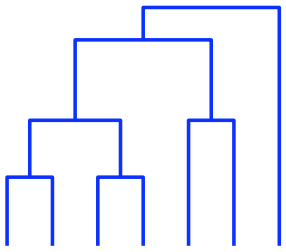
Lecture 20: Hierarchical Clustering. Dimensionality Reduction (I)

- Hierarchical clustering methods
- Overview of dimensionality reduction
- Principal component analysis

Hierarchical clustering

- Organizes data instances into trees.
- For visualization, exploratory data analysis.
- **Agglomerative methods** build the tree bottom-up, successively grouping together the clusters deemed most similar.
- **Divisive methods** build the tree top-down, recursively partitioning the data.



What is a hierarchical clustering?

- Given instances $D = \{\mathbf{x}_1, \ldots, \mathbf{x}_m\}$.
- A hierarchical clustering is a set of subsets (clusters) of D, $C = \{C_1, \ldots, C_K\}$, where
  - Every element in D is in at least one set of C
  - The C_j can be assigned to the nodes of a tree such that the cluster at any node is precisely the union of the clusters at the node's children (if any).

Example of a hierarchical clustering

- Suppose $D = \{1, 2, 3, 4, 5, 6, 7\}$.
- One hierarchical clustering is $C = \{\{1\}, \{2, 3\}, \{4, 5\}, \{1, 2, 3, 4, 5\}, \{6, 7\}, \{1, 2, 3, 4, 5, 6, 7\}\}$.
- In this example:
  - Leaves of the tree need not correspond to single instances.
  - The branching factor of the tree is not limited.
- However, most hierarchical clustering algorithms produce binary trees, and take single instances as the smallest clusters.

Agglomerative clustering

- Input: A set of instances and pairwise distances $d(\mathbf{x}, \mathbf{x}')$ between them.
- Output: A hierarchical clustering
- Algorithm:
  - Assign each instance as its own cluster on a working list W.
  - Repeat
    - Find the two clusters in W that are most "similar".
    - Remove them from W.
    - Add their union to W.

    Until W contains a single cluster with all the data objects.
  - The hierarchical clustering contains *all* clusters appearing in W at any stage of the algorithm.

How do we measure dissimilarity between clusters?

- Distance between nearest objects ("Single-linkage" agglomerative clustering, or "nearest neighbor"):

$$\min_{\mathbf{x} \in C, \mathbf{x}' \in C'} d(\mathbf{x}, \mathbf{x}')$$

- Distance between farthest objects ("Complete-linkage" agglomerative clustering, or "furthest neighbor"):

$$\max_{\mathbf{x} \in C, \mathbf{x}' \in C'} d(\mathbf{x}, \mathbf{x}')$$

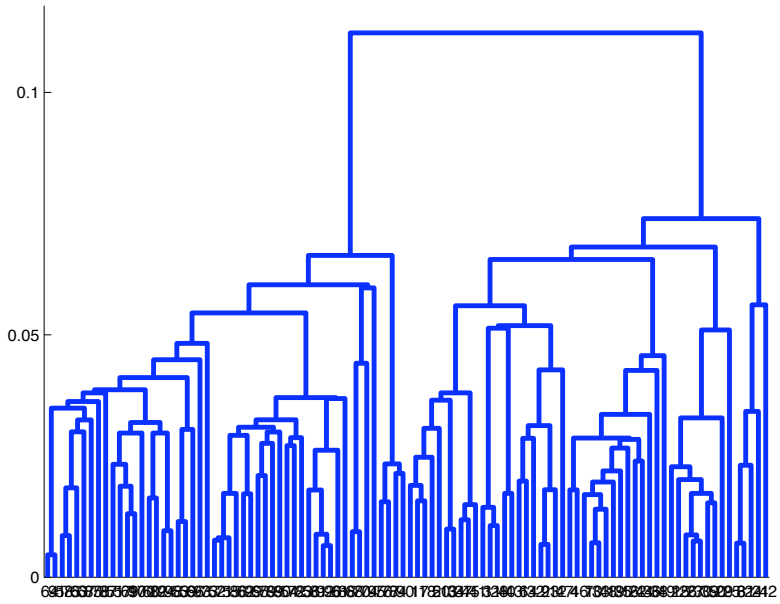
- Average distance between objects ("Group-average" agglomerative clustering):

$$\frac{1}{|C||C'|} \sum_{\mathbf{x} \in C, \mathbf{x}' \in C'} d(\mathbf{x}, \mathbf{x}')$$

