STAT 215A Fall 2020 Week 6

James Duncan, OH: M, Th 2-4pm

Slides in part thanks to past 215A GSIs (Tiffany Tang, Zoe Vernon, Rebecca Barter, and others.)

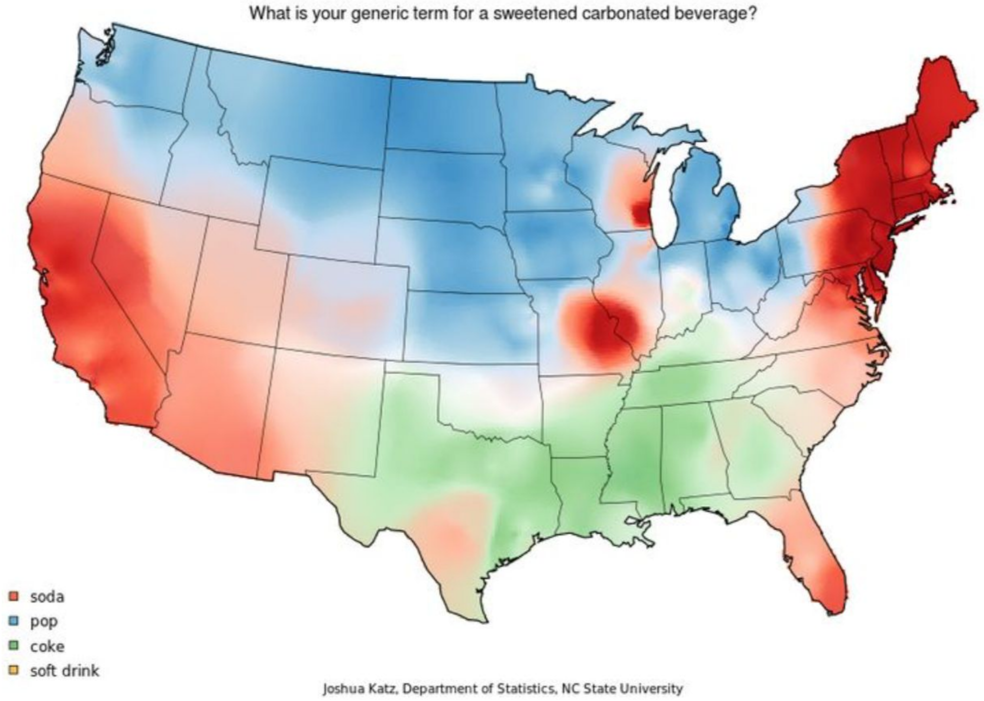
Announcements

- Lab 2 due in one week **10/08 at 11:59pm**
- Please respond to the discussion section feedback survey!
- Hoping to have grading done this weekend 🤞

Outline for today

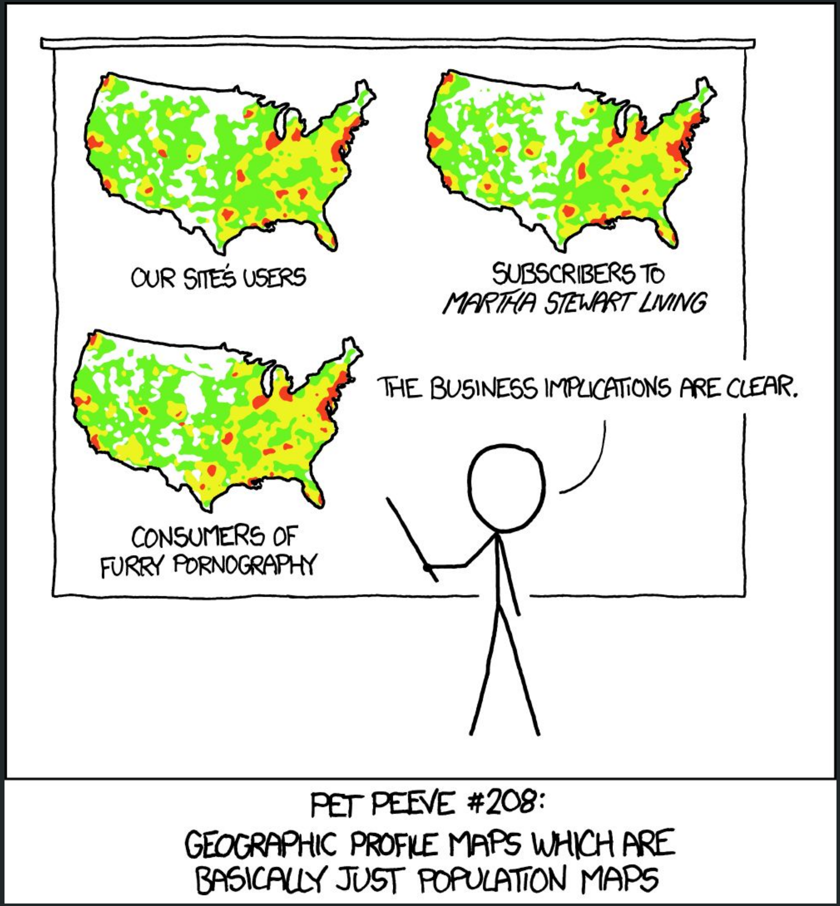
- Lab 2 check-in
- Choosing K for NMF
- Spectral clustering
- DBSCAN (time allowing)

