position of the ball tracked by each camera is depicted in each panel below.

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

ASIDE: CURSE OF DIMENSIONALITY

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).

In either case, most of the points in the space are "far" from the center.

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.

Q: What is the goal of dimensionality reduction?

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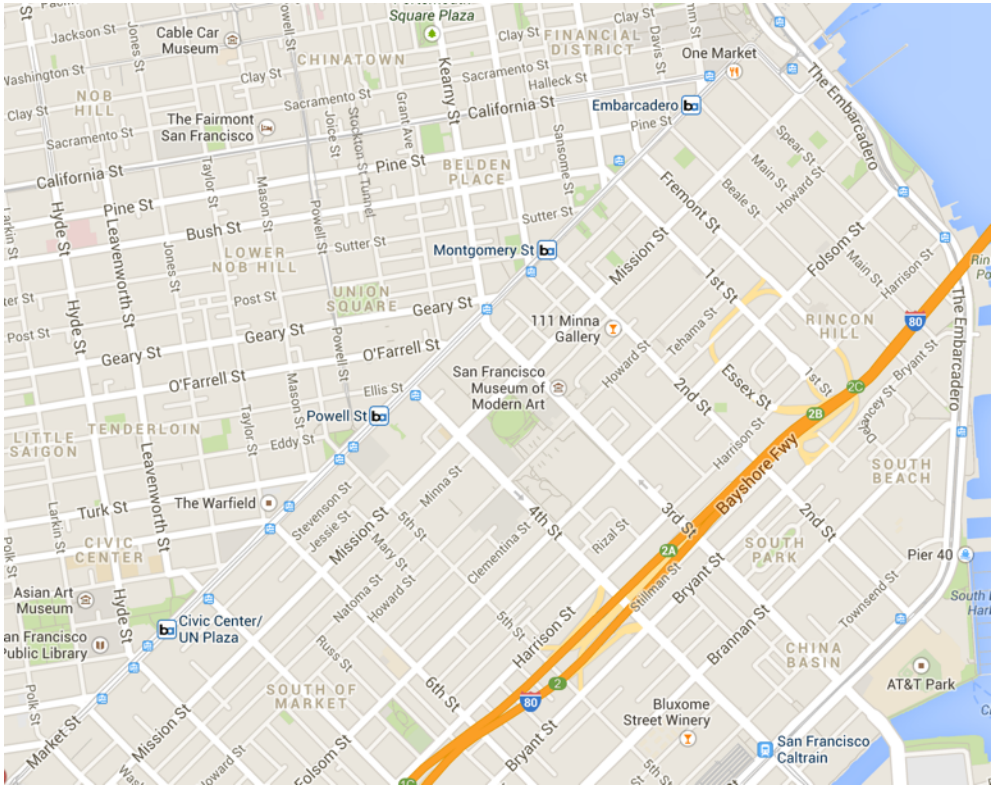
The goal of feature extraction is to create a new set of coordinates that *simplify the representation* of the data.

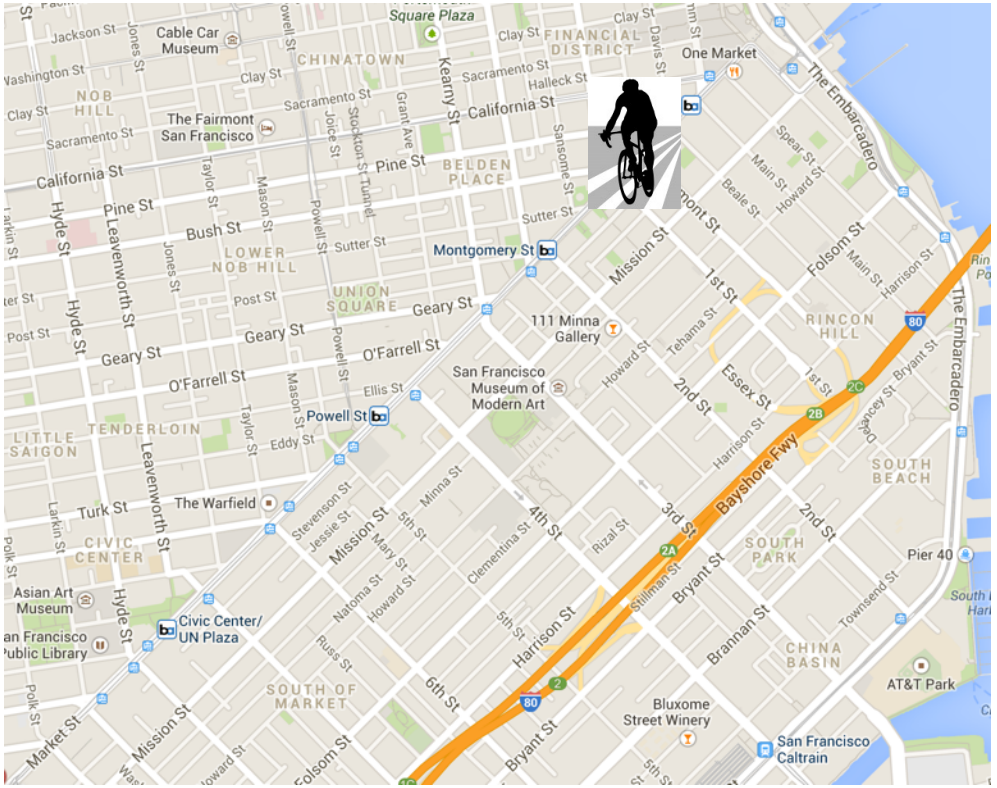
INTUITIVE EXAMPLE - BIKING DOWN MARKET STREET



