Lecture 20: Dimensionality Reduction

- Overview
- Self-organizing maps
- Principal component analysis

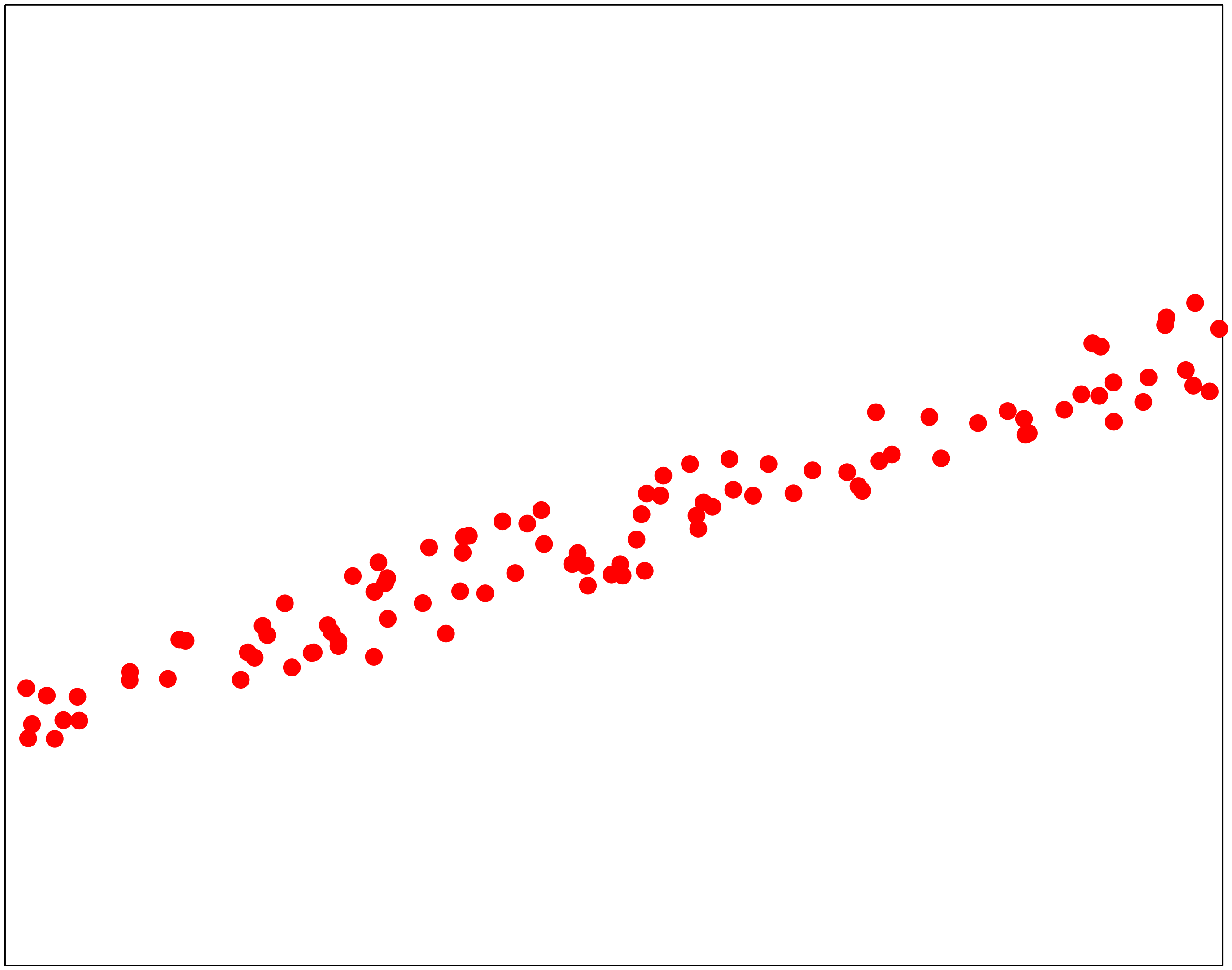
Motivation for dimensionality reduction

- Clustering, flat or hierarchical, can group the data according to similarity, helping visualization and discovery.
- But we still cannot *plot* high-dimensional (or non-numeric) data.
- We also have to guess at the number of clusters.
- We may want to “understand” better how the data was generated or how “variable” it is
- Dimensionality reduction (or embedding) techniques:
  - Assign instances to new coordinates, in a space that is much smaller-dimensional (even 2D or 3D for visualization).
  - Approximately preserve similarity/distance relationships between instances.
  - Allow us to “see” distance relationships more directly.

What is dimensionality reduction?

- Mapping instances to real vectors, usually with few dimensions
- Possible uses:
  - Visualization, comparison
  - Outlier detection
  - Further machine learning
- Some techniques:
  - Principal components analysis (linear)
  - Independent components analysis (linear or nonlinear)
  - Self-organizing maps (nonlinear)
  - Multi-dimensional scaling (nonlinear, allows non-numeric data objects)

What is the true dimensionality of this data?



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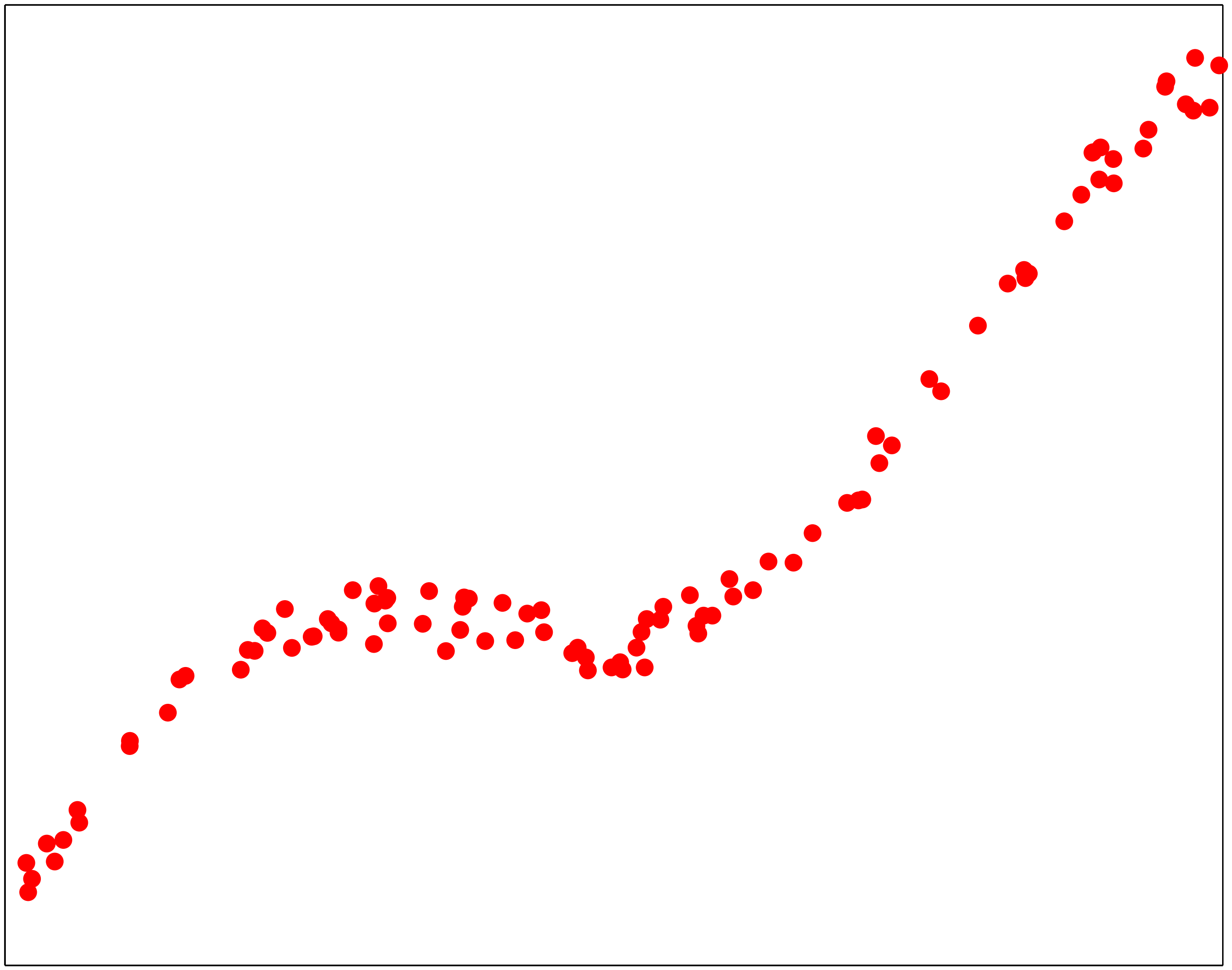