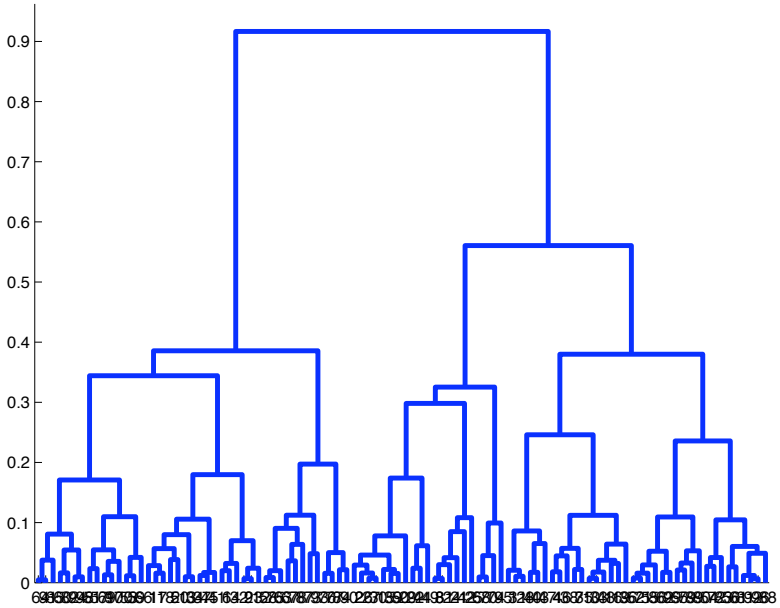
Dendrograms and monotonicity

- Single-linkage, complete-linkage and group-average dissimilarity measure all share a monotonicity property:
  - Let A, B, C be clusters.
  - Let d be one of the dissimilarity measures.
  - If $d(A, B) < d(A, C)$ and $d(A, B) < d(B, C)$, then $d(A, B) < d(A \cup B, C)$.
- Implication: every time agglomerative clustering merges two clusters, the dissimilarity of those clusters is $\geq$ the dissimilarity of all previous merges.
- Dendrograms (trees depicting hierarchical clusterings) are often drawn so that the height of a node corresponds to the dissimilarity of the merged clusters.

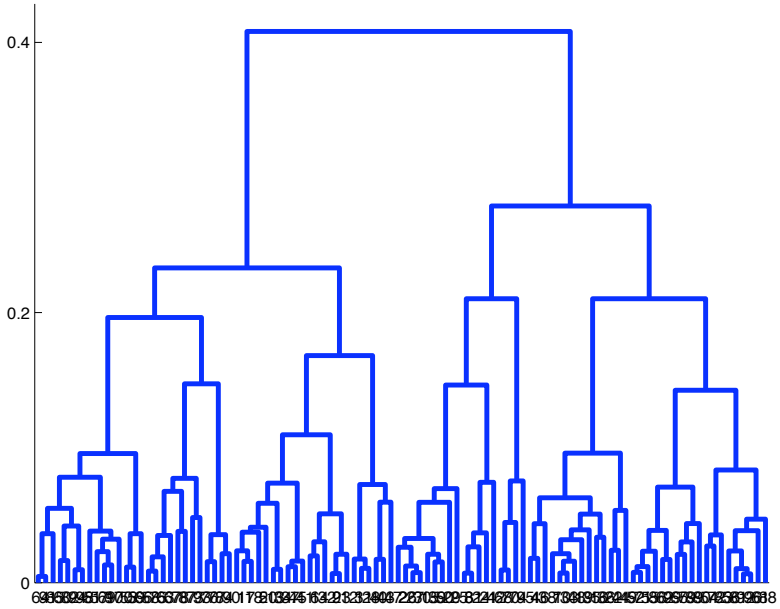
Example: Dendrogram for single-linkage clustering



Example: Dendrogram for complete-linkage clustering



Example: Dendrogram for average-linkage clustering



Remarks

- We can form a flat clustering by cutting the tree at any height.
- Jumps in the height of the dendrogram can suggest natural cutoffs.

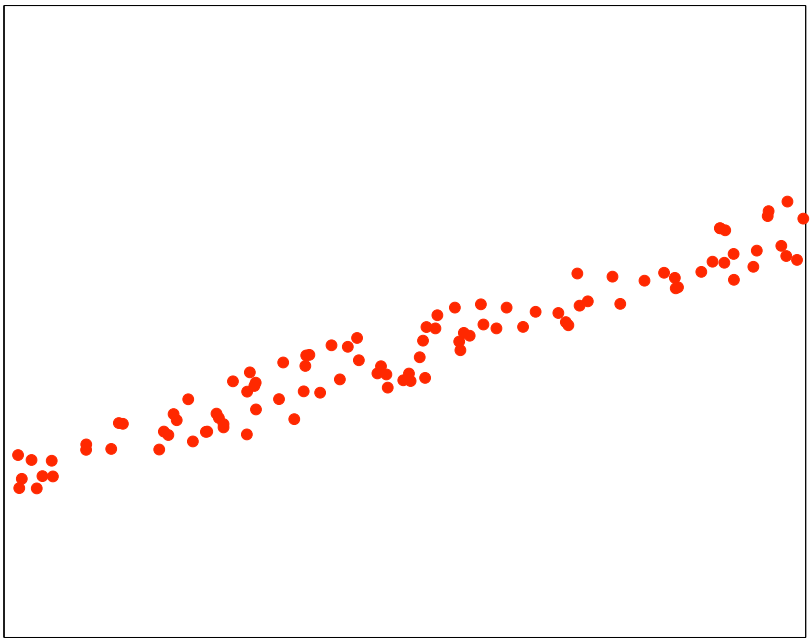
Divisive clustering

- Works by recursively partitioning the instances.
- But dividing such as to optimize one of the agglomerative criteria is computationally hard!
- Many heuristics for partitioning the instances have been proposed . . . but many violate monotonicity, making it hard to draw dendrograms.