W

S

INTUITIVE EXAMPLE - BIKING DOWN MARKET STREET



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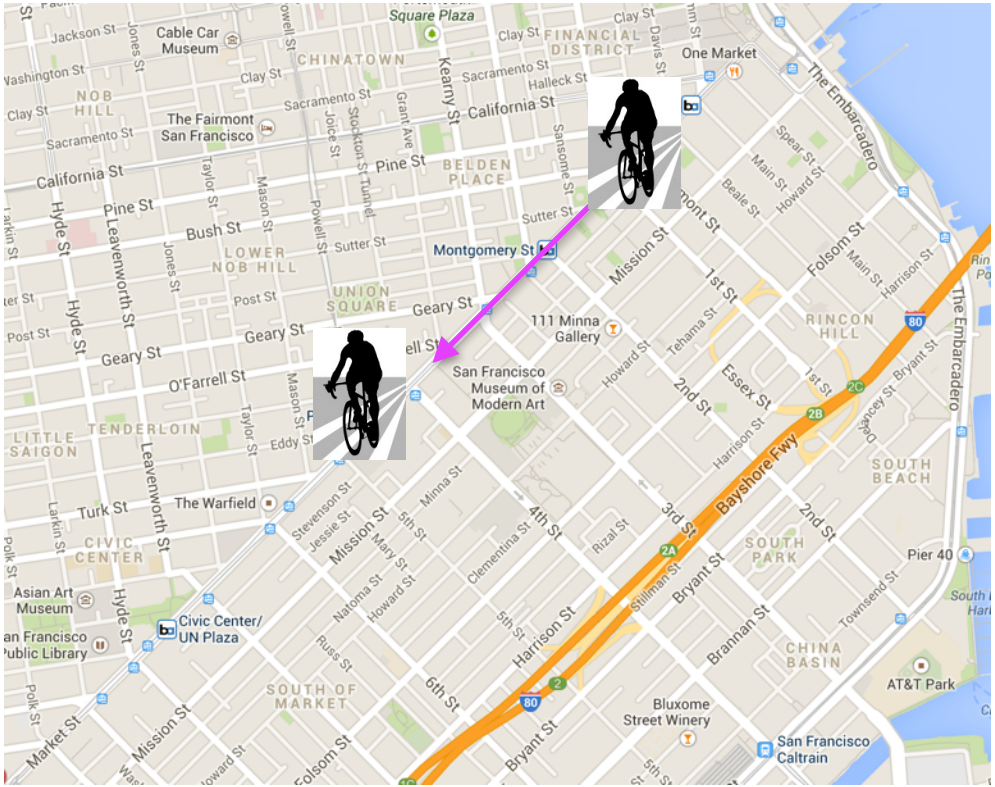
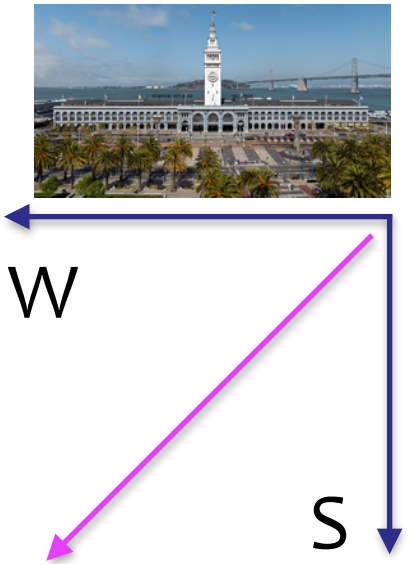
INTUITIVE EXAMPLE - BIKING DOWN MARKET STREET





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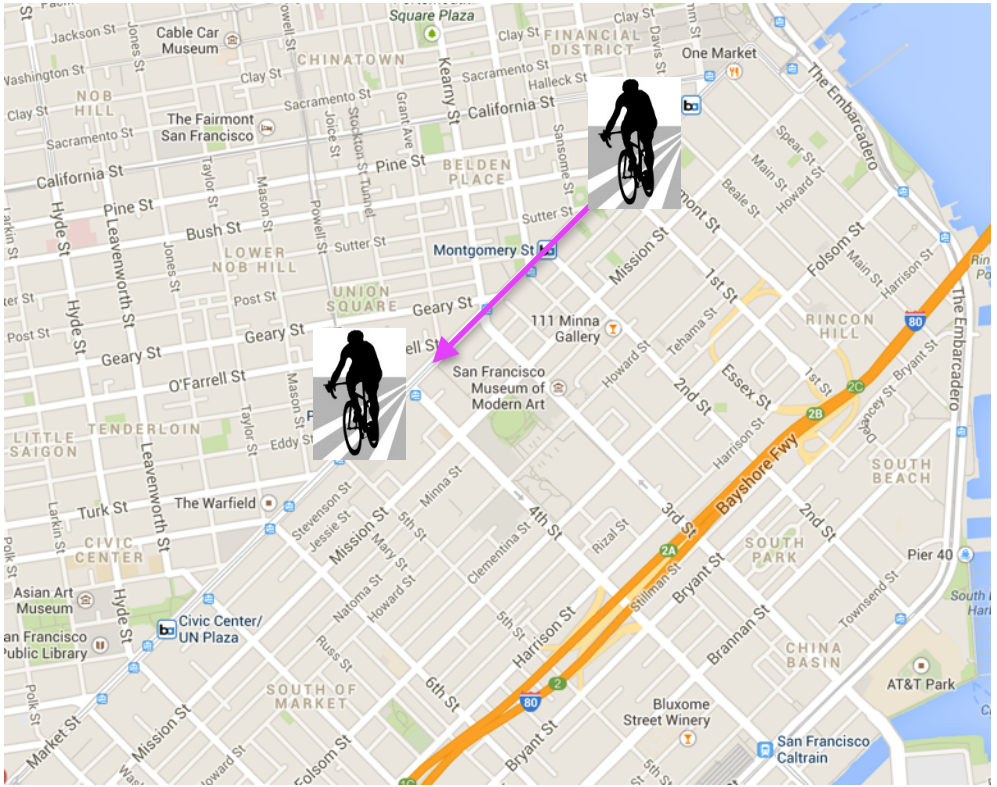

