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Self-Tuning Spectral Clustering

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Statistical Methods 2

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Basic Spectral Clustering Algorithm

To cluster n data points $\{\mathbf{x}_i\}_{i=1}^n$ into K clusters:

1. Form the affinity/similarity matrix $W \in \mathbb{R}^{n \times n}$ where $W_{ij} = \exp\left(-\frac{d^2(\mathbf{x}_i, \mathbf{x}_j)}{\sigma^2}\right)$ for $i \neq j$ and $W_{ii} = 0$.
2. Let G be the diagonal matrix with $G_{ii} = \sum_{j=1}^n W_{ij}$ (the degree of x_i). Let $\tilde{L} := G^{-1/2} W G^{-1/2}$ be the symmetric normalized Laplacian.
3. Form the matrix $Z \in \mathbb{R}^{n \times K}$ by stacking the eigenvectors corresponding to the K largest eigenvalues of $\tilde{L}$.
4. Cluster the rows of Z using K-means: assign x_i to cluster $k \in [K] := \{1, \ldots, K\}$ if and only if row i of Z was assigned to cluster k.

[Ng et al., 2001]

Parameters To Tune

Problem: we have to choose K and σ.

Self-Tuning Spectral Clustering [Zelnik-Manor and Perona, 2004] contributions:

(i) Selection of the appropriate scale to analyse the data.

(ii) Clustering data distributed at different scales.

(iii) Clustering with irregular background clutter.

(iv) Estimating the number of clusters.

Selecting a suitable σ will resolve (i)–(iii), whilst (iv) is just choosing K.

Selecting σ

Note that σ can be very sensitive.

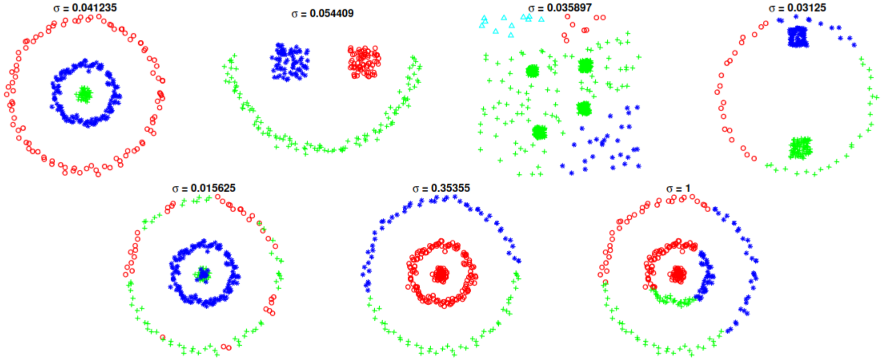


Figure: Fig. 1 from [Zelnik-Manor and Perona, 2004].

Local Scaling

Furthermore, different bandwidths σ may be needed for different clusters which are distributed at different scales. So we introduce local scaling:

1. For each data point x_i, define $\sigma_i = d(x_i, x_P)$, i.e. the distance from x_i to its Pth nearest neighbour, x_P. ($P = 7$ suggested.)
2. The *locally scaled* affinity matrix's non-diagonal entries are given by $\hat{W}_{ij} = \exp\left(-\frac{d^2(x_i, x_j)}{\sigma_i \sigma_j}\right)$.

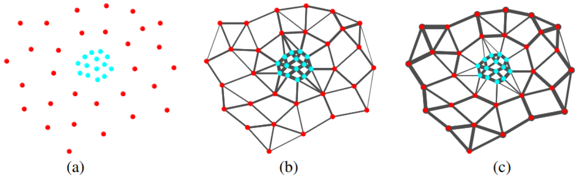


Figure: Fig. 2 from [Zelnik-Manor and Perona, 2004]: (a) Input data; (b) unscaled affinity; (c) locally-scaled affinity (edge thickness represents weight).

Selecting K

In the ideal case that there are some K completely disconnected clusters (i.e. $\hat{W}_{ij} > 0$ if and only if x_i and x_j are in the same cluster), then the eigenvalues of $\tilde{L}$, given by $\lambda_1 \geqslant \lambda_2 \geqslant \cdots \geqslant \lambda_n$, will be such that:

$$1 = \lambda_1 = \cdots = \lambda_K > \lambda_{K+1} \geqslant \cdots \geqslant \lambda_n \geqslant 0.$$

This leads to the “eigengap heuristic” for choosing K: choose K to be the smallest integer such that $\lambda_{K+1} - \lambda_K$ is large.

However, with real, noisy data, the above may not hold (“lacks a theoretical justification” [Zelnik-Manor and Perona, 2004])—so instead of looking at the eigenvalues, we’ll look further into the structure of $\tilde{L}$’s eigenvectors.