Questions on HW2 or Lab 2?



https://www.businessinsider.com/22-maps-that-show-the-deepest-linguistic-conflicts-in-america-2013-6#ok-this-one-is-crazy-everyone-pronounces-pecan-pie-differently-10

Is your map more than a map of population density?



Lab 2 reminders

- Use figure captions for cross-referencing: `fig.cap="My awesome caption"`
- Use png and adjust DPI, e.g.: `dev="png", dpi = 300`
- Folder structure for submission:
  - `stat-215-a/`
    - `lab2/`
      - `lab2.Rmd & .pdf`
      - `lab2_blind.Rmd & .pdf`
      - `R/`
      - `other/`

        Optional, for .bib files or other things necessary to reproduce your lab (but don't over do it!).
- Be careful when using section headers '#'

Nonnegative Matrix Factorization (NMF)

- Given a non-negative matrix $\mathbf{X}$, NMF solves

$$\underset{\mathbf{W}\geq 0, \mathbf{H}\geq 0}{\operatorname{argmin}} \ ||\mathbf{X} - \mathbf{W}\,\mathbf{H}||_F^2 = \sum_{i,j} (\mathbf{X}_{ij} - \mathbf{W}_i^\top \mathbf{H}_j)^2$$

- You can modify this to work for $\mathbf{X}$ with missing data (in R: `NNLM:nnmf()`[1]):

$$\underset{\mathbf{W}\geq 0, \mathbf{H}\geq 0}{\operatorname{argmin}} \ \sum_{\substack{(i,j) \\ \text{not missing}}} (\mathbf{X}_{ij} - \mathbf{W}_i^\top \mathbf{H}_j)^2$$

1. NNLM was archived on CRAN, so to install you need to use `devtools::install_github("linxihui/NNLM")`

Nonnegative Matrix Factorization (NMF)

Missing Data NMF: $$\underset{\mathbf{W}\geq 0, \mathbf{H}\geq 0}{\operatorname{argmin}} \sum_{\substack{(i,j) \\ \text{not missing}}} (\mathbf{X}_{ij} - \mathbf{W}_i^\top \mathbf{H}_j)^2$$

Idea for choosing K:

- Randomly leave out entries from the data matrix $\mathbf{X}$
- For each potential choice of K:
  1. Apply NMF to the data with missing values: $\mathbf{W}_M$ and $\mathbf{H}_M$
  2. Impute the missing values of $\mathbf{X}$ using corresponding entries of $\mathbf{W}_M\mathbf{H}_M$
  3. Compute the imputation error (MSE of difference between imputed and observed values)
  4. Repeat many times and compute the mean and SE for this K
- Choose K by taking the minimum or using the 1-SE rule (Breiman, 1984)