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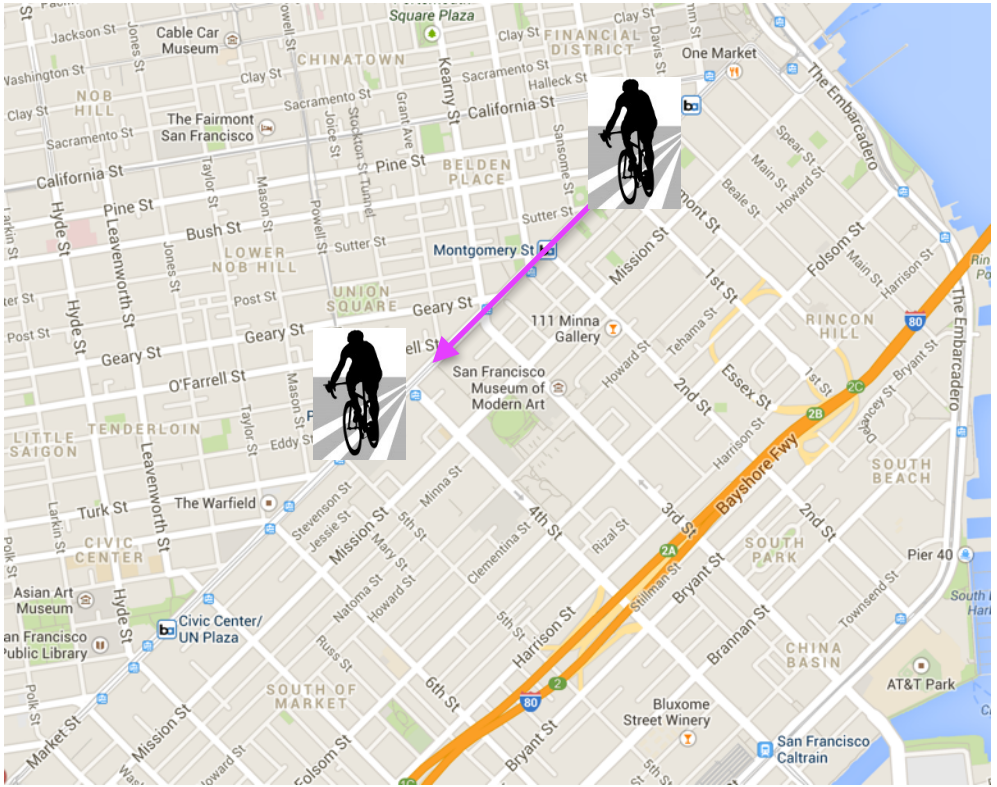
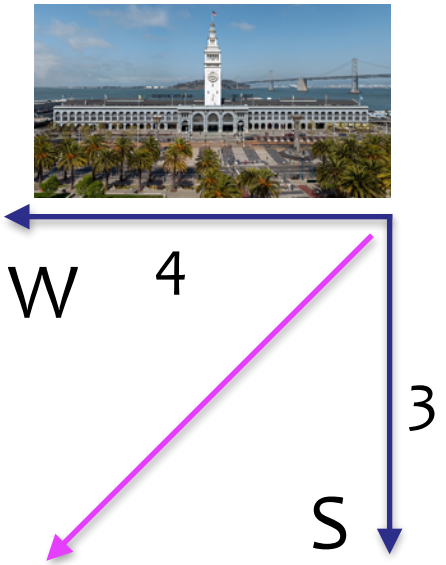
How many dimensions do we need to specify the position of this bike?