Analysing the Eigenvectors

In our ideal case (i.e. with K completely disconnected clusters), $\tilde{L}$ is block diagonal, with each block $\tilde{L}^{(k)}$ corresponding to a cluster $k \in [K]$. Therefore when we construct $Z \in \mathbb{R}^{n \times K}$ by stacking the eigenvectors of $\tilde{L}$ corresponding to the K largest eigenvalues of $\tilde{L}$, we obtain

$$Z = \begin{bmatrix} \mathrm{v}^{(1)} & \vec{0} & \vec{0} \\ \vec{0} & \dots & \vec{0} \\ \vec{0} & \vec{0} & \mathrm{v}^{(K)} \end{bmatrix} \in \mathbb{R}^{n \times K}$$

where $\mathrm{v}^{(k)}$ is the eigenvector corresponding to the largest eigenvalue (i.e. 1) of the submatrix $\tilde{L}^{(k)}$.

Analysing the Eigenvectors

$$Z = \begin{bmatrix} \mathrm{v}^{(1)} & \vec{0} & \vec{0} \\ \vec{0} & \dots & \vec{0} \\ \vec{0} & \vec{0} & \mathrm{v}^{(K)} \end{bmatrix} \in \mathbb{R}^{n \times K}$$

1. Each row i of Z has only one nonzero entry, lying in the column j corresponding to x_i's cluster—making the remaining task of cluster allocation trivial.
2. Taking more than K eigenvectors would result in more than one nonzero entry in some rows of Z, whilst taking fewer would result in some rows of Z having no nonzero entries.

With noisy, non-ideal data the rows of Z may have more than one nonzero entry, but there should hopefully be one entry significantly larger than the others.
Assign x_i to the cluster $k = \mathrm{argmax}_j \, Z_{ij}^2$.

A Problem With Z

Problem: The eigensolver we use may not return the K eigenvectors of $\tilde{L}$ in the standard basis—it could return any set of orthonormal vectors spanning the same space as Z's columns.
Solution: Find the rotation matrix $R \in \mathbb{R}^{K \times K}$ that minimises the cost function

$$J_K = \sum_{i=1}^{n} \sum_{j=1}^{K} \frac{\hat{Z}_{ij}^2}{\text{max}_l(\hat{Z}_{il}^2)}$$

where $\hat{Z} = ZR$ is the rotated matrix of eigenvectors.

Minimising this attempts to make the rows of $\hat{Z}$ as close to the standard basis as possible (i.e. with only one nonzero entry) and can be done via gradient descent (see [Zelnik-Manor and Perona, 2004] for details).

Selecting K from $\hat{Z}$

Choosing some large K' we can calculate the value of J_K for all $K \in [K']$ efficiently as follows:

1. Let $Z \in \mathbb{R}^{n \times 2}$ be the matrix of eigenvectors of $\tilde{L}$ corresponding to the two largest eigenvalues of $\tilde{L}$.
2. Find the rotation R that minimises J_K on $Z \in \mathbb{R}^{n \times 2}$ to obtain $\hat{Z}$.
3. Add the eigenvector corresponding to the next largest eigenvalue of $\tilde{L}$ as a column to $\hat{Z}$ and find the rotation R that minimises J_K for $K = 3$.
4. Repeat until we've found $J_{K'}$.

Finally, we choose $K_{\text{best}} = \text{argmin}_{K \in [K']} J_K$. (Although, if several Ks have very similar costs—e.g. within 0.01% of each other—then choose the largest of these Ks.)

Cluster Allocation

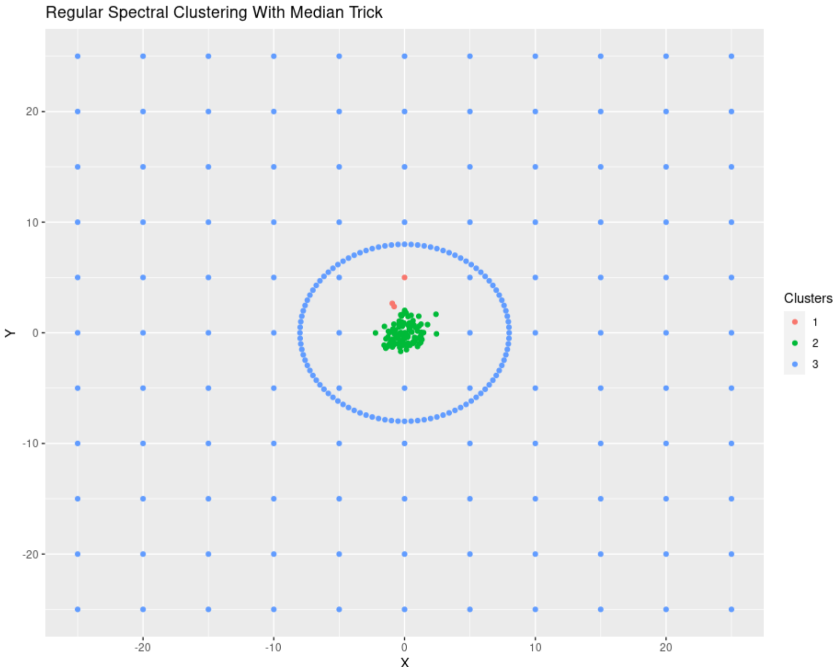
Now that we have K_{best}, using the rotated matrix $\hat{Z} \in \mathbb{R}^{n \times K_{\text{best}}}$ we can allocate each data point x_i to a cluster k in one of two ways:

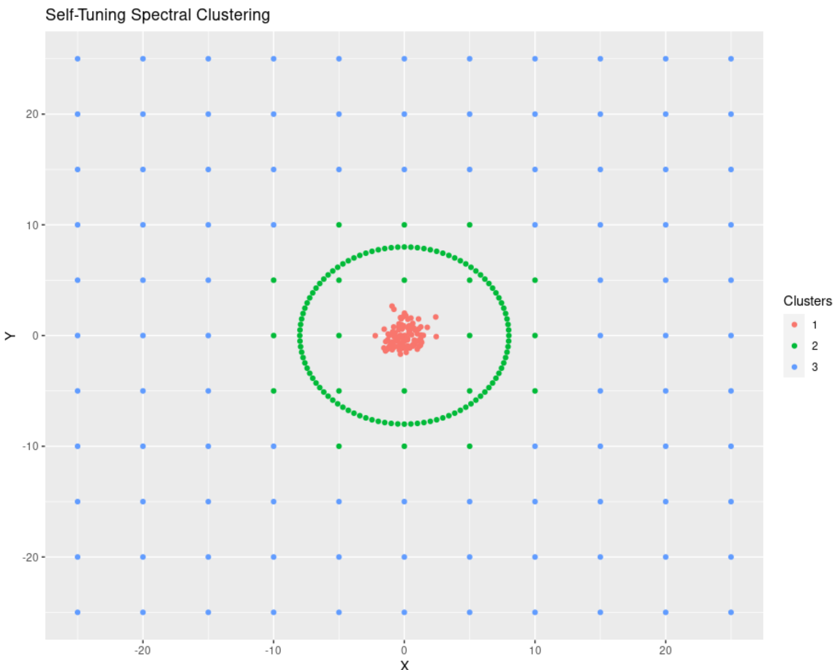
1. Assign x_i to the cluster $k = \text{argmax}_j \, \hat{Z}_{ij}^2$.
2. As in the old algorithm, perform K-means on the rows of $\hat{Z}$ to find the clusters (this should converge fairly quickly since $\hat{Z}$ is likely to be a good initialisation). This is particularly useful for very noisy data.

Self-Tuning Spectral Clustering Algorithm

1. Compute the local scale σ_i for each data point x_i.
2. Form the locally scaled affinity matrix $\hat{W} \in \mathbb{R}^{n \times n}$ where $\hat{W}_{ij} = \exp\left(-\frac{d^2(\mathbf{x}_i, \mathbf{x}_j)}{\sigma_i \sigma_j}\right)$ for $i \neq j$ and $\hat{W}_{ii} = 0$.
3. Let G be the diagonal matrix with $G_{ii} = \sum_{j=1}^{n} \hat{W}_{ij}$ (the degree of x_i) and $\tilde{L} := G^{-1/2}\, \hat{W}\, G^{-1/2}$ be the symmetric normalized Laplacian.
4. For some large K', form the matrix $Z \in \mathbb{R}^{n \times K'}$ by stacking the eigenvectors corresponding to the K' largest eigenvalues of $\tilde{L}$ and use gradient descent to find the rotation matrix $R \in \mathbb{R}^{K' \times K'}$ that minimizes $J_{K'} = \sum_{i=1}^{n} \sum_{j=1}^{K'} (Z_{ij}^2 / \max_l Z_{il}^2)$.
5. Choose $K_{\text{best}} = \operatorname{argmin}_K J_K$ (or largest such K if several give very similar costs).
6. Assign x_i to cluster k if and only if $\max_j Z_{ij}^2 = Z_{ik}^2$. (Or, for very noisy data, use K-means to cluster the rows of Z as in the standard algorithm.)

[Zelnik-Manor and Perona, 2004]


Regular Spectral Clustering With Median Trick
Y
X
20
10
0
-10
-20
-20
-10
0
10
20
Clusters
1
2
3


Self-Tuning Spectral Clustering
20
10
0
-10
-20
Y
-20
-10
0
10
20
X
Clusters
1
2
3

Conclusion

- Self-tuning spectral clustering allows us to determine suitable values of σ and K automatically.
- We do have to choose P and K', but these are much simpler to tune (and we can usually just set K' to be ‘big enough’ in some sense).
- The local scaling implemented to deal with σ also allows us to perform clustering noisy, multi-scale data.

References

Ng, A. Y., Jordan, M. I., and Weiss, Y. (2001).
On Spectral Clustering: Analysis and an algorithm.

Zelnik-Manor, L. and Perona, P. (2004).
Self-Tuning Spectral Clustering.

Thank you

Any questions?