What is dimensionality reduction?

- Dimensionality reduction (or embedding) techniques:
  - Assign instances to real-valued vectors, in a space that is much smaller-dimensional (even 2D or 3D for visualization).
  - Approximately preserve similarity/distance relationships between instances.
- Some techniques:
  - Linear: Principal components analysis
  - Non-linear
    - Kernel PCA
    - Independent components analysis
    - Self-organizing maps
    - Multi-dimensional scaling

What is the true dimensionality of this data?



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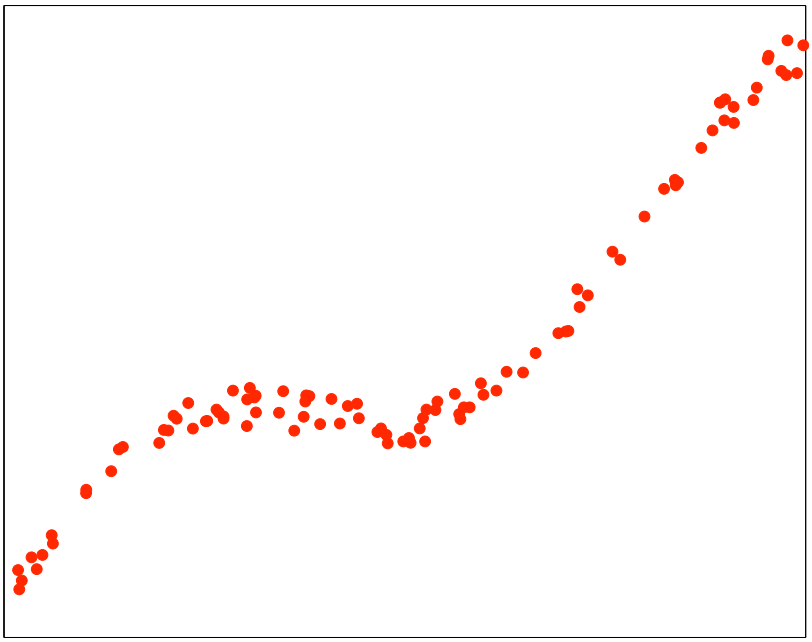

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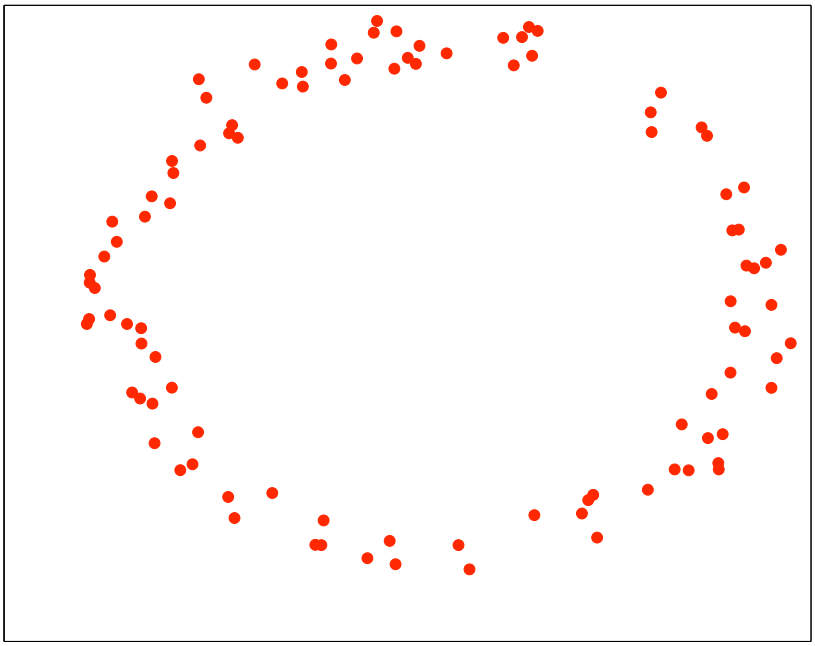