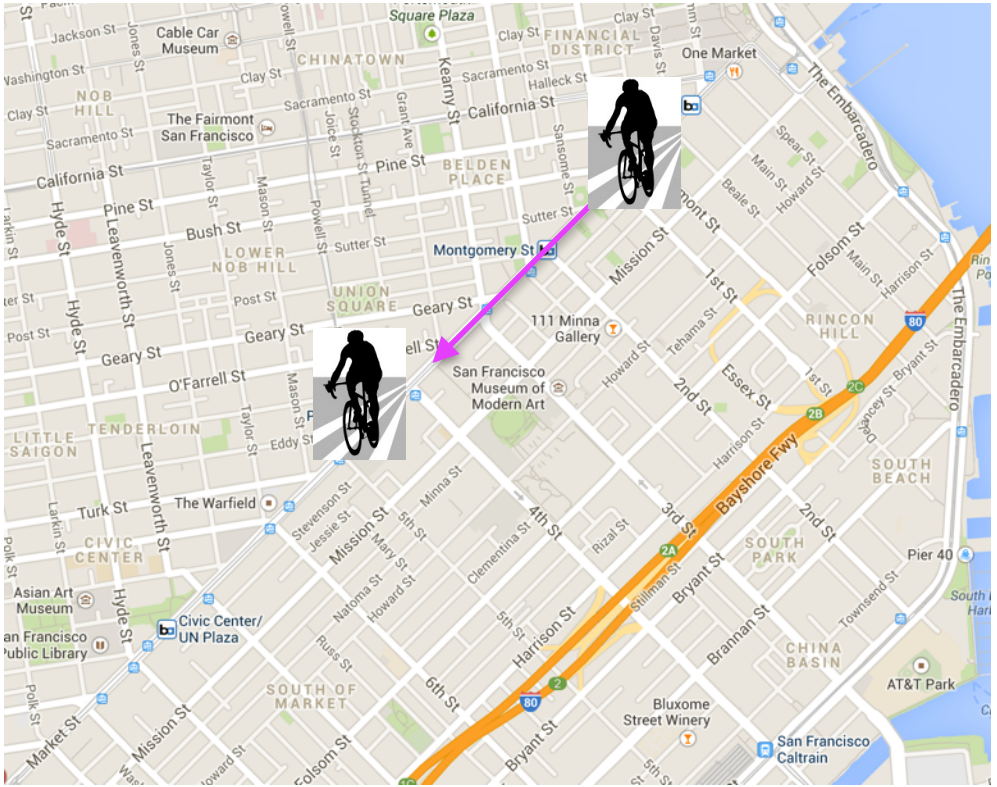
INTUITIVE EXAMPLE - BIKING DOWN MARKET STREET





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

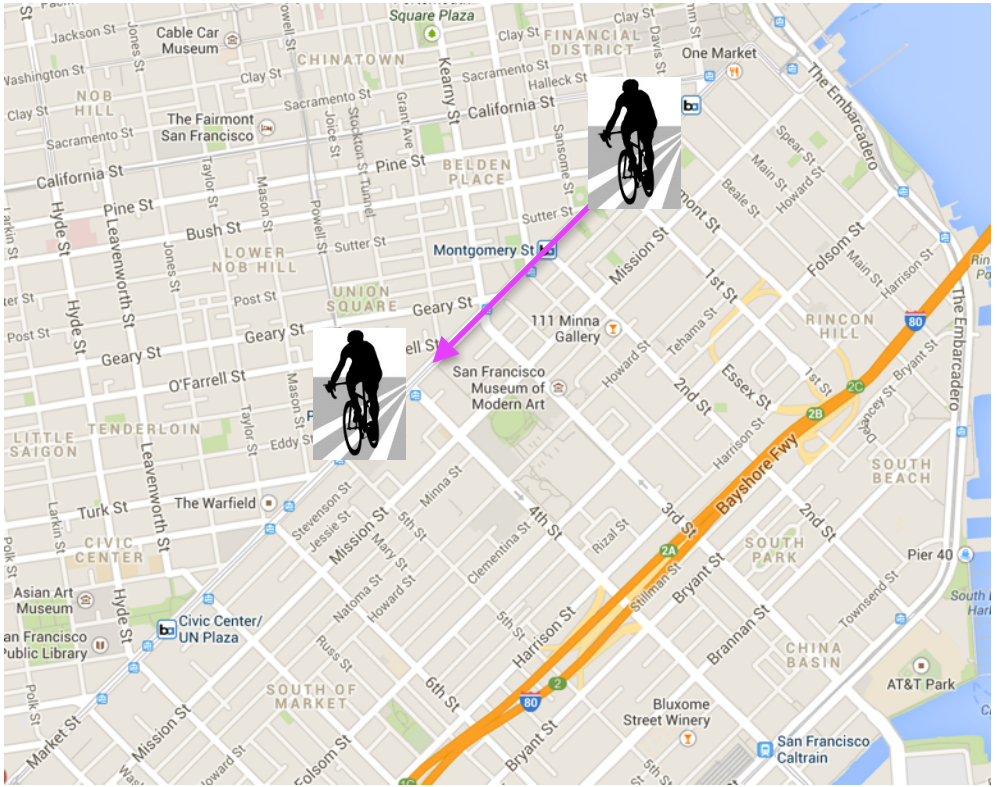
INTUITIVE EXAMPLE - BIKING DOWN MARKET STREET