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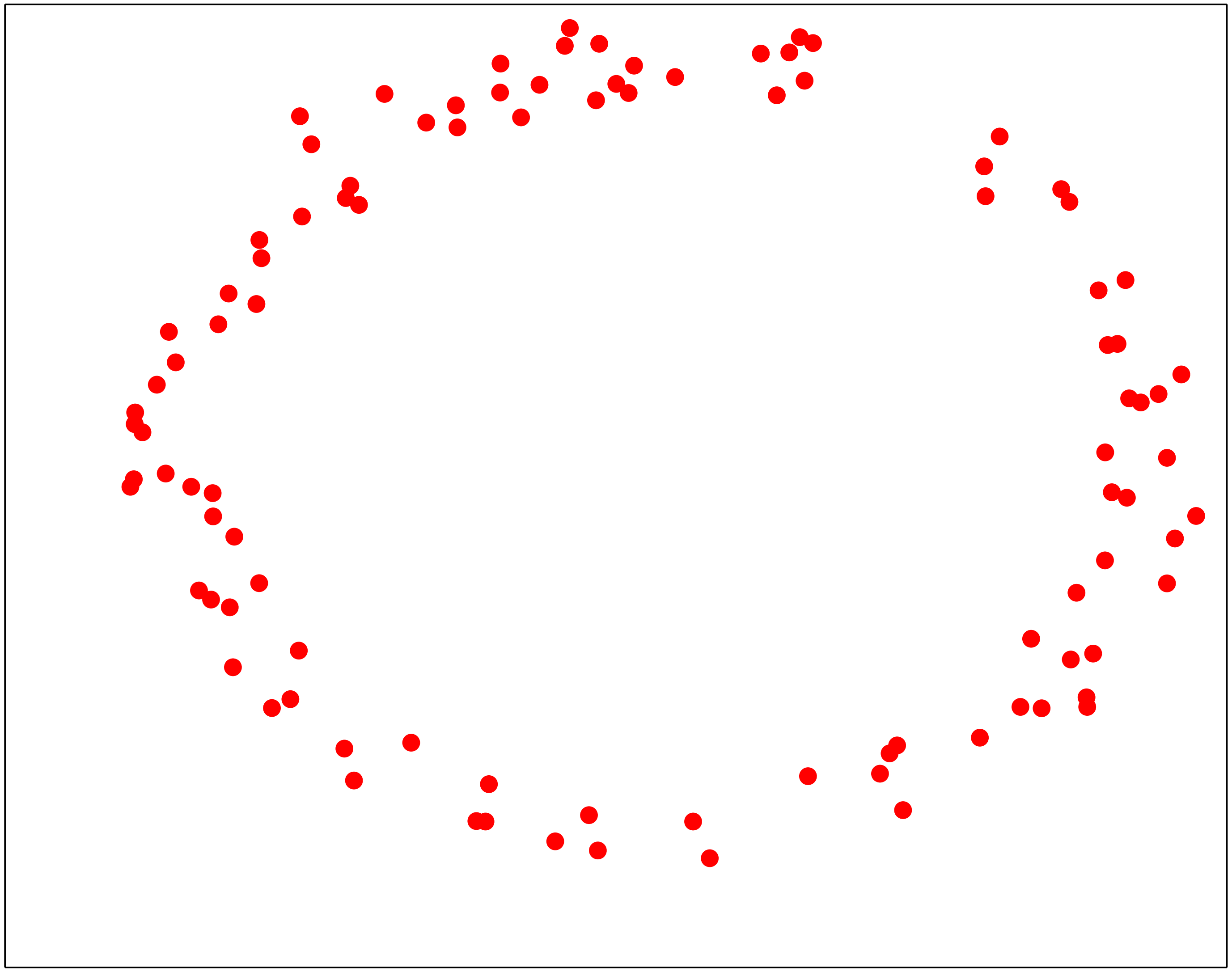

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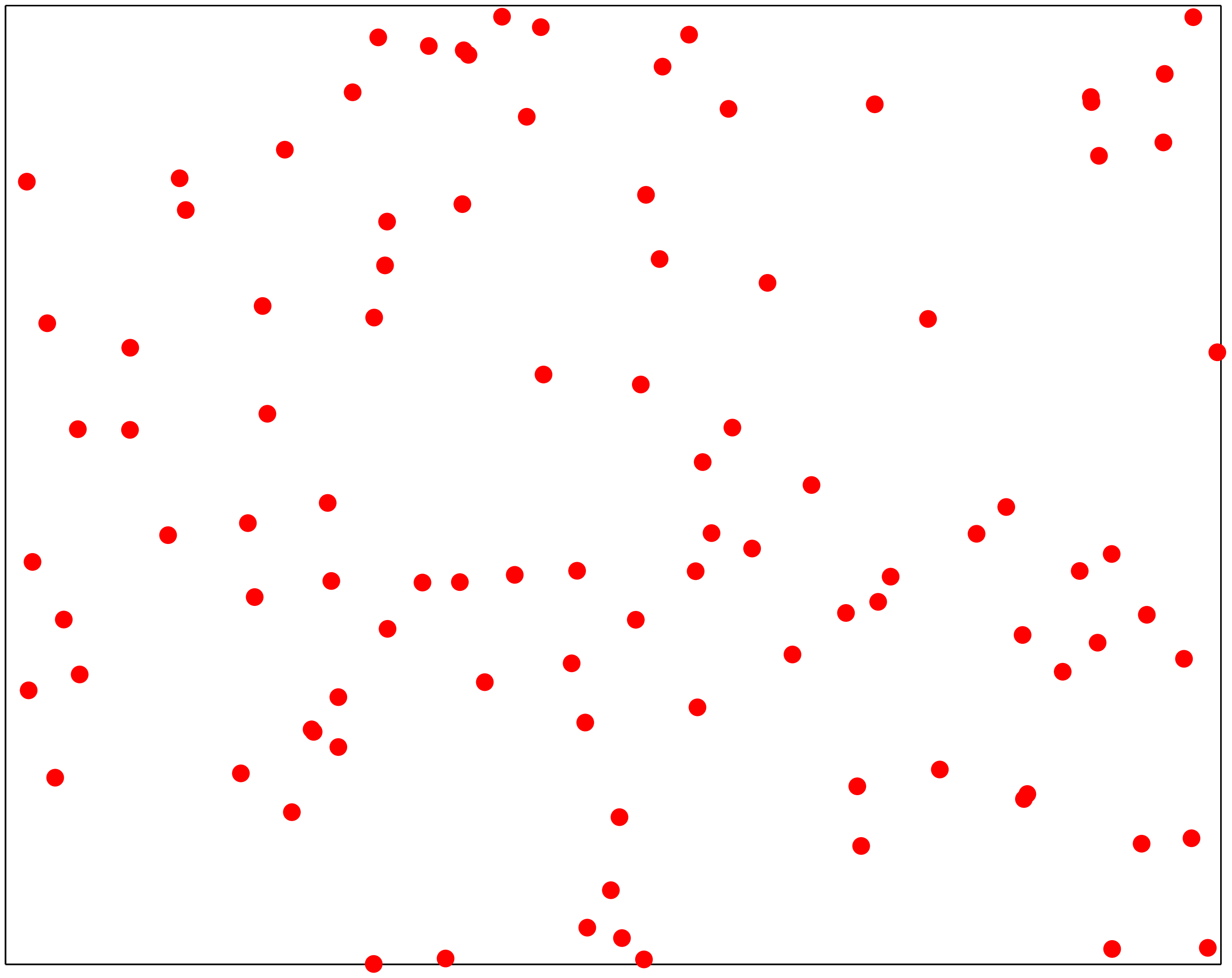


Remarks

- All dimensionality reduction techniques are based on an implicit assumption that the data lies along some *low-dimensional manifold*
- This is the case for the first three examples, despite being plotted in 2D
- In the last example, the data has been generated randomly in 2D, so no dimensionality reduction is possible without losing information
- The first three cases are in increasing order of difficulty, from the point of view of existing techniques.

Self-organizing maps

- Assume the data objects are real vectors of length n.
- Try to stretch a “grid” of points in n-dimensional space to approximate the data.
- The indices of the grid points indicate *neighborhood* relationships
- E.g., in 2D, $G(i, j)$ is neighbor with $G(i - 1, j)$, $G(i + 1, j)$, $G(i, j - 1)$, $G(i, j + 1)$.
- The grid points are iteratively moved, ”pulled”, by data points, similar to how the centroids of K-means clustering move around.
- The data can then be visualized by mapping each object to the nearest grid point.