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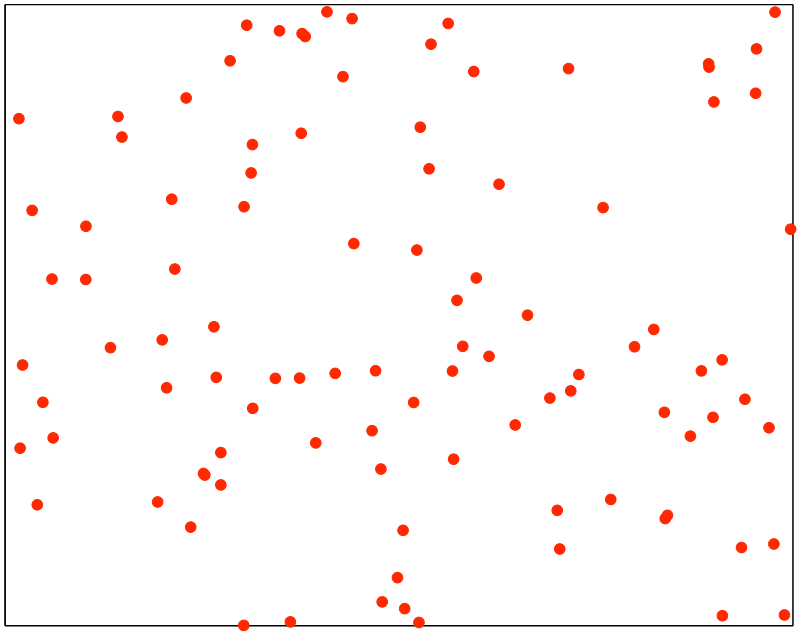


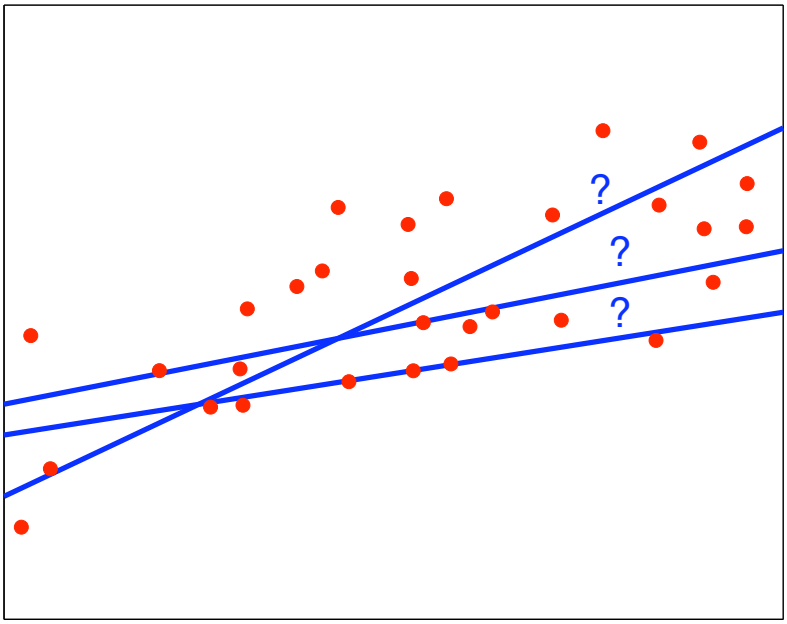
Remarks

- 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, which lie along a 1-dimensional manifold 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.

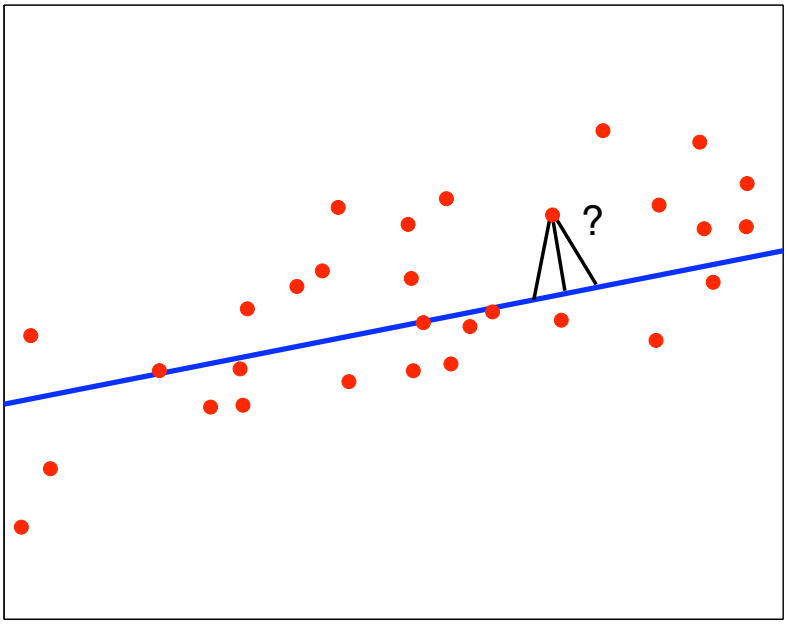
Simple Principal Component Analysis (PCA)

- 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?



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 $\hat{\mathbf{x}}_i = \mathbf{b} + \alpha_i\mathbf{v}$.
- We want to choose $\mathbf{b}$, $\mathbf{v}$, and the α_i to minimize the total reconstruction error over all data points, measured using Euclidean distance:

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

A constrained optimization problem!