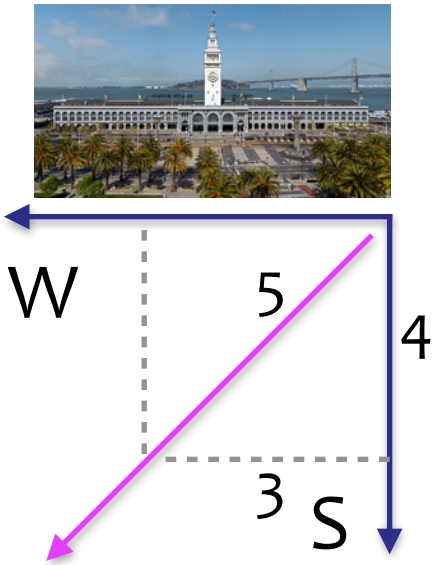


dist = 5

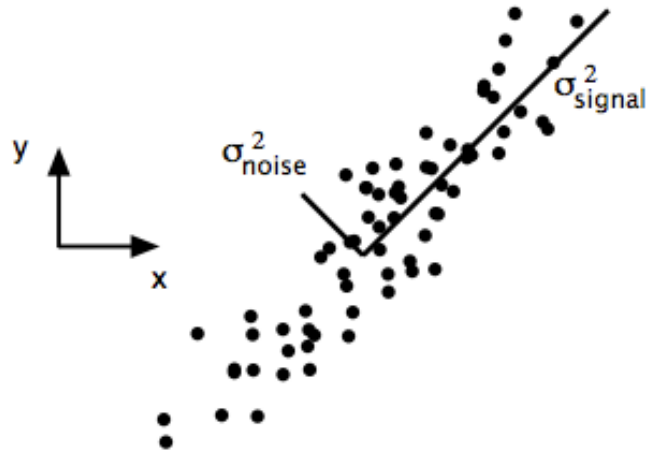
What if we just used distance down Market St.?

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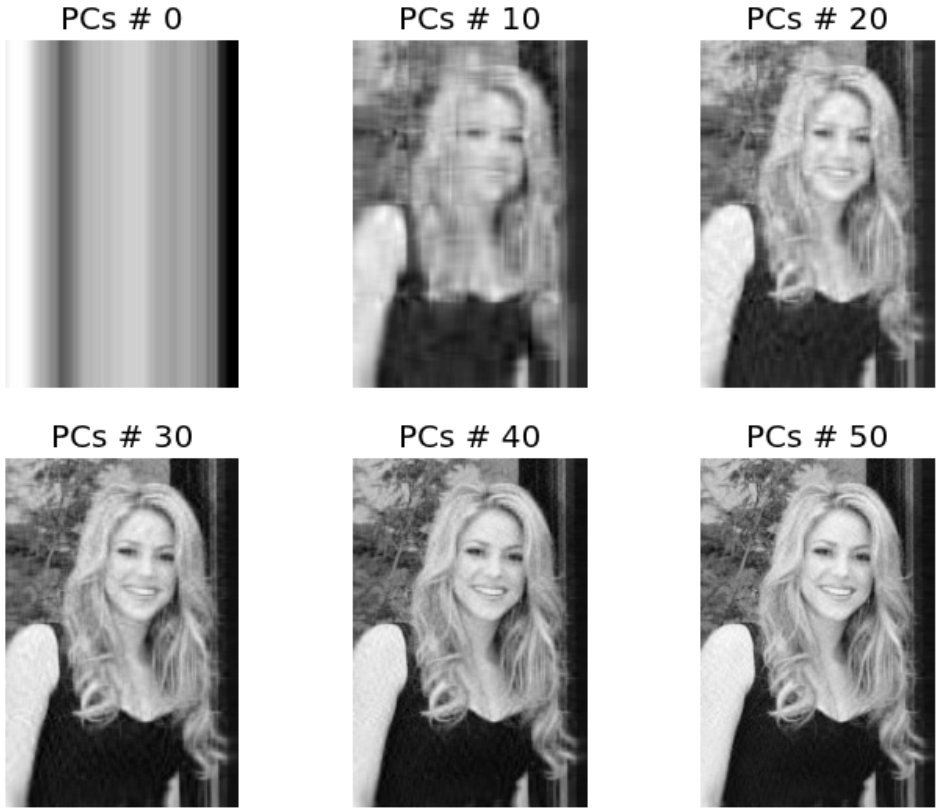
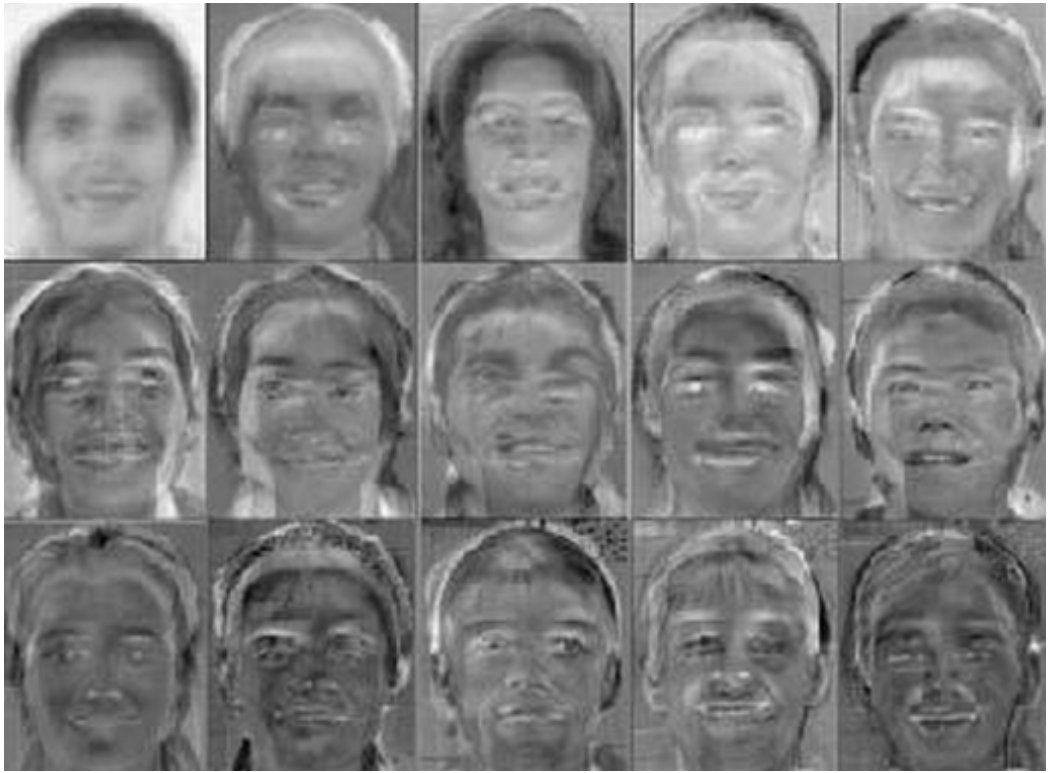
- topic models (document clustering)
- image recognition/computer vision
- bioinformatics (microarray analysis)
- speech recognition
- astronomy (spectral data analysis)
- recommender systems



