COMPSCI 589
Lecture 21: Kernel Principal Components Analysis and Spectral Clustering

Benjamin M. Marlin

College of Information and Computer Sciences
University of Massachusetts Amherst

Slides by Benjamin M. Marlin (marlin@cs.umass.edu).
Created with support from National Science Foundation Award# IIS-1350522.

Limitations of LDR

- All the dimensionality reduction methods we've seen so far find optimal linear sub-spaces under different constraints.
- **Question:** How can we move beyond linear sub-spaces?

Basis Expansion

- One way to move beyond linear dimensionality reduction is to first apply a non-linear basis expansion to the data vectors, and then apply linear dimensionality reduction.
- Any basis expansion can be applied including polynomials, etc., just as in the case of classification and regression.

Basis Expansion + SVD

Given a data set $\mathbf{X} \in \mathbb{R}^{N \times D}$ and a basis expansion function $\phi : \mathbb{R}^{D} \rightarrow \mathbb{R}^{D'}$ for $D' > D$, we obtain the following SVD-based algorithm:

1. Compute $\mathbf{U}, \mathbf{S}, \mathbf{V} = \text{SVD}(\phi(\mathbf{X}))$
2. Return $Z = \mathbf{US}$

Basis Expansion + PCA

Given a data set $\mathbf{X} \in \mathbb{R}^{N \times D}$ and a basis expansion function $\phi : \mathbb{R}^D \rightarrow \mathbb{R}^{D'}$ for $D' > D$, we obtain the following PCA-based algorithm:

1. Compute $\Sigma = (\phi(\mathbf{X}) - \mu)^T(\phi(\mathbf{X}) - \mu)$ where $\mu = 1/N \sum \phi(\mathbf{X}_i)$.
2. Compute the K leading eigenvectors $w_1, ..., w_K$ of Σ where $\mathbf{w}_k \in \mathbb{R}^{D'}$.
3. Stack the eigenvectors together into a $D' \times K$ matrix $\mathbf{W}$ where each column k of $\mathbf{W}$ corresponds to $\mathbf{w}_k$.
4. Project the matrix $\phi(\mathbf{X})$ into the rank-K sub-space of maximum variance by computing the matrix product $\mathbf{Z} = \phi(\mathbf{X})\mathbf{W}$.

Kernel PCA

- As in the classification case, it becomes very expensive to use an explicit basis function expansion that maps data into a high-dimensional space.
- In the basic SVD-based algorithm, there's no way to avoid this problem.
- In the PCA-based algorithm, it's not hard to show that the sample covariance matrix obtained after the basis expansion depends only on inner products of the form $\langle \phi(\mathbf{X}_i), \phi(\mathbf{X}_j) \rangle$.
- Kernel functions can often provide a much more efficient computation of these inner products without explicitly computing the basis expansion: $\mathcal{K}(\mathbf{X}_i, \mathbf{X}_j) = \langle \phi(\mathbf{X}_i), \phi(\mathbf{X}_j) \rangle$

Kernel PCA Algorithm

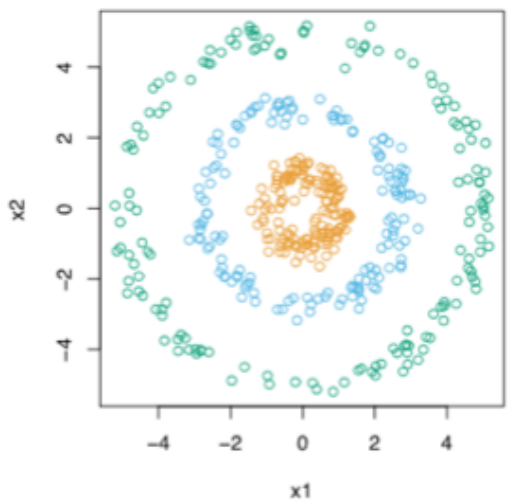
Given a data set $\mathbf{X} \in \mathbb{R}^{N \times D}$ and a kernel function $\mathcal{K}$, Kernel PCA can be computed as follows:

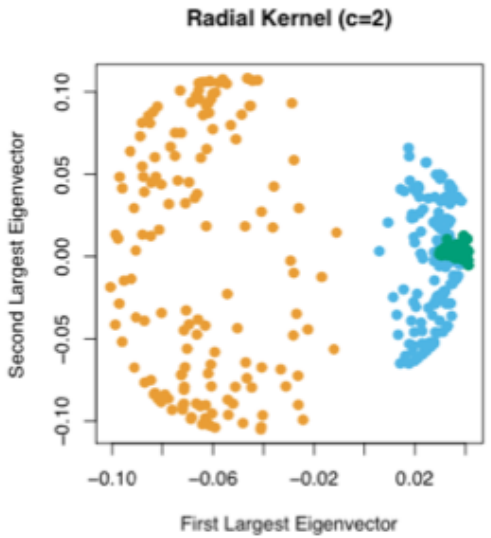
1. Compute $\mathbf{K}_{ij} = \mathcal{K}(\mathbf{X}_i, \mathbf{X}_j)$ for all i, j
2. Compute $\Sigma = (I - 1_N)\mathbf{K}(I - 1_N)$ where 1_N is an NxN matrix where every entry is $1/N$.
3. Compute the K leading eigenvectors $w_1, ..., w_K$ of Σ where $\mathbf{w}_k \in \mathbb{R}^N$ along with their eigenvalues $\lambda_1, ..., \lambda_K$
4. Compute the elements of the matrix of projected data vectors using