Self-organizing maps

- Inputs:
  - A set $D = \{\mathbf{x_1}, \ldots, \mathbf{x_m}\}$ of n-dimensional real vectors.
  - A dimension for the grid (1,2 or 3 if we want to plot it.)
  - Number of grid points along each dimension.
- Output: Coordinates G in $\Re^n$ for each grid-point.

  E.g., for the 2D grid case, $G(i, j) \in \Re^n$ specifies the coordinates of grid-point (i, j).

SOM learning algorithm

- Initialize the grid points.
- Repeat
  - Choose a data point $\mathbf{x}$ at random.
  - Find the nearest grid point; e.g., in 2D:

$$\mathbf{G}^* = G(i^*, j^*) = \arg\min_{i,j} \|G(i,j) - \mathbf{x}\|$$

  - Find the "neighborhood" of $\mathbf{G}^*$
  - Move all points $\mathbf{G}$ in the neighborhood towards $\mathbf{x}$:

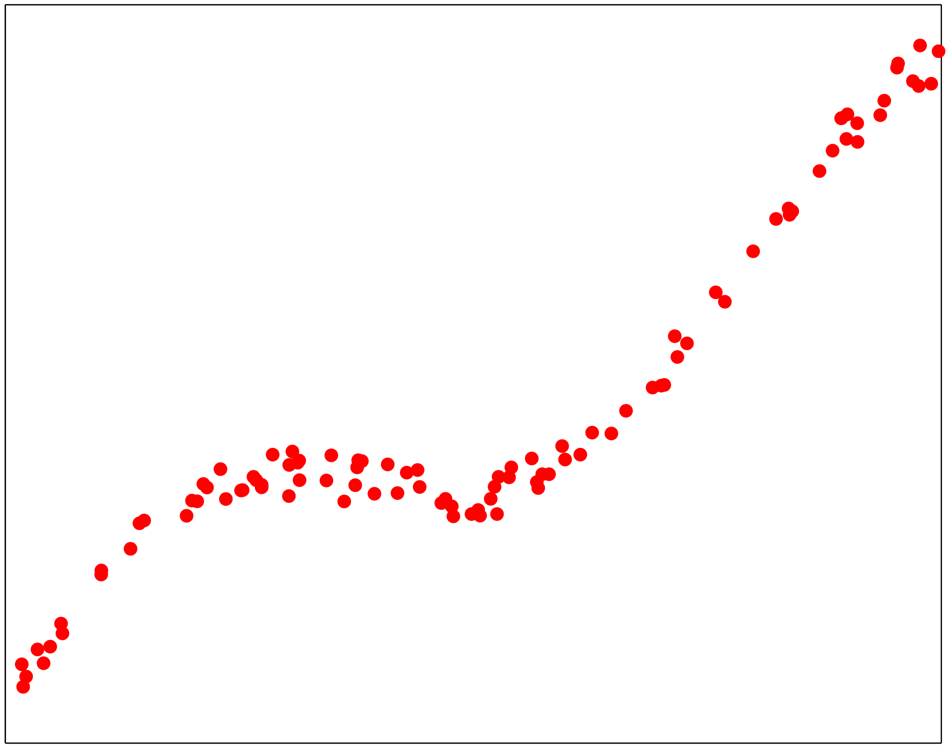
$$\mathbf{G} \leftarrow \mathbf{G} + \alpha e(\mathbf{x}, \mathbf{G})(\mathbf{x} - \mathbf{G})$$

    where $e(\mathbf{x}, \mathbf{G})$ is a similarity function, equal to 1 if $\mathbf{x} = \mathbf{G}$ and decreasing with $|\mathbf{x} - \mathbf{G}|$ (e.g. Gaussian)

Remarks

- DHS has nice pictures of SOMs at work
- Typically the learning rate $\alpha \to 0$ with time
- The SOM builds a *topographical map* of the input space, putting more points where the data is dense
- Instances that are close in the input space will be mapped to units which are neighbors in the grid.
- If the data approximately lies on a curve or surface, the SOM may capture that structure, but:
  - Different runs can find different solutions.
  - If we try to fit data on a 2D surface with a 1D grid, well...
- More sophisticated versions of SOMs use different updating rules, different neighboring functions

Back to the example

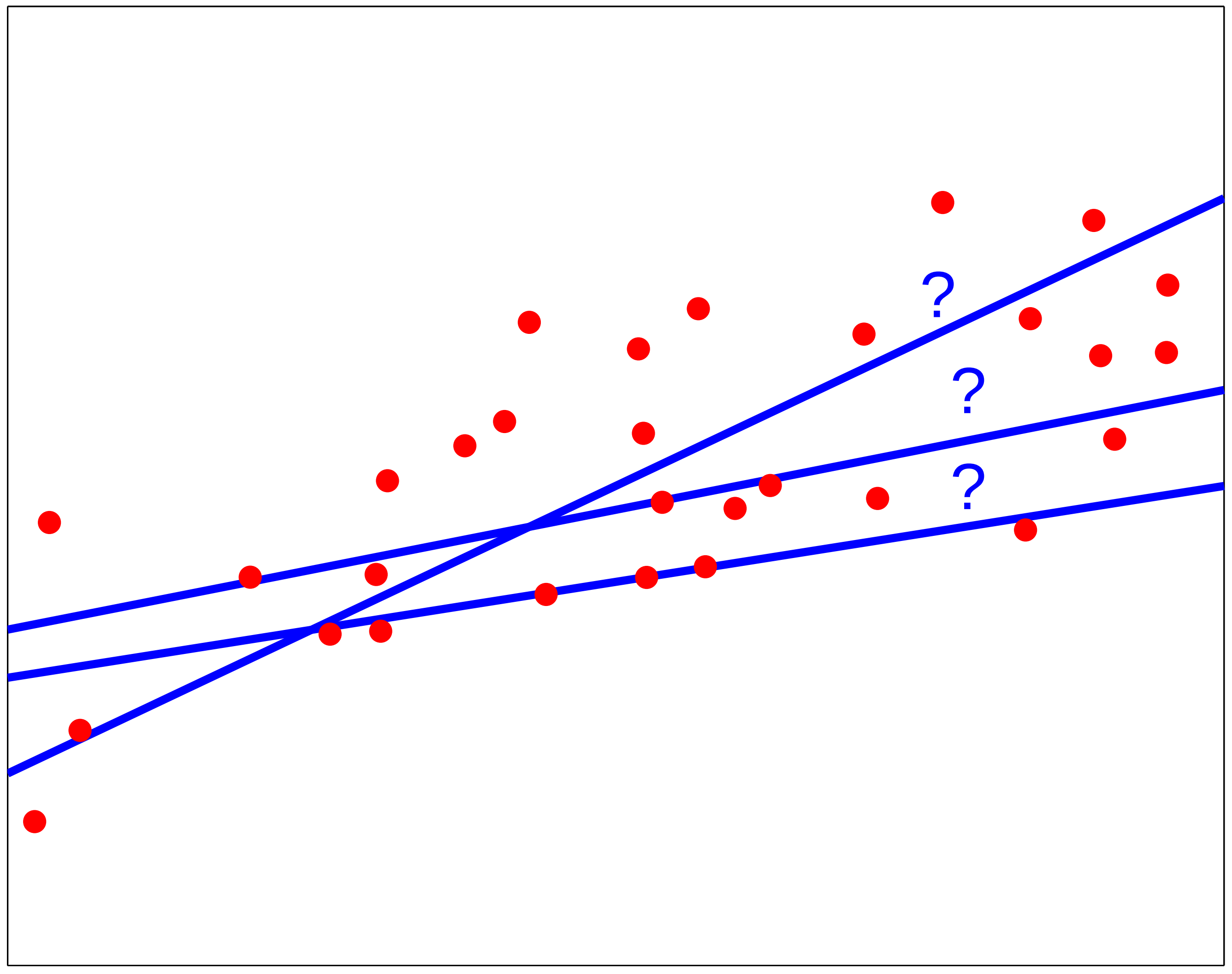


- SOMs will put units along the curve, where the data lies
- But there are other interesting things about this data!
- Can we find a good model for it?