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

The covariance matrix C of a matrix A 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?

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

For that matter, what is covariance?

Remember variance?

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

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

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

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COVARIANCE MATRICES

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ASIDE: EIGENVALUE DECOMPOSITION

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NOTE

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

For an eigenvector v of A and its eigenvalue λ, we have the important relation:

$$Av = \lambda v$$

The eigenvectors form a basis of the vector space on which A acts (e.g., 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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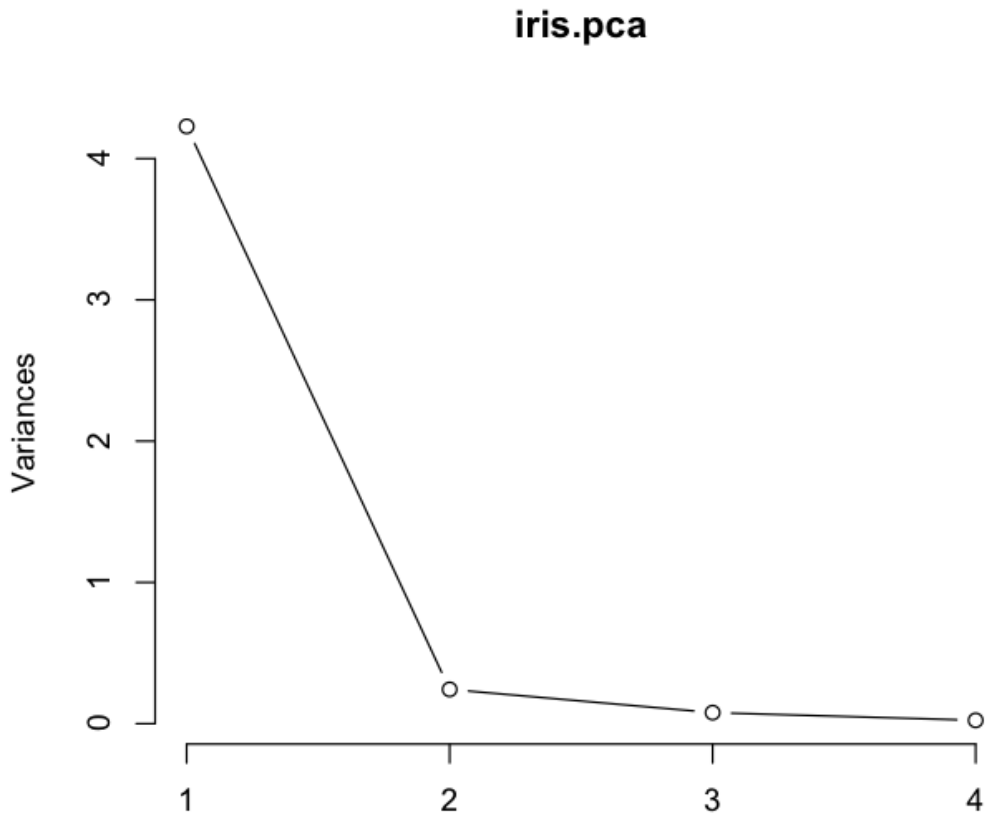
This can be visualized in a scree plot, which shows the amount of variance explained by each basis vector.