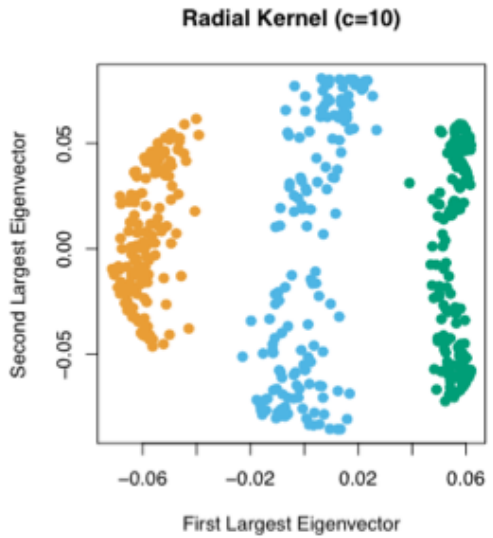
$$\mathbf{Z}_{nk} = \sum_{i=1}^{N} \frac{\mathbf{w}_{ik}}{\lambda_k} \mathcal{K}(\mathbf{X}_n, \mathbf{X}_i)$$

Example

Consider the case of using the radial basis function kernel $\mathcal{K}(\mathbf{x}, \mathbf{y}) = \exp(-\frac{1}{c}||\mathbf{x} - \mathbf{y}||_2^2)$.







Summary

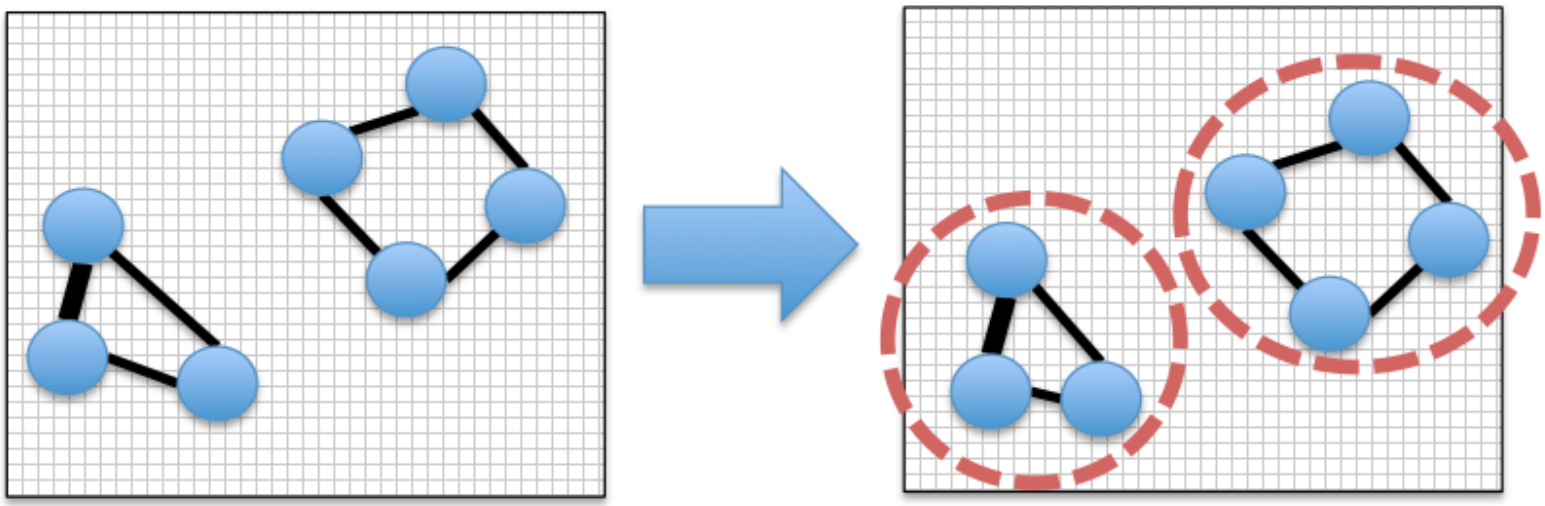
- Kernel PCA provides a non-linear dimensionality reduction method that can be used to extract directions of variation after applying high-dimensional basis function expansions, without explicitly performing the basis expansion.
- Kernel PCA can be thought of as looking for directions of variation in the space of similarities between data cases, and can extract components that correspond to fairly complex structures.
- When a good kernel is known a priori, kernel PCA can provide an effective pre-processing step for clustering methods as well as linear classification and regression methods.
- However, exact computation of kernel PCA can be expensive because the size of the matrix that is decomposed is NxN.

