Self-Tuning Spectral Clustering

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Statistical Methods 2

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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.

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Parameters To Tune

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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.

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

Selecting σ

Note that σ can be very sensitive.

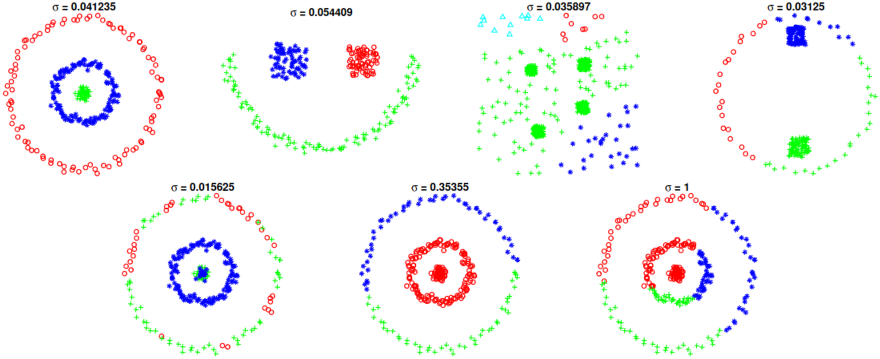

Figure: Fig. 1 from [Zelnik-Manor and Perona, 2004].

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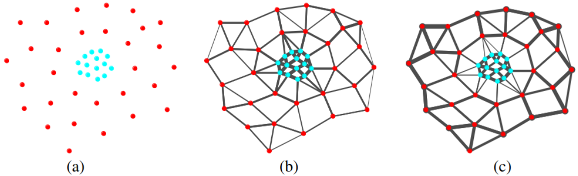

Figure: Fig. 2 from [Zelnik-Manor and Perona, 2004]: (a) Input data; (b) unscaled affinity; (c) locally-scaled affinity (edge thickness represents weight).

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:

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

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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

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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 $\tilde{L}^{(k)}$.

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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 $k = \operatorname{argmax}_j Z_{ij}^2$.

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.

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Solution: Find the rotation matrix $R \in \mathbb{R}^{K \times K}$ that minimises the cost function

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

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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).

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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 $K = 3$.

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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.)

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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.

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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 $J_{K'} = \sum_{i=1}^{n} \sum_{j=1}^{K'} (Z_{ij}^2 / \max_l Z_{il}^2)$.

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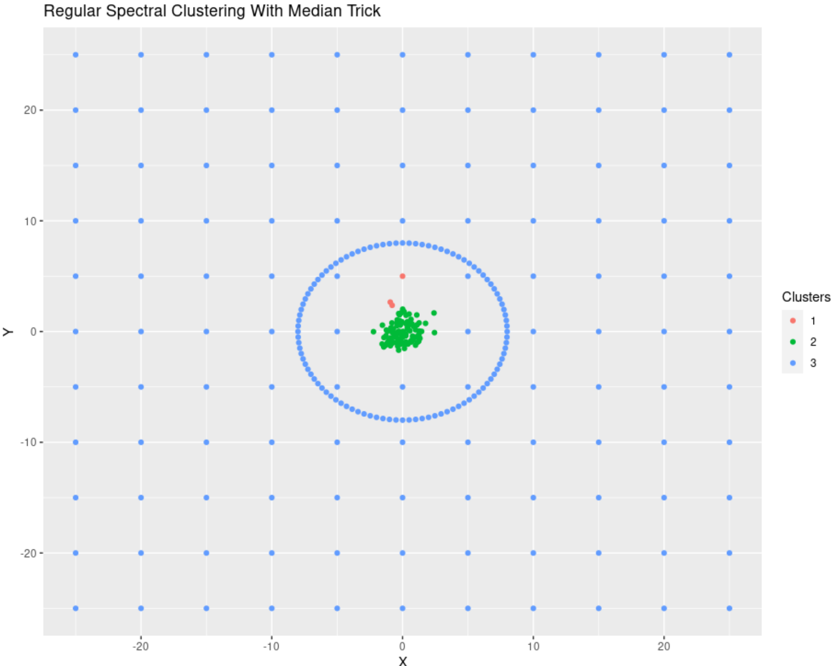
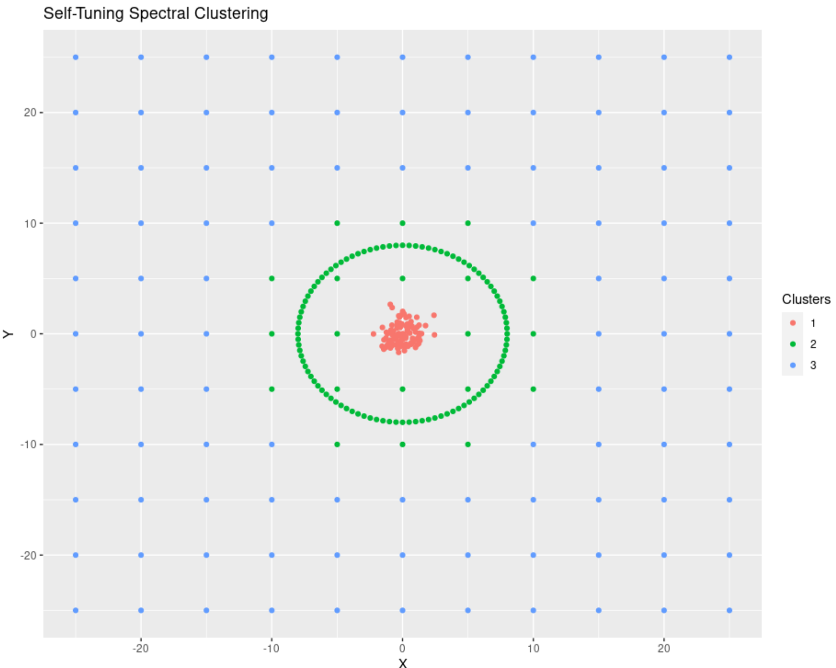
6. Assign x_i to cluster k if and only if $\max_j Z_{ij}^2 = Z_{ik}^2$. (Or, for very noisy data, use K-means to cluster the rows of Z as in the standard algorithm.)

[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



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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).
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Self-Tuning Spectral Clustering.

Thank you

Any questions?