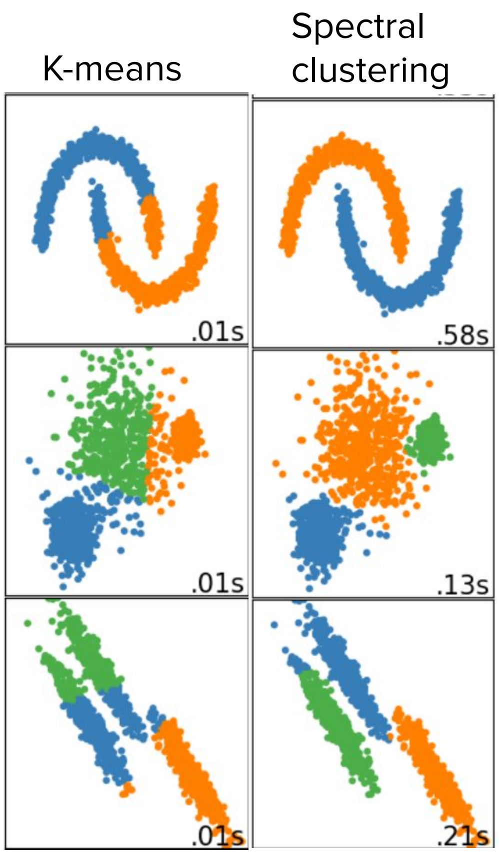
Spectral clustering: a “good” method

Advantages:

- Simple to implement
- Stable to underlying data generation mechanism

Disadvantages

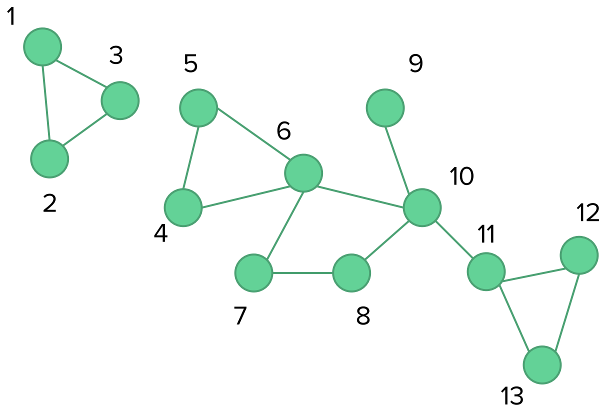
- Need to represent the data as a graph
- Still need to choose K
- Not advised for problems with large numbers of clusters



More details: http://people.csail.mit.edu/dsontag/courses/ml14/notes/Luxburg07_tutorial_spectral_clustering.pdf
Nice summary: https://eric-bunch.github.io/blog/spectral-clustering

Setup

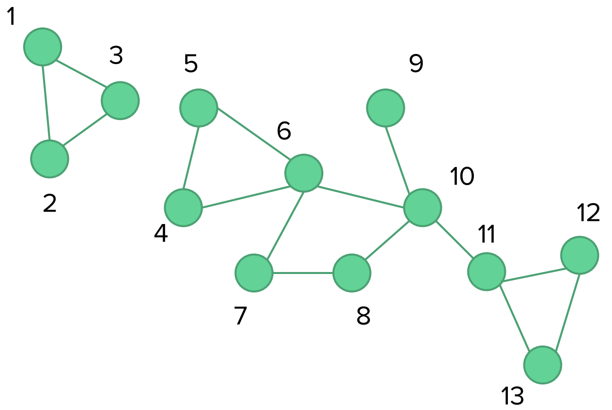
- Graph: $G = (E,V)$
- Weighted adjacency matrix: $W = (w_{ij})_{i,j=1,\dots,n}$
  - 0 on the diagonal
  - $w_{ij} = 0$ if there is no edge between v_i and v_j
- Diagonal degree matrix $D: D_{ii} = \sum_j W_{ij}$
- (Unnormalized) graph Laplacian: $L = D - W$



What can the graph Laplacian tell us?

