Machine learning: lecture 16

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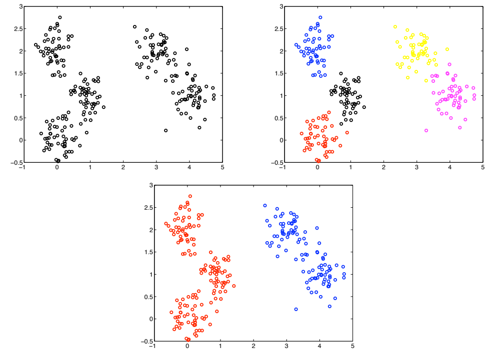
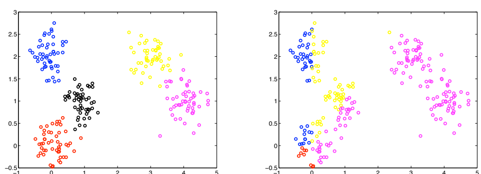
Finding structure in the data: clustering

- We can find structure in the data by isolating groups of examples that are similar in some well-defined sense



Clustering: metric



- Clustering results are crucially dependent on the measure of similarity (or distance) between the "points" to be clustered

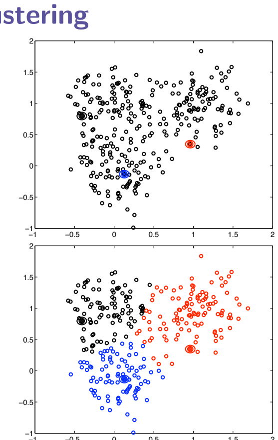
Overview of clustering methods

- Flat clustering methods
  - e.g., mixture models, k-means clustering
- Hierarchical clustering methods:
  - Top-down (splitting)
    - ∗ e.g., hierarchical mixture models
  - Bottom-up (merging)
    - ∗ e.g., hierarchical agglomerative clustering
- Spectral clustering
- Semi-supervised clustering
- Clustering by dynamics

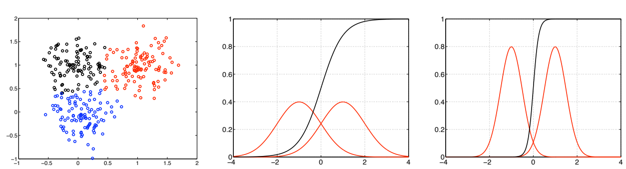
Etc.

K-means clustering

- The procedure:
  1. Pick k arbitrary centroids (cluster means)
  2. Assign each example to its "closest" centroid (**E-step**)
  3. Adjust the centroids to be the means of the examples assigned to them (**M-step**)
  4. Goto step 2 (until no change)
- The algorithm is guaranteed to converge in a finite number of iterations

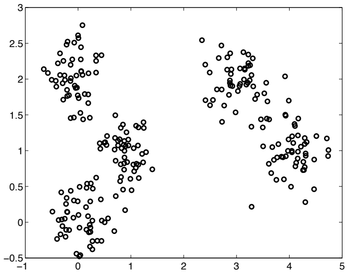


K-means clustering cont'd



- K-means clustering corresponds to estimating a Gaussian mixture model with EM provided that the covariance matrices are fixed, $\Sigma_j = \sigma^2 I$, for all $j = 1, \ldots, m$, and σ^2 is small.

Spectral clustering: motivation



Spectral clustering: outline

- Spectral clustering (as described here) relies on a random walk over the points

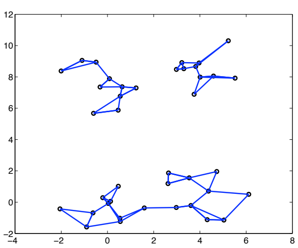
  We find the random walk via the following steps

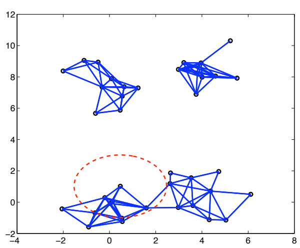
  1. construct a neighborhood graph
  2. assign weights to the edges in the graph
  3. define a transition probability matrix based on the weights

- The points are clustered on the basis of the eigenvectors of the resulting transition probability matrix

Step 1: neighborhood graph

- We can connect each point to its k-nearest neighbors, or connect each point to all neighbors within distance ϵ

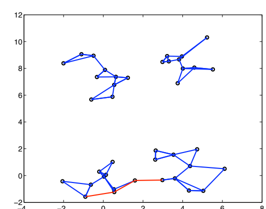




Step 2: edge weights

- We assign symmetric non-negative edge weights W_{ij}:

$$\begin{aligned} W_{ij} &= \exp\{-\beta\|\mathbf{x}_i - \mathbf{x}_j\|\}, \text{ if } i \text{ and } j \text{ connected} \\ W_{ij} &= 0, \text{ otherwise} \end{aligned}$$



Note: we do not use a squared distance in the exponent so that a weight for a path is computed analogously to the edge weights

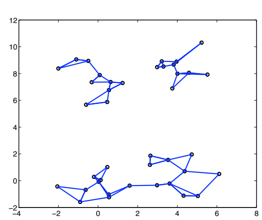
Step 3: transition probability matrix

- Finally, we define a Markov random walk over the neighborhood graph by constructing a transition probability matrix from the edge weights

$$P_{ij} = \frac{W_{ij}}{W_{i\cdot}}, \text{ where } W_{i\cdot} = \sum_j W_{ij}$$

and $\sum_j P_{ij} = 1$ for all i.