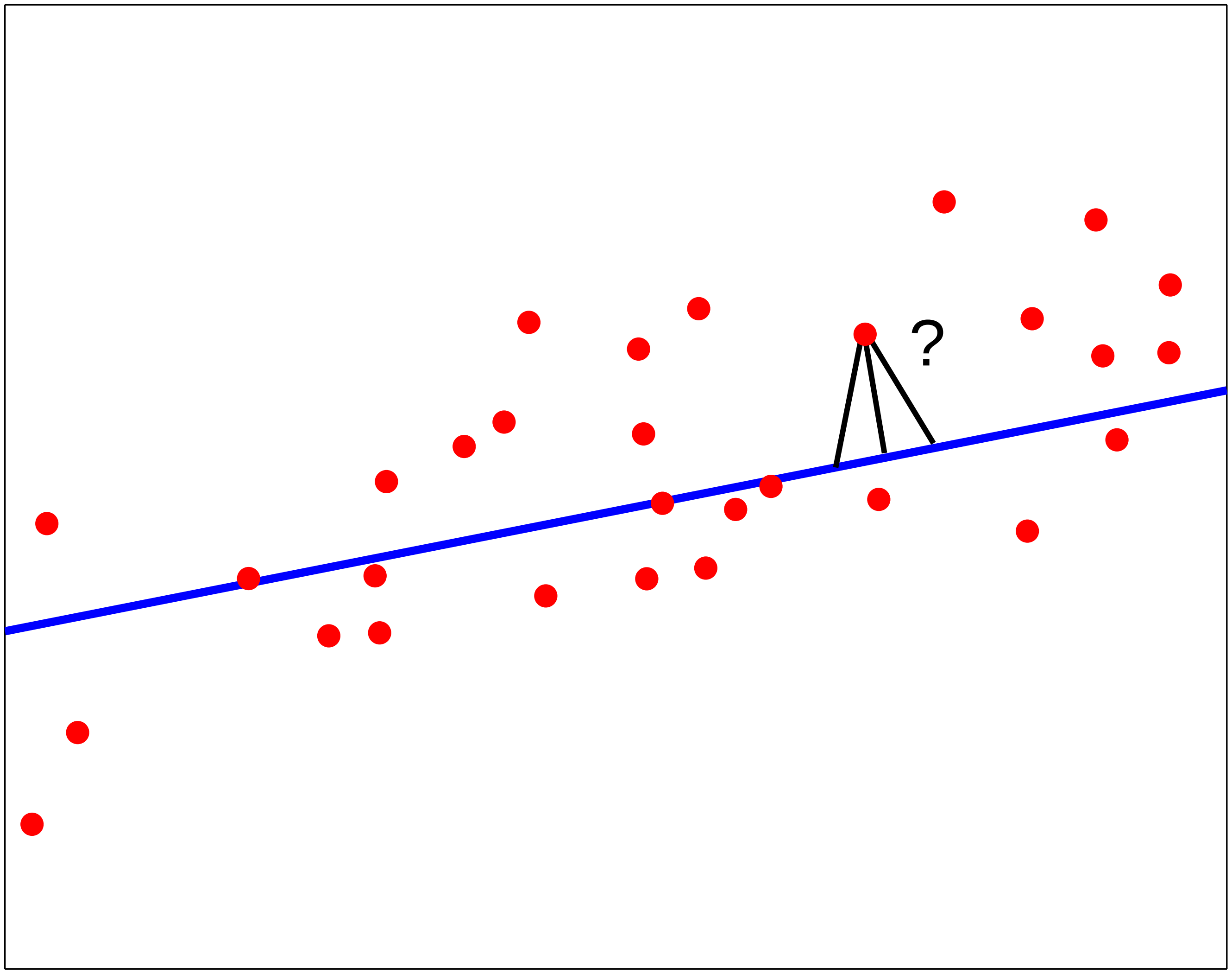
Simple Principal Component Analysis (PCA)

- Given: m data objects, each a length-n real vector.
- Suppose we want a 1-dimensional representation of that data, instead of n-dimensional.
- Specifically, we will:
  - Choose a line in $\Re^n$ that “best represents” the data.
  - Assign each data object to a point along that line.

Which line is best?



How do we assign points to lines?



Recall a useful tool: Covariance

- Covariance quantifies a linear relationship (if any) between two random variables X and Y.

$$Cov(X,Y) = E\{(X - E(X))(Y - E(Y))\}$$

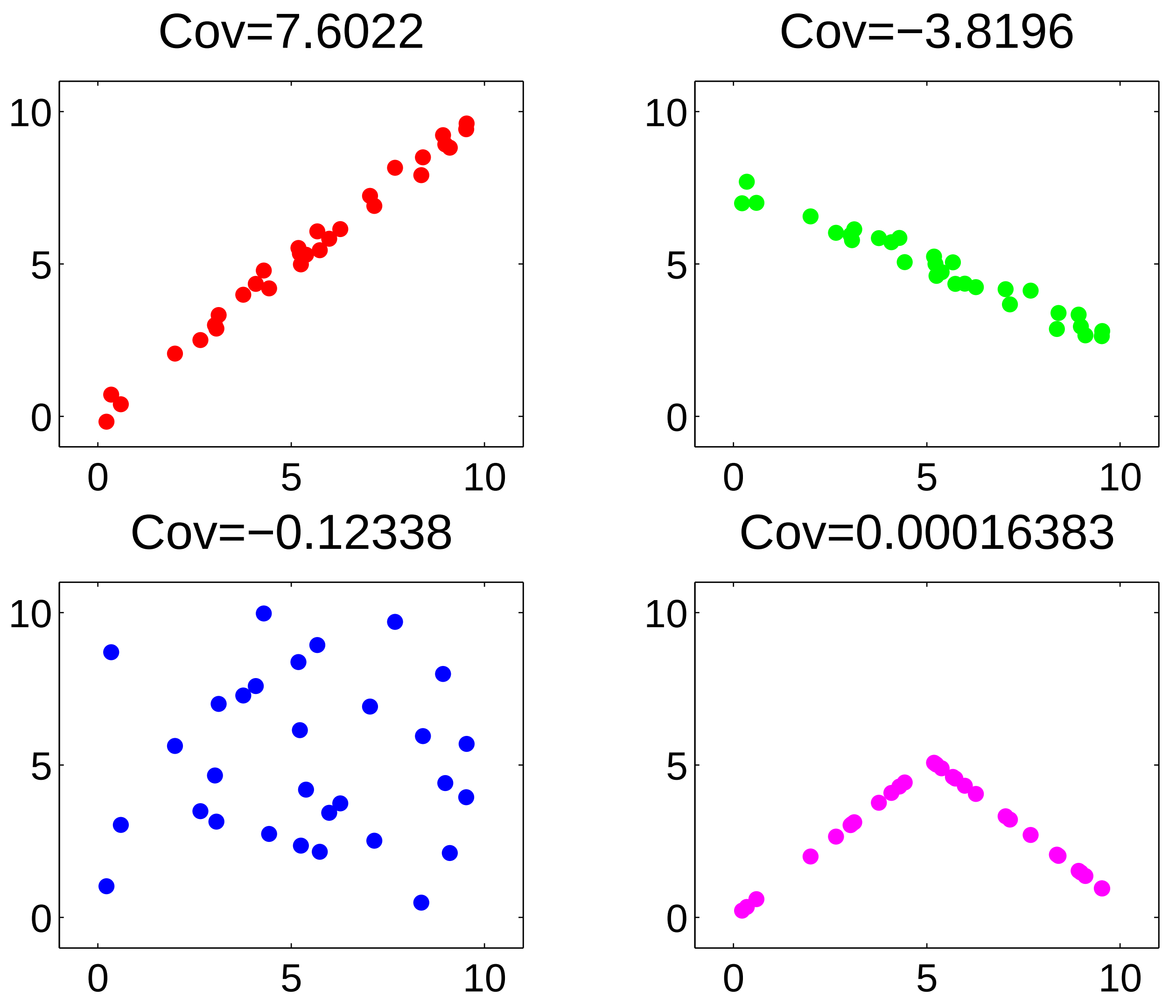
- Given m samples of X and Y, covariance can be estimated as

$$\frac{1}{m-1}\sum_{i=1}^{m}(x_i - \mu_X)(y_i - \mu_Y) \ ,$$

where $\mu_X = \sum_{i=1}^{m} x_i$ and $\mu_Y = \sum_{i=1}^{m} y_i$.

- Note: $Cov(X,X) = Var(X)$.