iris.pca
Variances
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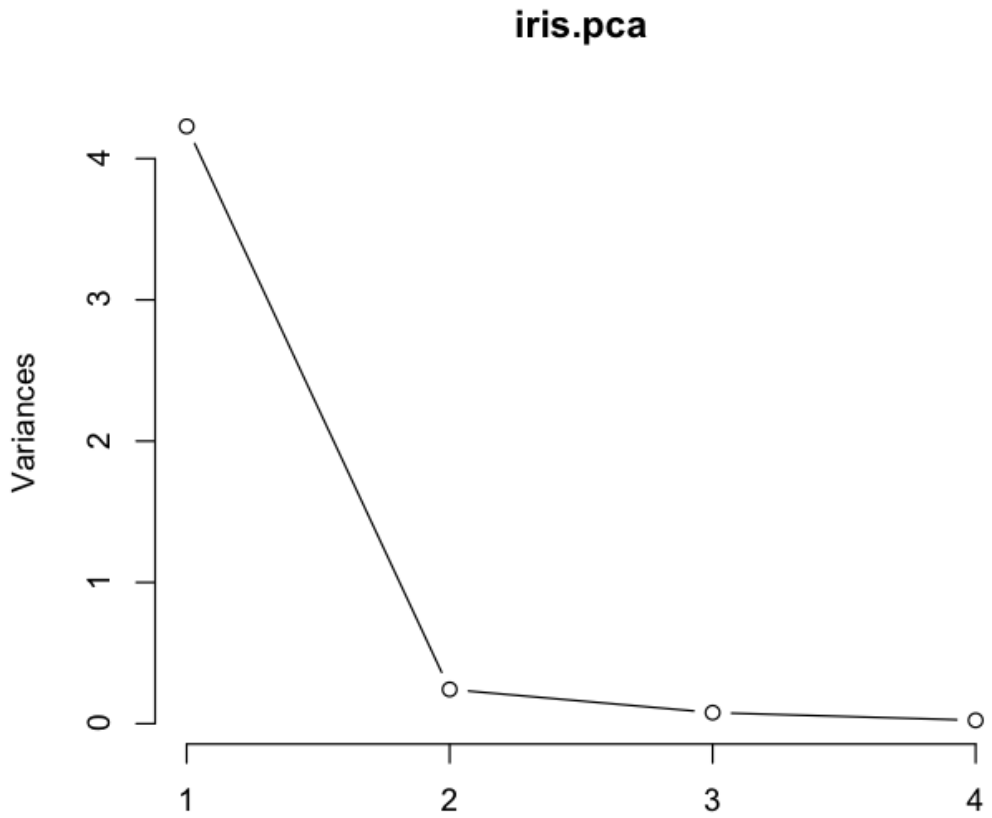
PRINCIPAL COMPONENT ANALYSIS



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.

PRINCIPAL COMPONENT ANALYSIS - ASSUMPTIONS

1. **Linearity** – The change in basis is a linear projection

2. **Large variances have important structure** – e.g. large signal-to-noise ratio. In other words, we assume that principal components with larger associated variances are signal, while those with lower variances represent noise. NOTE: this is a strong (and not always correct) assumption!

3. **The principal components are orthogonal** – A simplification that makes PCA soluble with linear algebra matrix decomposition techniques

III. SINGULAR VALUE DECOMPOSITION

Notice: Lots of math / linear algebra notation ahead!

It's okay if it does not all immediately make sense.

Take a deep breath…

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Take a deep breath…

That's better! Okay, then…

Consider a matrix A with n rows and d features.

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$$A = U \Sigma V^T$$

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st. U, V are orthogonal matrices and Σ is a diagonal matrix.

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

The singular value decomposition of A is given by:

$$A = U \Sigma V^T$$

(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 A.

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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 A.

These singular vectors provide orthonormal bases for the spaces K_n & K_d (columns of U & V, respectively).

The singular value decomposition of *A* is given by:

$$A = U \Sigma V^T$$

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

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

The singular value decomposition of A is g

$$A = U \Sigma V^T$$

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

NOTE

The number of singular values is equal to the *rank* of A.

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

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

For a general SVD, the columns of U are the eigenvectors of AA^T, and the columns of V are the eigenvectors of A^TA.

Also, the singular values of A are the square roots of the eigenvalues of AA^T and A^TA.

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

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NOTE

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

Q: How do you interpret the SVD?

A: Recall that given a set of n points in d-dimensional space (eg, a matrix A), 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.

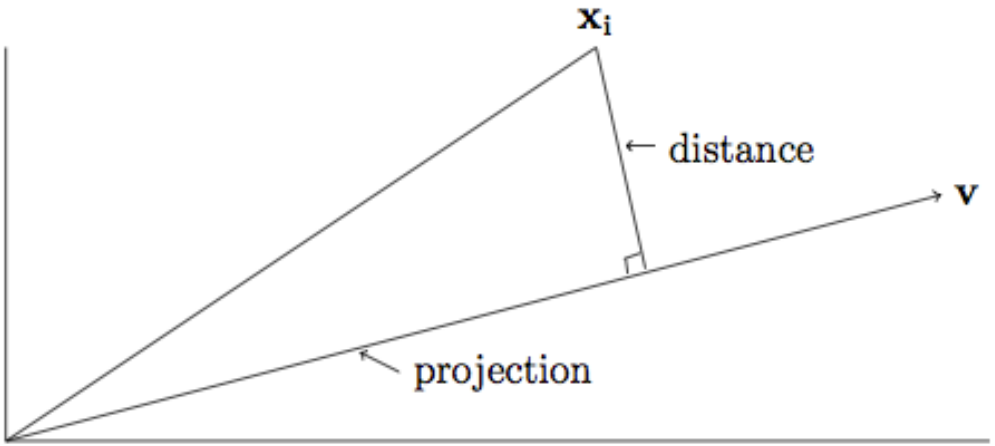

Figure 4.1: The projection of the point $\mathbf{x_i}$ onto the line through the origin in the direction of $\mathbf{v}$

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.