Spectra Clustering

- Applying kernel PCA followed by K-means clustering is closely related to a clustering method called spectral clustering.
- Spectral clustering works by defining a weighted similarity graph on the data cases.
- It's very common to use $\mathcal{K}(\mathbf{x}, \mathbf{y}) = \exp(-\frac{1}{c}||\mathbf{x} - \mathbf{y}||_2^2)$ as the weighting function and to include edges corresponding to the K nearest neighbors of each point.
- Unlike the kernel PCA case, the similarity values for edges not included in the graph are set to 0. The matrix of edge weights is denoted by $\mathbf{W}$.

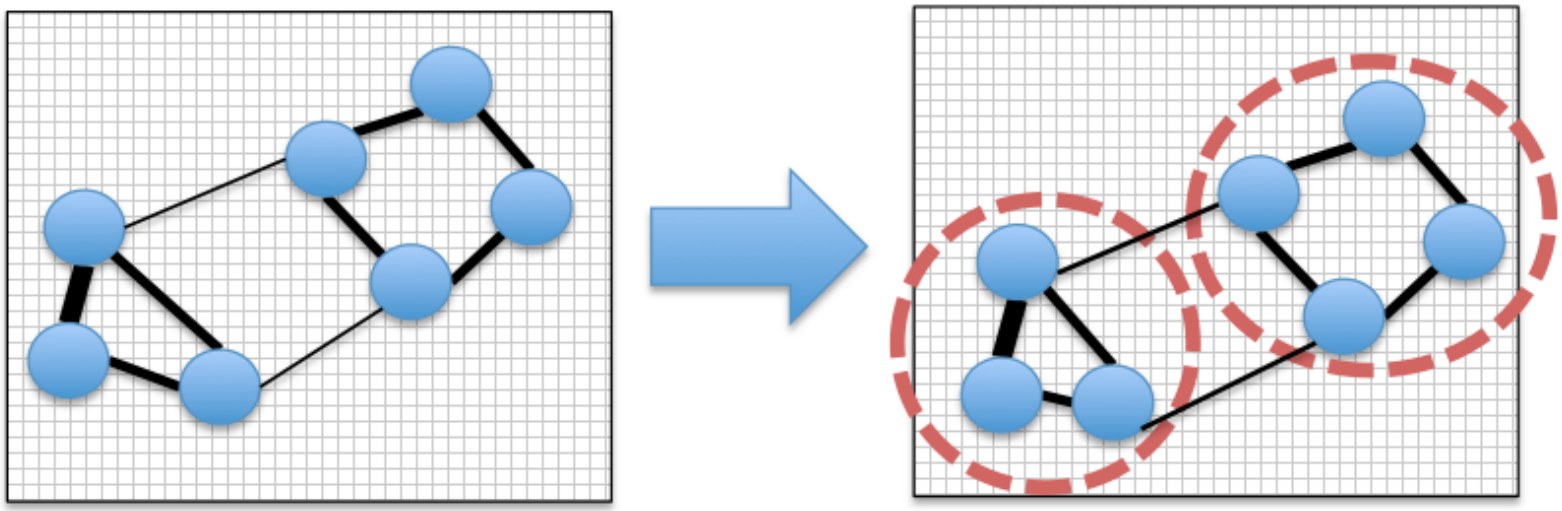
Connected Components

- In the simple case, the resulting graph has multiple connected components, and we can create one cluster for each connected component.



Minimum Weight Balanced Cut

- In the more complex case, the graph has only one connected component, and the goal is to identify a minimum weight balanced cut:



Spectral Clustering Algorithm

- Define the weighted node degree matrix $\mathbf{D}$ such that $\mathbf{D}_{ii} = \sum_n \mathbf{W}_{in}$.
- Define the graph laplacian $\mathbf{L} = \mathbf{D} - \mathbf{W}$.
- Compute the eigendecomposition of $\mathbf{L}$ and extract the M eigenvectors corresponding to the M smallest eigenvalues.
- Just like in kernel PCA, each eigenvector is length N. The collection of M of them forms an alternative dimensionality reduced representation for $\mathbf{X}$, which we can call $\mathbf{Z}$.
- Run K-means on $\mathbf{Z}$ to extract K clusters.
- This algorithm is an approximation to the exact K-way min-cut in the graph, which has exponential complexity to compute.