Examples



Reconstruction error

- Let our line be represented as $\mathbf{b} + \alpha\mathbf{v}$ for $\mathbf{b}, \mathbf{v} \in \Re^n$, $\alpha \in \Re$. For later convenience, assume $\|\mathbf{v}\| = 1$.
- Each instance $\mathbf{x}_i$ is assigned a point on the line $\hat{\mathbf{x}}_i = \mathbf{b} + \alpha_i\mathbf{v}$.
- The (squared Euclidean) reconstruction error for instance i is

$$\|\mathbf{x}_i - \hat{\mathbf{x}}_i\|^2 = \sum_{j=1}^{n} (\mathbf{x}_i(j) - \hat{\mathbf{x}}_i(j))^2$$

- We want to choose $\mathbf{b}$, $\mathbf{v}$, and the α_i to minimize the total reconstruction error over all data points:

$$R = \sum_{i=1}^{m} \|\mathbf{x}_i - \hat{\mathbf{x}}_i\|^2$$

A constrained optimization problem!

$$\begin{array}{rl} \text{min} & \|\mathbf{x}_i - (\mathbf{b} + \alpha_i \mathbf{v})\|^2 \\ \text{w.r.t.} & \mathbf{b}, \mathbf{v}, \alpha_i, i = 1, \ldots n \\ \text{s.t.} & \|v\|^2 = 1 \end{array}$$

We can write down the Lagrangian and try to solve directly, but this gets a bit difficult... (see homework 7)

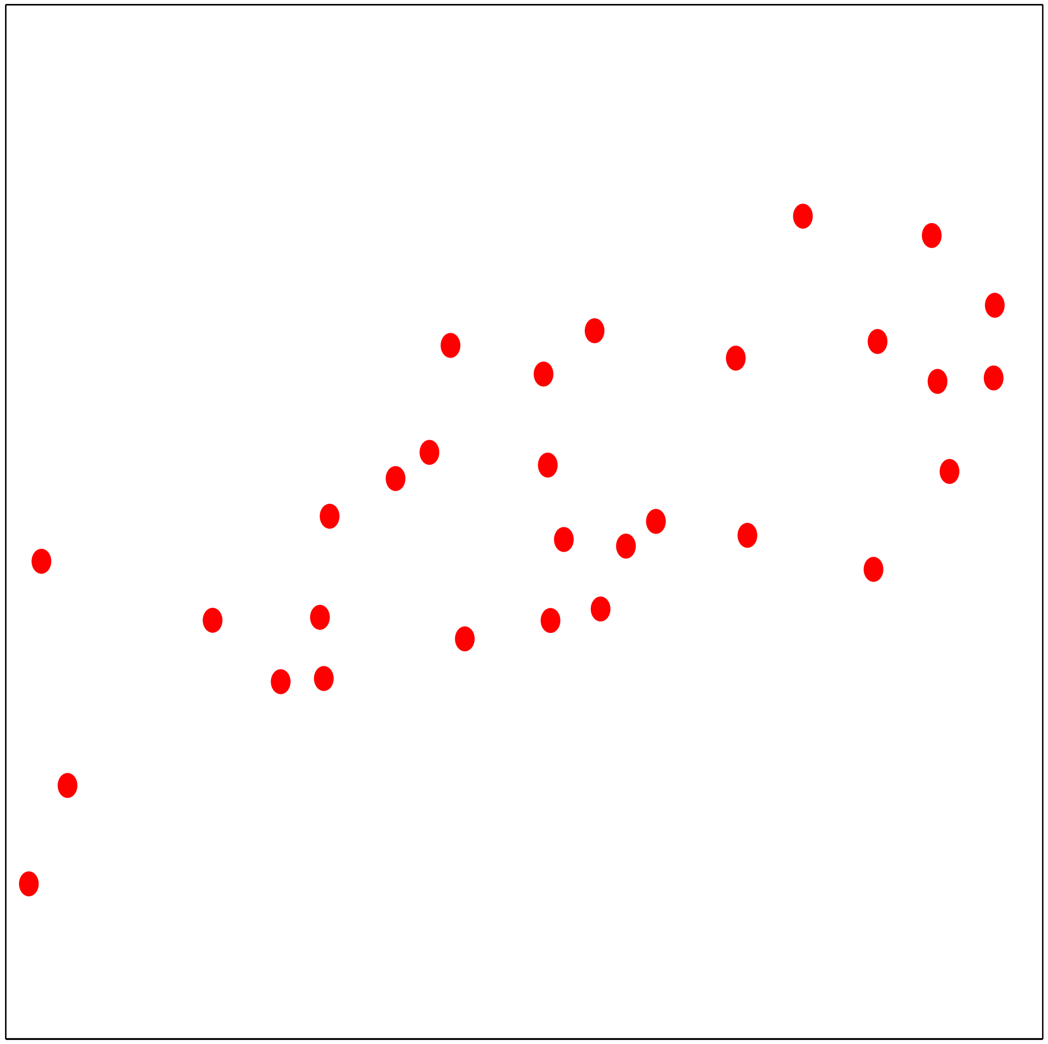
Minimizing reconstruction error: b and the α_i

- Suppose we fix $\mathbf{v}$. Now we have an unconstrained optimization problem!
- By taking the gradient of the reconstruction error and setting it to 0 we get that an optimal choice for $\mathbf{b}$ is

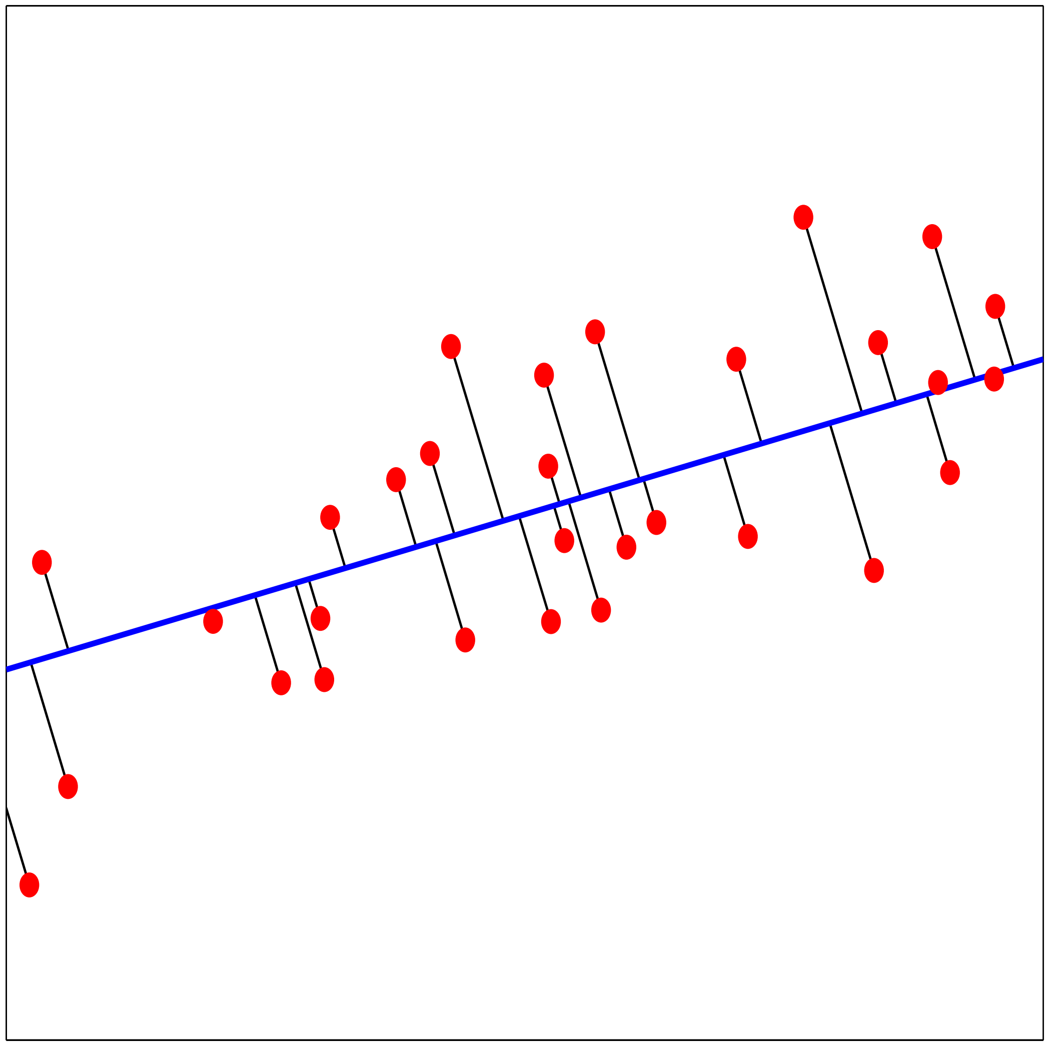
$$\mathbf{b} = \frac{1}{m}\sum_{i=1}^{m}\mathbf{x}_i ,$$

- From this, we get $\alpha_i = \mathbf{v}\cdot(\mathbf{x}_i - \mathbf{b})$
- By substituting, we get: $\hat{\mathbf{x}}_i = \mathbf{b} + \mathbf{v}\cdot(\mathbf{x}_i - \mathbf{b})$.
- Intuitively:
  - The line goes through the centroid of the data.
  - Instances are projected orthogonally on the line to get the associated point.