SINGULAR VALUE DECOMPOSITION

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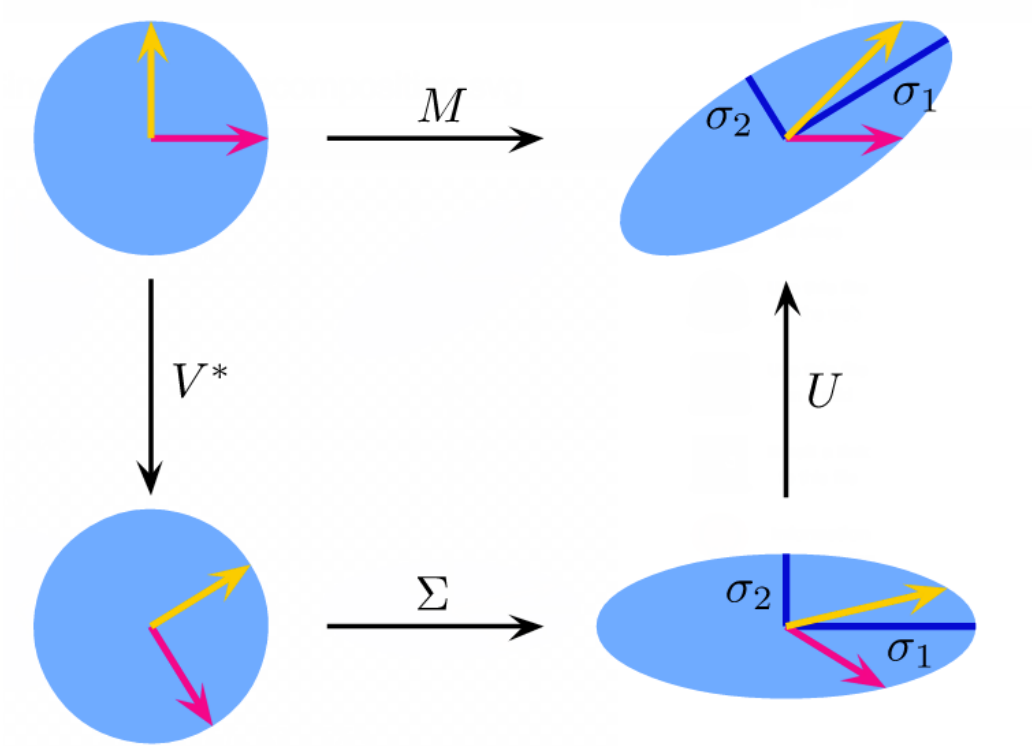
The singular vectors of T correspond to the lengths of the axes of the d-dimensional ellipsoid.

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

SINGULAR VALUE DECOMPOSITION



$$M = U \cdot \Sigma \cdot V^*$$

source: http://en.wikipedia.org/wiki/Singular_value_decomposition

III. OTHER METHODS

Whereas PCA and SVD create new coordinates by transform the old coordinates, factor analysis requires new coordinates to be specified externally.

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These new coordinates are associated with *hidden* or *latent* features that we think our data depends on.

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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$$X_i = \lambda_1 f_1 + \lambda_2 f_2 + \varepsilon$$

This would allow us to analyze the data in a more fundamental way.

SVD, PCA, and factor analysis are all linear techniques (eg, we use a linear transformation to embed the in a lower-dimensional space).

However, sometimes linear techniques are not sufficient.

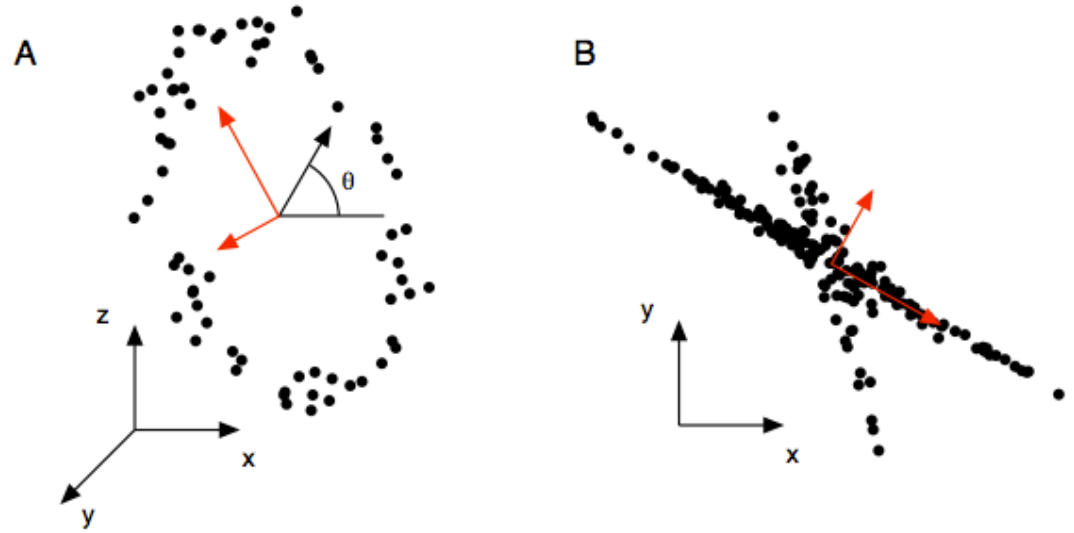

FIG. 6 Example of when PCA fails (red lines). (a) Tracking a person on a ferris wheel (black dots). All dynamics can be described by the phase of the wheel θ, a non-linear combination of the naive basis. (b) In this example data set, non-Gaussian distributed data and non-orthogonal axes causes PCA to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

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

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

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

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

IV. EXAMPLE: DIMENSIONALITY REDUCTION IN SKLEARN