The random walk proceeds by successively selecting points according to $j \sim P_{ij}$, where i specifies the current location



Random walk: properties

- If we start from i_0, the distribution of points i_t that we end up in after t steps is given by

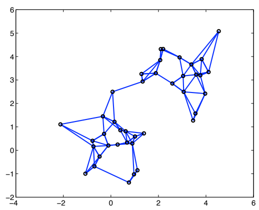
$$\begin{aligned} & i_1 \sim P_{i_0 i_1}, \\ & i_2 \sim \sum_{i_1} P_{i_0,i_1} P_{i_1 i_2} = [P^2]_{i_0 i_2}, \\ & i_3 \sim \sum_{i_1}\sum_{i_2} P_{i_0,i_1} P_{i_1 i_2} P_{i_2 i_3} = [P^3]_{i_0 i_3}, \\ & \ldots \\ & i_t \sim [P^t]_{i_0 i_t} \end{aligned}$$

where $P^t = PP\ldots P$ (t matrix products) and $[\cdot]_{ij}$ denotes the i,j component of the matrix.

Random walk and clustering

- The distribution of points we end up in after t random steps converge as t increases. If the graph is connected (and ergodic), the resulting distribution becomes independent of the starting point

  Even for large t, the transition probabilities $[P^t]_{ij}$ have a slightly higher probability of transitioning within "clusters" than across; we want to recover this effect from eigenvalues/vectors



Eigenvalues/vectors and spectral clustering

- Let W be the matrix with components W_{ij} and D a diagonal matrix such that $D_{ii} = \sum_j W_{ij}$. Then

$$P = D^{-1}W$$

- To find out how P^t behaves for large t it is useful to examine the eigen-decomposition of the following symmetric matrix

$$D^{-\frac{1}{2}}WD^{-\frac{1}{2}} = \lambda_1 \mathbf{z}_1\mathbf{z}_1^T + \lambda_2 \mathbf{z}_2\mathbf{z}_2^T + \ldots + \lambda_n \mathbf{z}_n\mathbf{z}_n^T$$

  where the ordering is such that $|\lambda_1| \geq |\lambda_2| \geq \ldots \geq |\lambda_n|$.

Eigenvalues/vectors cont'd

- The symmetric matrix is related to P^t since

$$(D^{-\frac{1}{2}}WD^{-\frac{1}{2}})\cdots(D^{-\frac{1}{2}}WD^{-\frac{1}{2}}) = D^{\frac{1}{2}}\,(P\cdots P)\,D^{-\frac{1}{2}}$$

  This allows us to write the t step transition probability matrix in terms of the eigenvalues/vectors of the symmetric matrix

$$\begin{aligned} P^t &= D^{-\frac{1}{2}}\left(D^{-\frac{1}{2}}WD^{-\frac{1}{2}}\right)^t D^{\frac{1}{2}} \\ &= D^{-\frac{1}{2}}\left(\lambda_1^t \mathbf{z}_1\mathbf{z}_1^T + \lambda_2^t \mathbf{z}_2\mathbf{z}_2^T + \ldots + \lambda_n^t \mathbf{z}_n\mathbf{z}_n^T\right) D^{\frac{1}{2}} \end{aligned}$$

  where $\lambda_1 = 1$ and

$$P^\infty = D^{-\frac{1}{2}}\left(\mathbf{z}_1\mathbf{z}_1^T\right) D^{\frac{1}{2}}$$

Eigenvalues/vectors and spectral clustering

- We are interested in the largest correction to the asymptotic limit

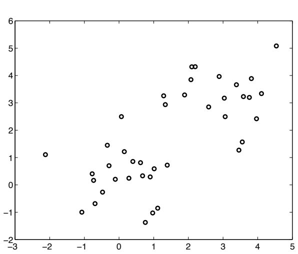
$$P^t \approx P^\infty + D^{-\frac{1}{2}}\left(\lambda_2^t\,\mathbf{z}_2\mathbf{z}_2^T\right) D^{\frac{1}{2}}$$

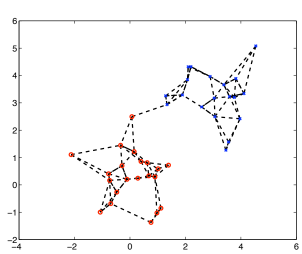
  Note: $[\mathbf{z}_2\mathbf{z}_2^T]_{ij} = z_{2i}z_{2j}$ and thus the largest correction term increases the probability of transitions between points that share the same sign of z_{2i} and decreases transitions across points with different signs

- Binary spectral clustering: we divide the points into clusters based on the sign of the elements of $\mathbf{z}_2$

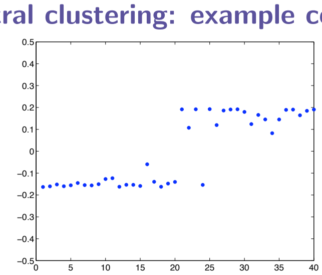
  $z_{2j} > 0 \Rightarrow$ cluster 1, otherwise cluster 0

Spectral clustering: example





Spectral clustering: example cont'd



Components of the eigenvector corresponding to the second largest eigenvalue