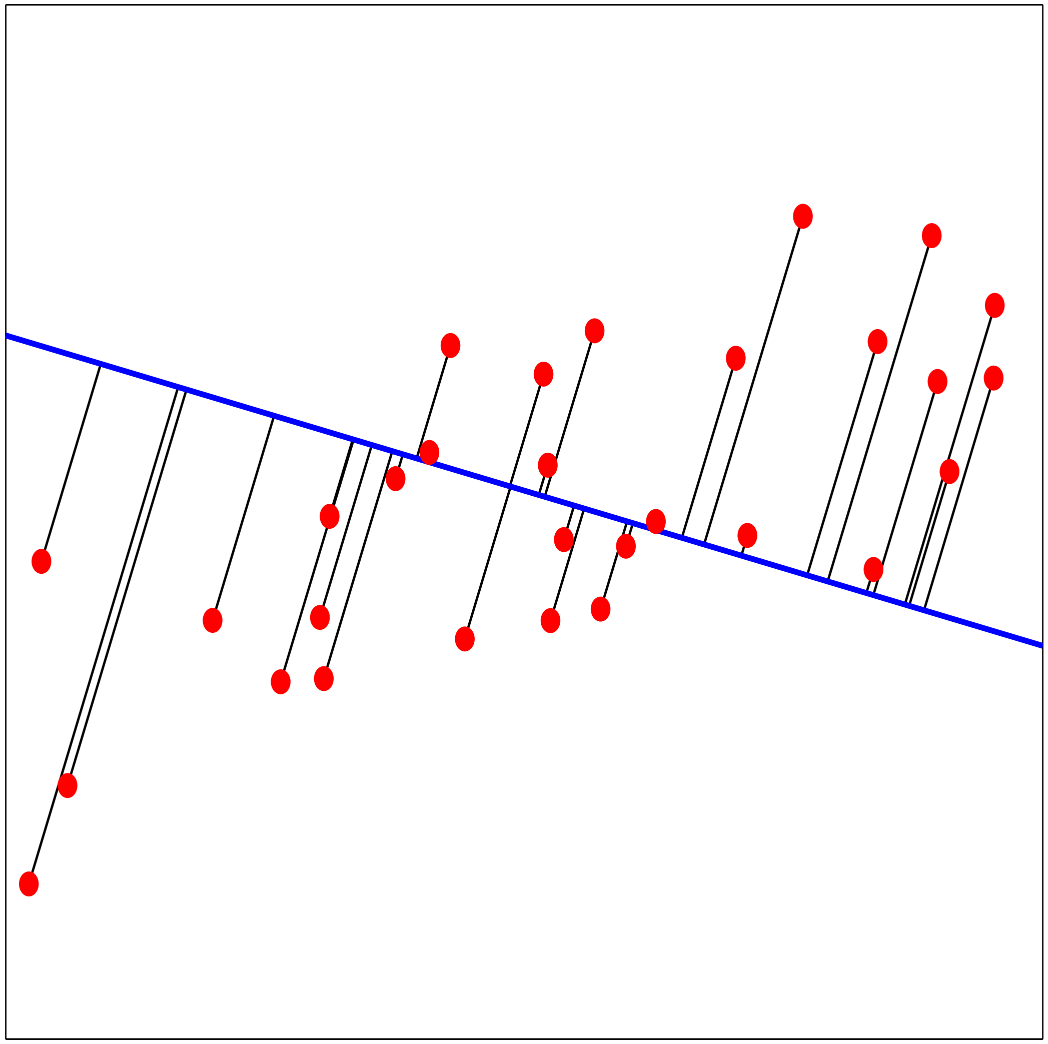
Example data



Example with $\mathbf{v} \propto (1, 0.3)$



Example with $\mathbf{v} \propto (1, -0.3)$



Minimizing reconstruction error: the scatter matrix

- Substituting back into the formula for the reconstruction error, we get that $\mathbf{v}$ should maximize

$$\mathbf{v}^T S \mathbf{v} \ ,$$

where S is an $n \times n$ matrix with

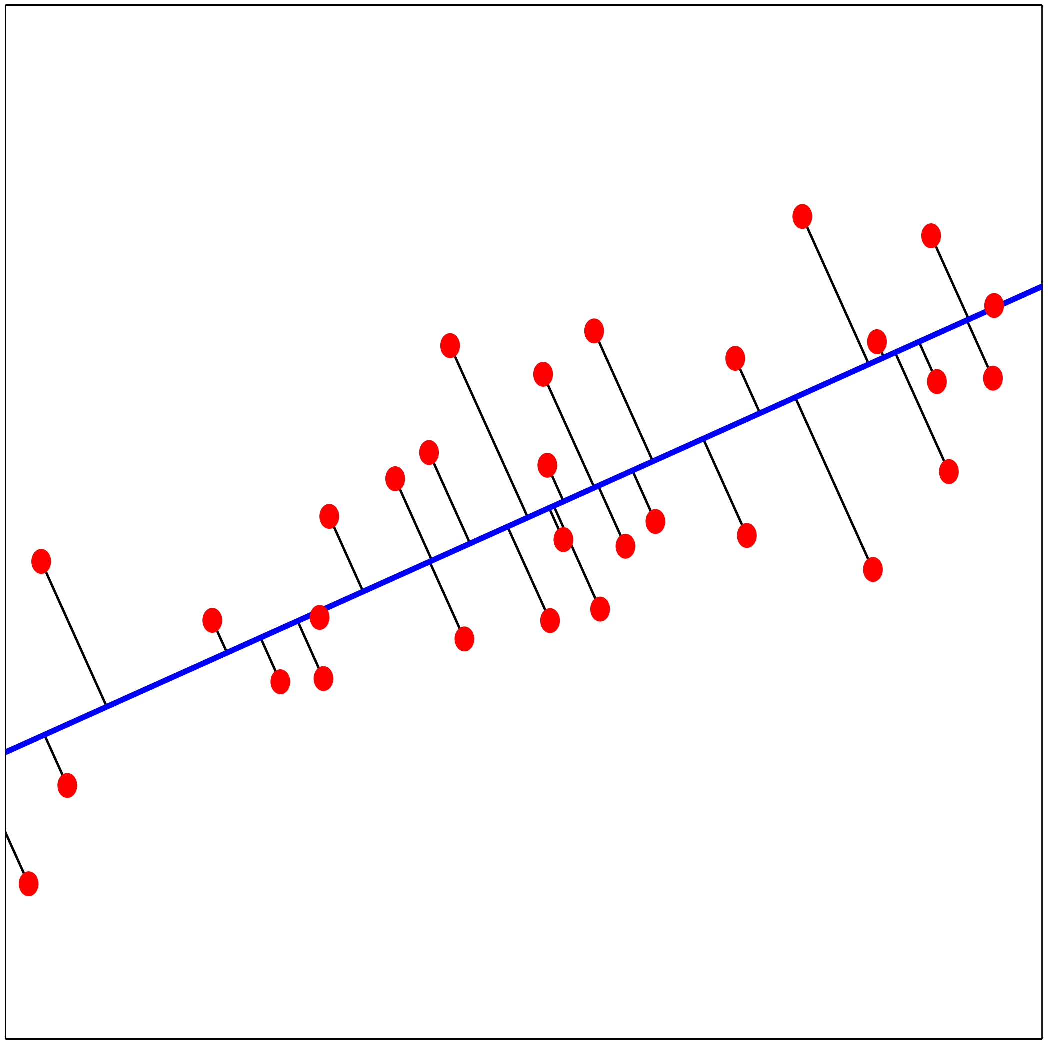
$$S(k,l) = \sum_{i=1}^{m} (\mathbf{x}_i(k) - \mathbf{b}(k))(\mathbf{x}_i(l) - \mathbf{b}(l))$$

- Note that $S(k,l)$ is proportional to the estimated covariance between the kth and lth dimension in the data.
- S is called the **scatter matrix**.

