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

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Outline

Limitations of LDR

- All the dimensionality reduction methods we've seen so far find optimal linear sub-spaces under different constraints.

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- **Question:** How can we move beyond linear sub-spaces?

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- Any basis expansion can be applied including polynomials, etc., just as in the case of classification and regression.

Basis Expansion + SVD

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2. Return $Z = \mathbf{US}$

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4. Project the matrix $\phi(\mathbf{X})$ into the rank-K sub-space of maximum variance by computing the matrix product $\mathbf{Z} = \phi(\mathbf{X})\mathbf{W}$.

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- 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: $\mathcal{K}(\mathbf{X}_i, \mathbf{X}_j) = \langle \phi(\mathbf{X}_i), \phi(\mathbf{X}_j) \rangle$

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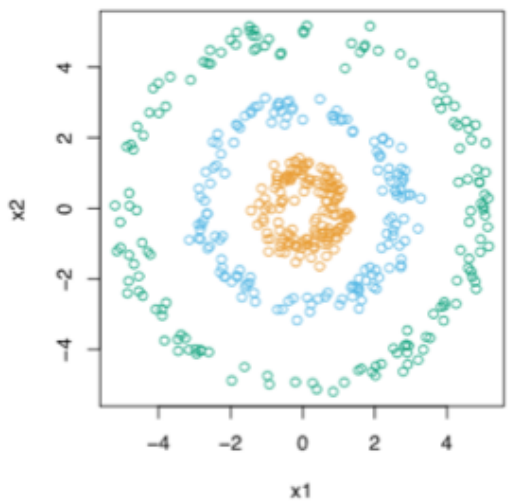
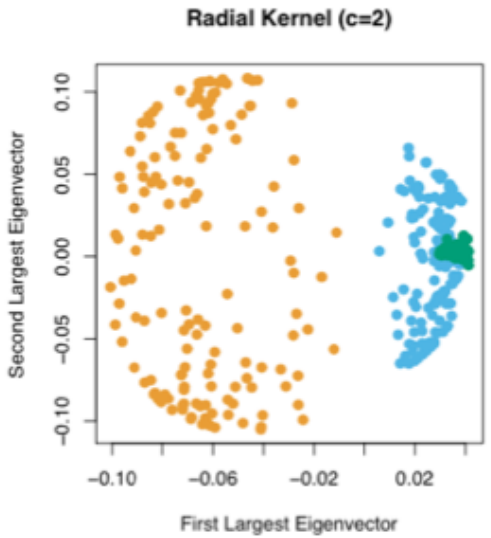
4. Compute the elements of the matrix of projected data vectors using

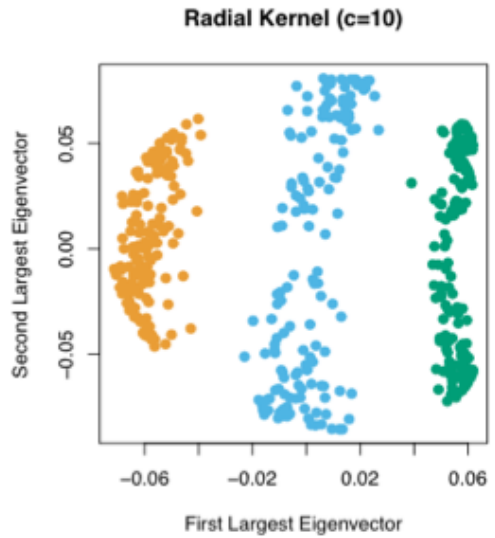
$$\mathbf{Z}_{nk} = \sum_{i=1}^{N} \frac{\mathbf{w}_{ik}}{\lambda_k} \mathcal{K}(\mathbf{X}_n, \mathbf{X}_i)$$

Example

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







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- 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.