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

We write down the Lagrangian (see SVM lectures):

$$\begin{aligned} L(\mathbf{b}, \mathbf{v}, \lambda, \alpha_1, \ldots \alpha_m) &= \sum_{i=1}^{m} \|\mathbf{x}_i - (\mathbf{b} + \alpha_i \mathbf{v})\|^2 + \lambda(\|\mathbf{v}\|^2 - 1) \\ &= \sum_{i=1}^{m} \|\mathbf{x}_i\|^2 + m\|\mathbf{b}\|^2 + \|\mathbf{v}\|^2 \sum_{i=1}^{m} \alpha_i^2 \\ &- 2\mathbf{b} \sum_{i=1}^{m} \mathbf{x}_i - 2\mathbf{v} \sum_{i=1}^{m} \alpha_i \mathbf{x}_i + 2\mathbf{b}\mathbf{v} \sum_{i=1}^{m} \alpha_i \\ &- \lambda\|\mathbf{v}\|^2 + \lambda \end{aligned}$$

Solving the optimization problem

- The most straightforward approach would be to write the KKT conditions and solve the resulting equations
- Unfortunately, we get equations which have multiple variables in them, and the resulting system is not linear (you can check this)
- Instead, we will fix $\mathbf{v}$.
- For a given $\mathbf{v}$, finding the best $\mathbf{b}$ and α_i is now an unconstrained optimization problem:

$$\min R = \min \sum_{i=1}^{m} \|\mathbf{x}_i - (\mathbf{b} + \alpha_i \mathbf{v})\|^2$$

Solving the optimization problem (II)

- We write the gradient of R wrt to α_i and set it to 0:

$$\frac{\partial R}{\partial \alpha_i} = 2\|\mathbf{v}\|^2\alpha_i - 2\mathbf{v}\mathbf{x}_i + 2\mathbf{b}\mathbf{v} = 0 \Rightarrow \alpha_i = \mathbf{v} \cdot (\mathbf{x}_i - \mathbf{b})$$

  where we take into account that $\|\mathbf{v}\|^2 = 1$.

- We write the gradient of R wrt $\mathbf{b}$ and set it to 0:

$$\nabla_{\mathbf{b}} R = 2m\mathbf{b} - 2\sum_{i=1}^{m}\mathbf{x}_i + 2\left(\sum_{i=1}^{m}\alpha_i\right)\mathbf{v} = 0 \qquad (1)$$

- From above:

$$\sum_{i=1}^{m}\alpha_i = \sum_{i=1}^{m}\mathbf{v}^T(\mathbf{x}_i - \mathbf{b}) = \mathbf{v}^T\left(\sum_{i=1}^{m}\mathbf{x}_i - m\mathbf{b}\right) \qquad (2)$$

Solving the optimization problem (III)

- By plugging (2) into (1) we get:

$$\mathbf{v}^T\left(\sum_{i=1}^{m}\mathbf{x}_i - m\mathbf{b}\right)\mathbf{v} = \left(\sum_{i=1}^{m}\mathbf{x}_i - m\mathbf{b}\right)$$

- This is satisfied when:

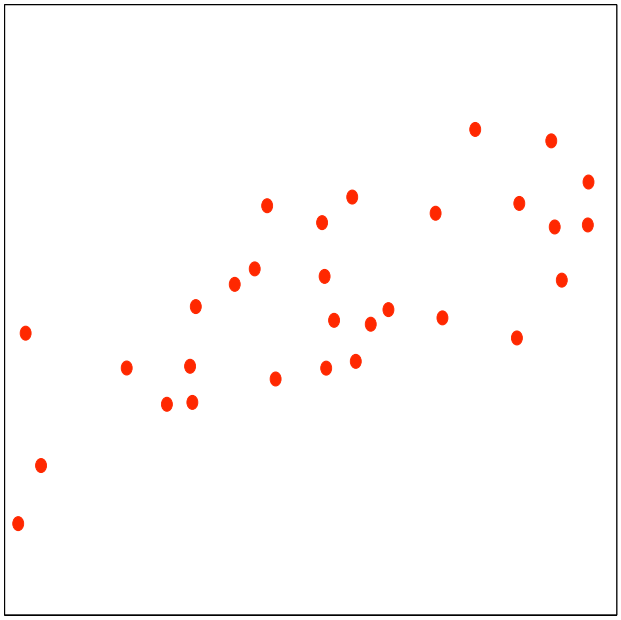
$$\sum_{i=1}^{m}\mathbf{x}_i - m\mathbf{b} = 0 \Rightarrow \mathbf{b} = \frac{1}{m}\sum_{i=1}^{m}\mathbf{x}_i$$

- This means that the line goes through the mean of the data
- By substituting α_i, we get:

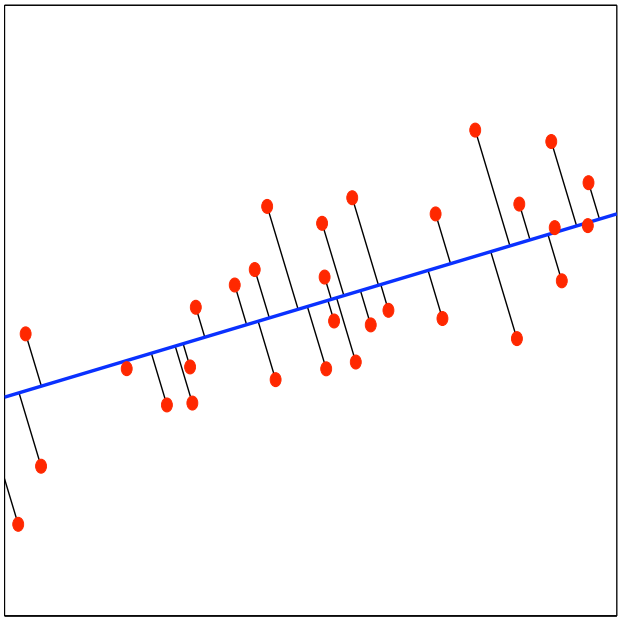
$$\hat{\mathbf{x}}_i = \mathbf{b} + (\mathbf{v}^T(\mathbf{x}_i - \mathbf{b}))\mathbf{v}$$

- This means that instances are projected orthogonally on the line to get the associated point.

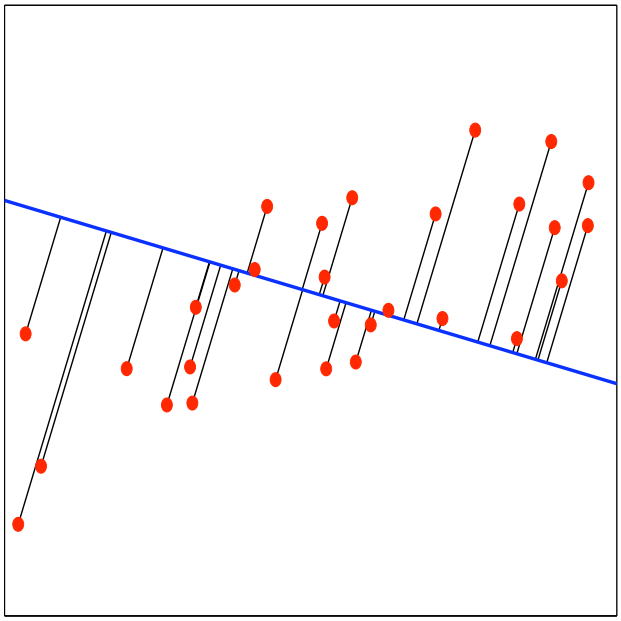
Example data



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



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



Finding the direction of the line

- Substituting $\alpha_i = \mathbf{v}^T(\mathbf{x}_i - \mathbf{b}) = (\mathbf{x}_i - \mathbf{b})^T\mathbf{v}$ into our optimization problem we obtain a new optimization problem:

$$\begin{aligned} \min_{\mathbf{v}} \quad & \sum_{i=1}^m \|\mathbf{x}_i - \mathbf{b} - (\mathbf{v}^T(\mathbf{x}_i - \mathbf{b}))\mathbf{v}\|^2 \\ \text{s.t.} \quad & \|\mathbf{v}\|^2 = 1 \end{aligned}$$

- The optimization criterion can be re-written as:

$$\sum_{i=1}^m (\|\mathbf{x}_i - \mathbf{b}\|^2 + \alpha_i^2\|\mathbf{v}\|^2 - 2\alpha_i(\mathbf{x}_i - \mathbf{b})^T\mathbf{v}) = \sum_{i=1}^m (\|\mathbf{x}_i - \mathbf{b}\|^2 - \alpha_i^2)$$

- Hence, the we can solve the equivalent problem:

$$\begin{aligned} \max_{\mathbf{v}} \quad & \sum_{i=1}^m \alpha_i^2 \\ \text{s.t.} \quad & \|\mathbf{v}\|^2 = 1 \end{aligned}$$

Finding the direction of the line

- Optimization problem re-written:

$$\max_{\mathbf{v}} \quad \sum_{i=1}^{m} \mathbf{v}^T(\mathbf{x}_i - \mathbf{b})(\mathbf{x}_i - \mathbf{b})^T\mathbf{v}$$

$$\text{s.t.} \quad \|\mathbf{v}\|^2 = 1$$

- The Lagrangian is:

$$L(\mathbf{v}, \lambda) = \sum_{i=1}^{m} \mathbf{v}^T(\mathbf{x}_i - \mathbf{b})(\mathbf{x}_i - \mathbf{b})^T\mathbf{v} + \lambda - \lambda\|\mathbf{v}\|^2$$

- Let $S = \sum_{i=1}^{m}(\mathbf{x}_i - \mathbf{b})(\mathbf{x}_i - \mathbf{b})^T$ be an n-by-n matrix, which we will call the **scatter matrix**
- The solution to the problem, obtained by setting $\nabla_{\mathbf{v}} L = 0$, is: $S\mathbf{v} = \lambda\mathbf{v}$.