Optimal choice of $\mathbf{v}$

- Recall: an **eigenvector** $\mathbf{u}$ of a matrix A satisfies $A\mathbf{u} = \lambda\mathbf{u}$, where $\lambda \in \Re$ is the **eigenvalue**.
- Fact: the scatter matrix, S, has n non-negative eigenvalues and n orthogonal eigenvectors.
- The $\mathbf{v}$ that maximizes $\mathbf{v}^T S\mathbf{v}$ is the eigenvector of S with the largest eigenvalue (homework 7)

Example with optimal line: $\mathbf{b} = (0.54, 0.52)$, $\mathbf{v} \propto (1, 0.45)$



Remarks

- The line $\mathbf{b} + \alpha\mathbf{v}$ is the **first principal component**.
- The variance of the data along the line $\mathbf{b} + \alpha\mathbf{v}$ is as large as along any other line.
- $\mathbf{b}$, $\mathbf{v}$, and the α_i can be computed easily in polynomial time.

Reduction to d dimensions

- More generally, we can create a d-dimensional representation of our data by projecting the instances onto a hyperplane $bfb + \alpha^1 \mathbf{v}_1 + \ldots + \alpha^d \mathbf{v}_d$.
- If we assume the $\mathbf{v}_j$ are of unit length and orthogonal, then the optimal choices are:
  - $\mathbf{b}$ is the mean of the data (as before)
  - The $\mathbf{v}_j$ are orthogonal eigenvectors of S corresponding to its d largest eigenvalues.
  - Each instance is projected orthogonally on the hyperplane.

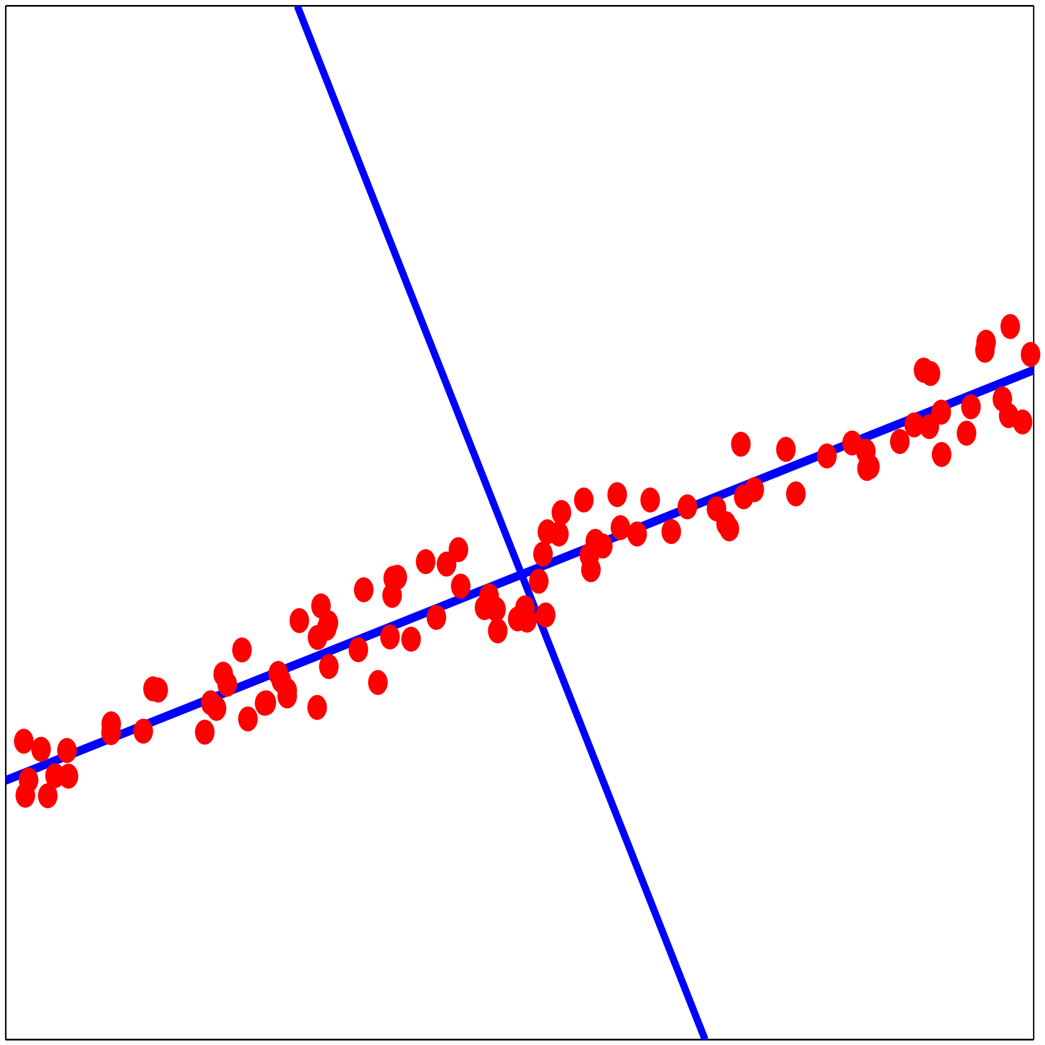
Remarks

- $\mathbf{b}$, the eigenvalues, the $\mathbf{v}_j$, and the projections of the instances can all be computing in polynomial time.
- The magnitude of the j^{th}-largest eigenvalue, λ_j, tells you how much variability in the data is captured by the j^{th} principal component
- So you have feedback on how to choose d!
- When the eigenvalues are sorted in decreasing order, the proportion of the variance captured by the first d components is:

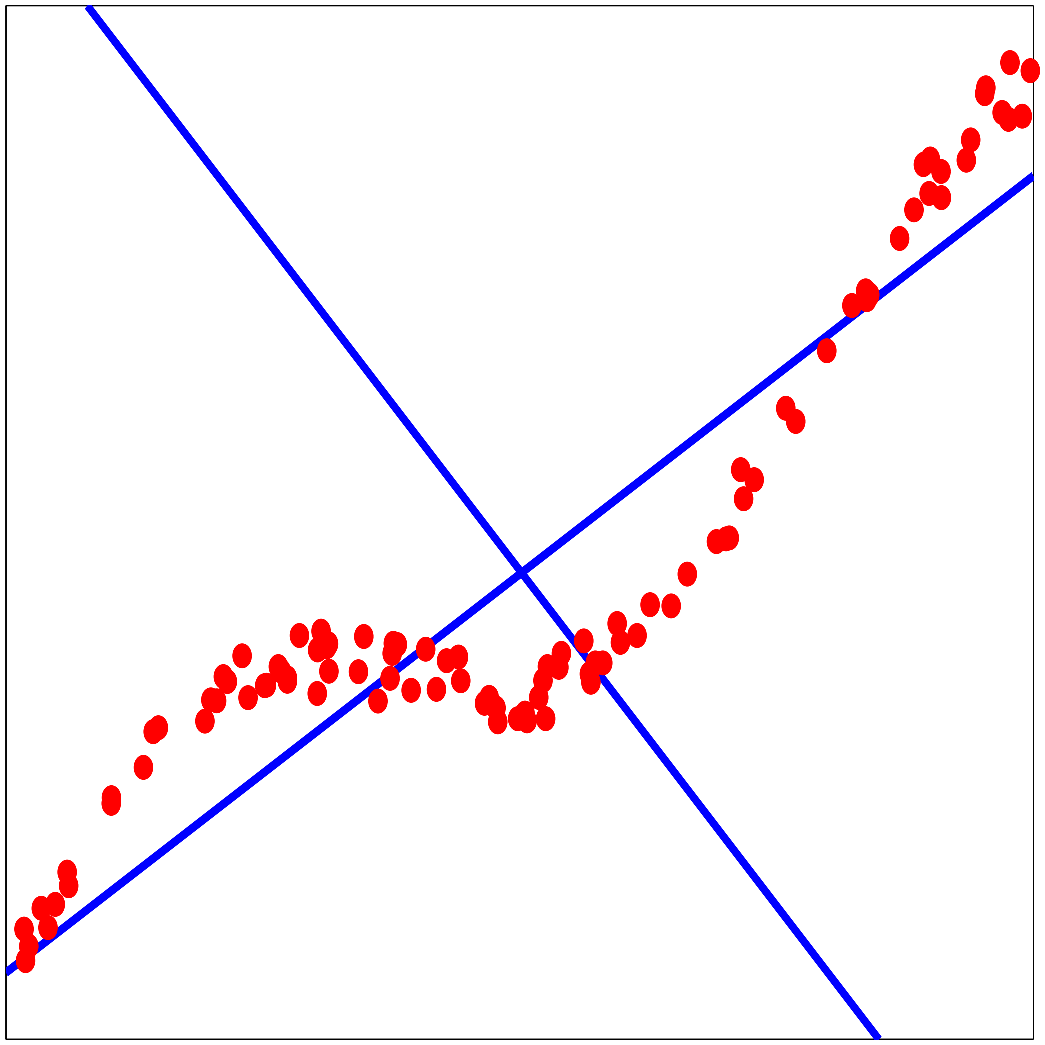
$$\frac{\lambda_1 + \cdots + \lambda_d}{\lambda_1 + \cdots + \lambda_d + \lambda_{d+1} + \cdots + \lambda_n}$$