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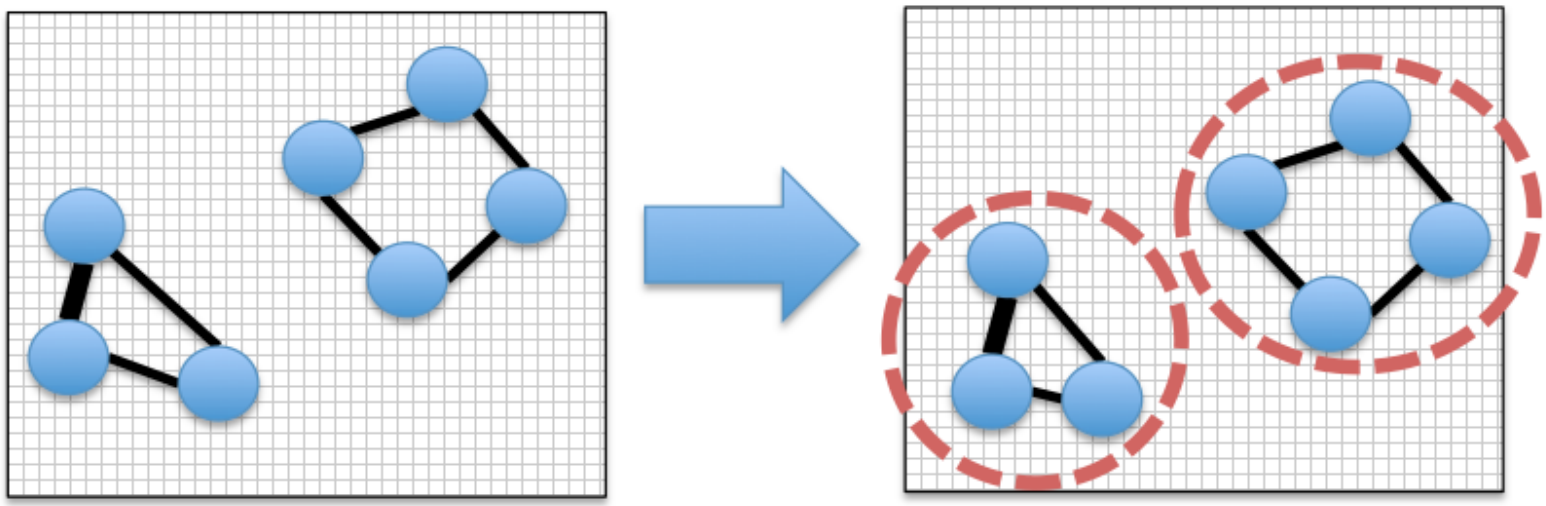
- Unlike the kernel PCA case, the similarity values for edges not included in the graph are set to 0. The matrix of edge weights is denoted by $\mathbf{W}$.

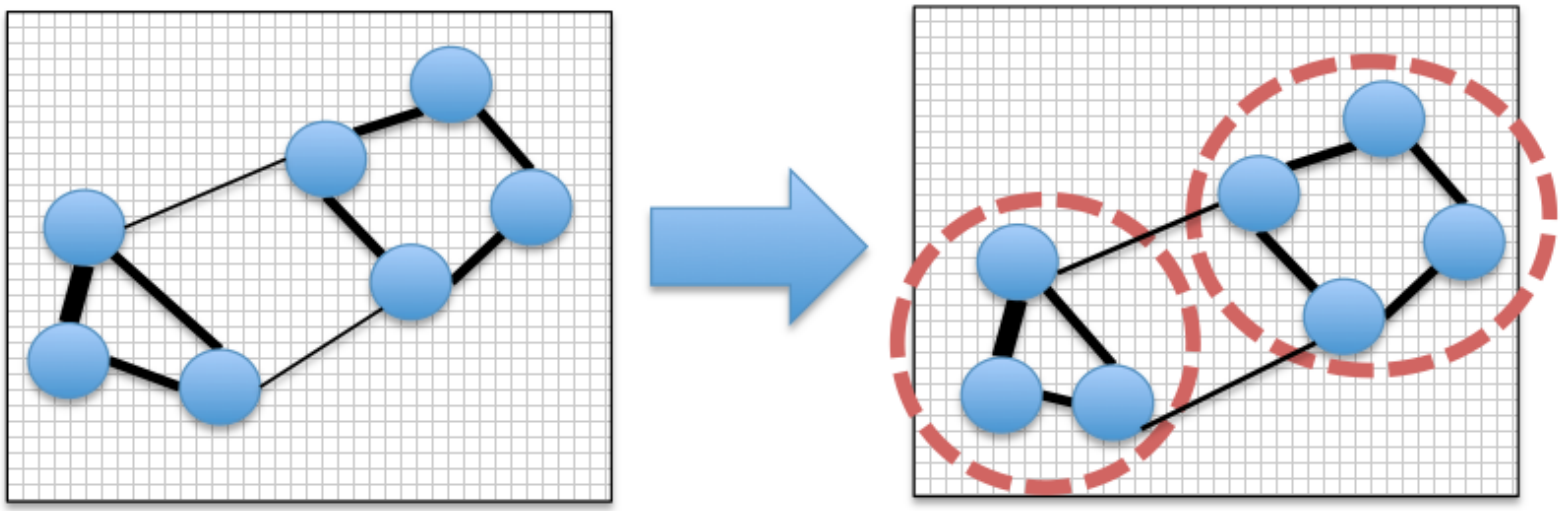
Connected Components

- 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:



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- This algorithm is an approximation to the exact K-way min-cut in the graph, which has exponential complexity to compute.