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 equation obtained for $\mathbf{v}$ tells us that it should be an eigenvector of S.
- The $\mathbf{v}$ that maximizes $\mathbf{v}^T S\mathbf{v}$ is the eigenvector of S with the largest eigenvalue

What is the scatter matrix

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

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

- Hence, $S(k,l)$ is proportional to the *estimated covariance* between the kth and lth dimension in the data.

Recall: Covariance

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

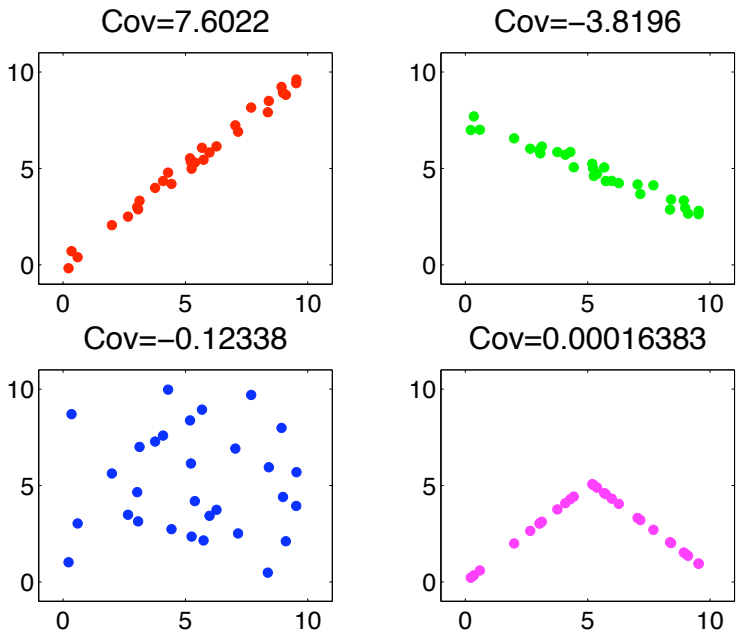
$$Cov(X,Y) = E\{(X - E(X))(Y - E(Y))\}$$

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

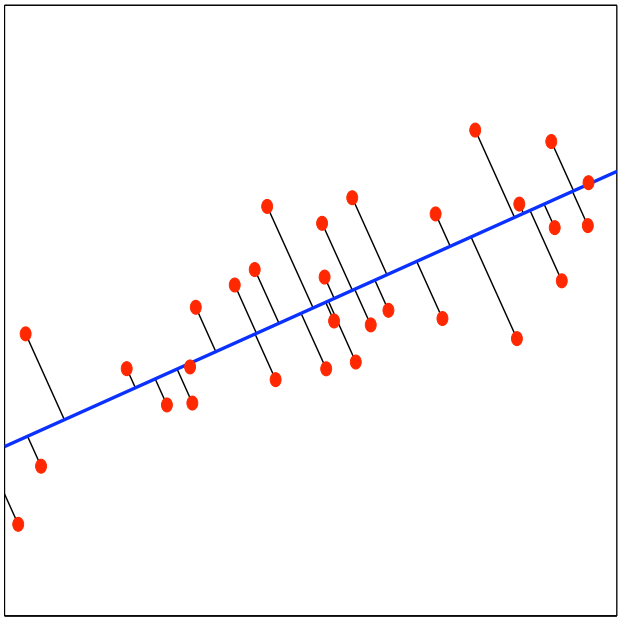
$$\frac{1}{m} \sum_{i=1}^{m} (x_i - \mu_X)(y_i - \mu_Y) \ ,$$

  where $\mu_X = (1/m) \sum_{i=1}^{m} x_i$ and $\mu_Y = (1/m) \sum_{i=1}^{m} y_i$.
- Note: $Cov(X,X) = Var(X)$.

Covariance example



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 $\mathbf{b} + \alpha^1\mathbf{v}_1 + \ldots + \alpha^d\mathbf{v}_d$.
- 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.

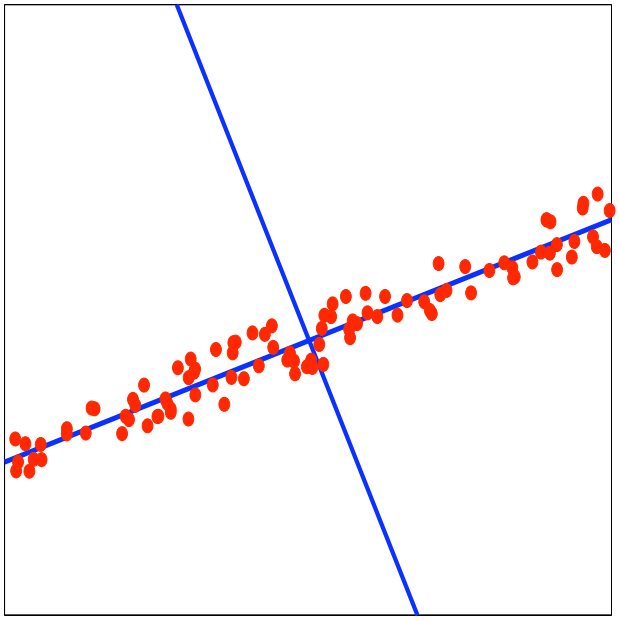
Remarks

- $\mathbf{b}$, 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:

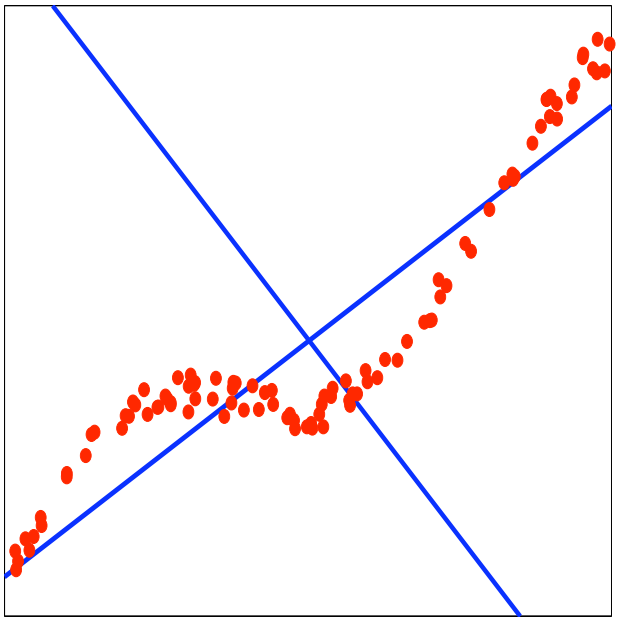
$$\frac{\lambda_1 + \cdots + \lambda_d}{\lambda_1 + \cdots + \lambda_d + \lambda_{d+1} + \cdots + \lambda_n}$$

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

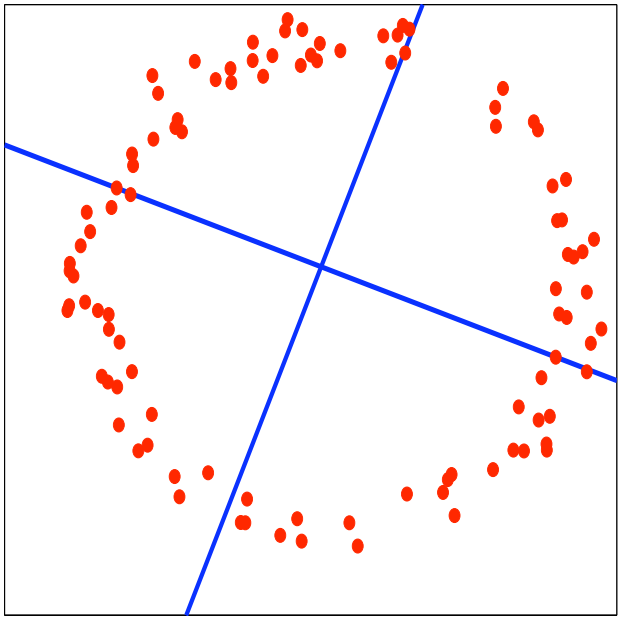
Example: $\lambda_1 = 0.0938, \lambda_2 = 0.0007$



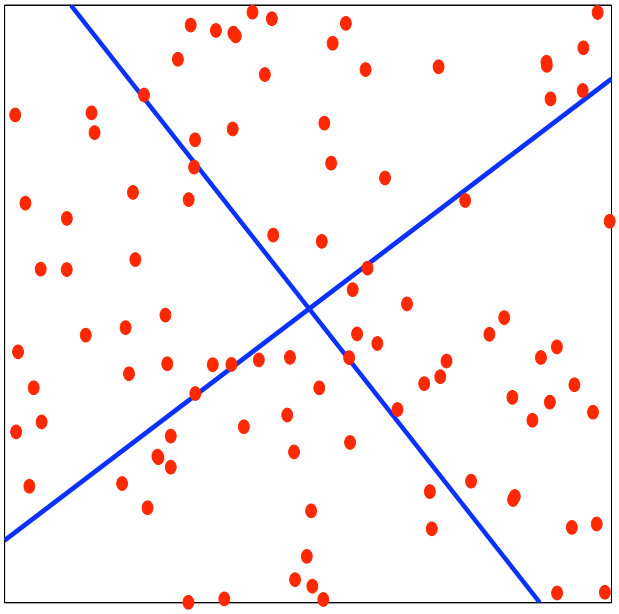
Example: $\lambda_1 = 0.1260, \lambda_2 = 0.0054$



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)