- So if a “big” drop occurs in the eigenvalues at some point, that suggests a good dimension cutoff

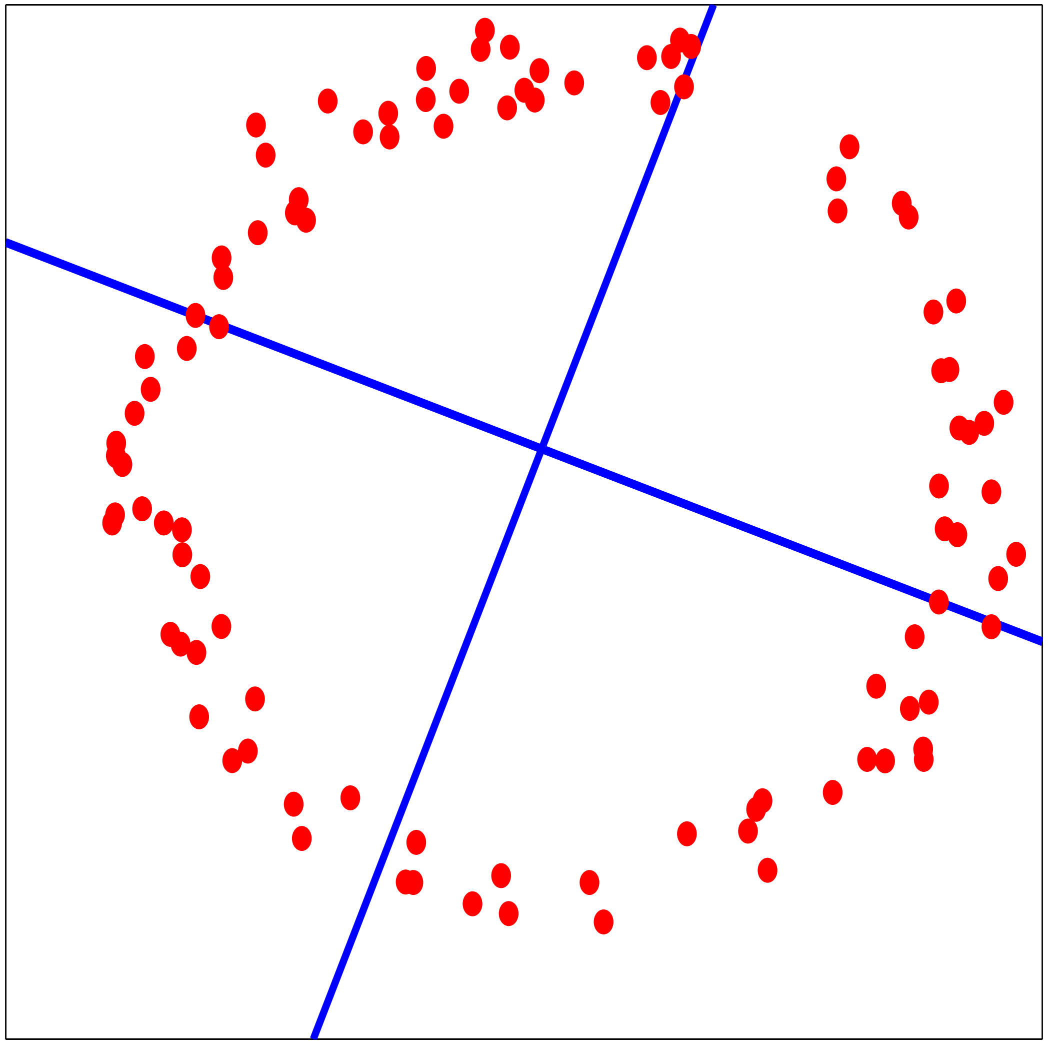
Example: $\lambda_1 = 0.0938, \lambda_2 = 0.0007$



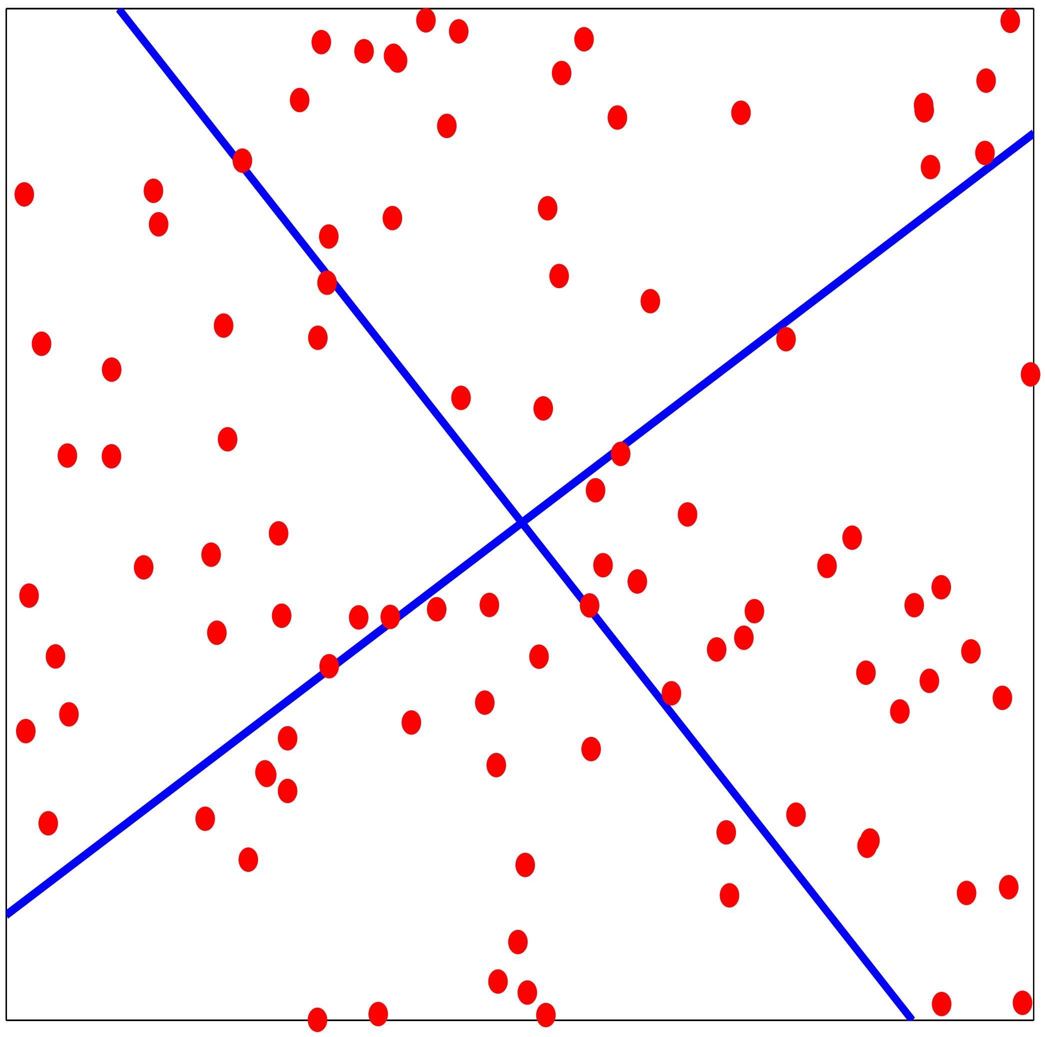
Example: $\lambda_1 = 0.1260, \lambda_2 = 0.0054$



Example: $\lambda_1 = 0.0884, \lambda_2 = 0.0725$



Example: $\lambda_1 = 0.0881, \lambda_2 = 0.0769$



More remarks

- Outliers have a big effect on the covariance matrix, so they can affect the eignevectors quite a bit
- A simple examination of the pairwise distances between instances can help discard points that are very far away (for the purpose of PCA)
- If the variances in the original dimensions vary considerably, they can “muddle” the true correlations. There are two solutions:
  - work with the correlation of the original data, instead of covariance matrix
  - normalize the input dimensions individually before PCA
- In certain cases, the eigenvectors are meaningful; e.g. in vision, they can be displayed as images (“eigenfaces”)

Uses of PCA

- Pre-processing for a supervised learning algorithm, e.g. for image data, robotic sensor data
- Used with great success in image and speech processing
- Visualization
- Exploratory data analysis
- Removing the linear component of a signal (before fancier non-linear models are applied)