- Let's try to find eigenvectors $Lx = \lambda x$

$$L = \begin{pmatrix} \sum_j w_{1j} & -w_{12} & -w_{13} & 0 & \cdots \\ -w_{12} & \sum_j w_{2j} & -w_{23} & 0 & \cdots \\ -w_{13} & -w_{23} & \sum_j w_{3j} & 0 & \cdots \\ 0 & 0 & 0 & \ddots & \\ \vdots & \vdots & \vdots & & \end{pmatrix}$$



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$\mathbb{1}$, the vector with all entries equal to 1

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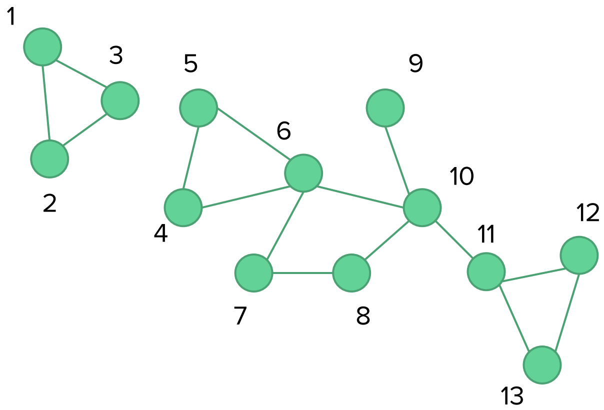

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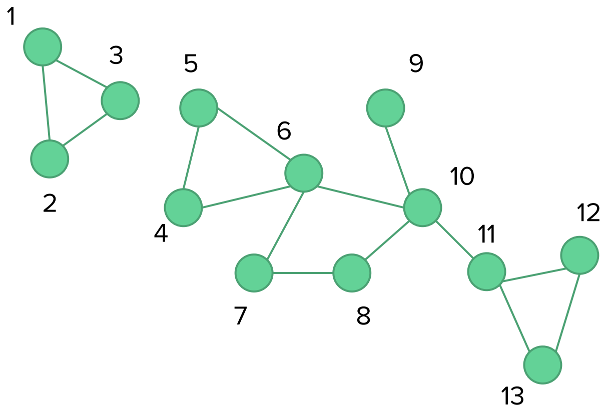
$$\begin{pmatrix} 1 & 1 & 1 & 0 \cdots 0 \end{pmatrix}^\top$$



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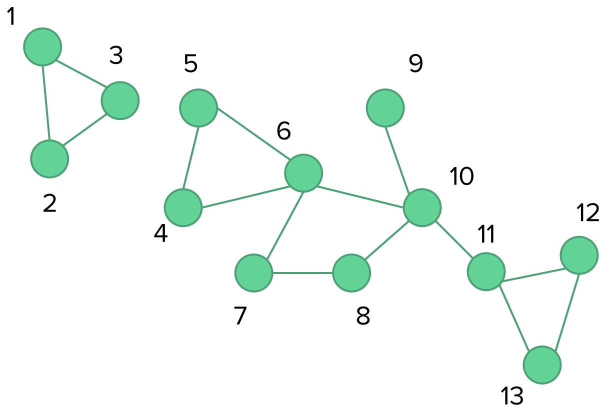

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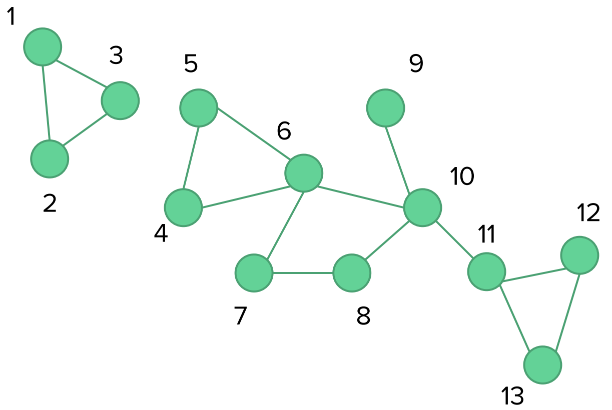

$\lambda_1 = 0$ in these cases, so the multiplicity of the eigenvalue 0 tells us about the number of **connected components** in the graph.

What about the other eigenvectors of L ?

- Fact[1]: $$\lambda_2 = \min_{x:||x||=1} x^\top M x$$

Second smallest eigenvalue

M symmetric

1 See https://math.stackexchange.com/questions/1403920/second-smallest-eigenvalue-as-min-x-fracxtaxxtx for a proof

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- So, $$\lambda_2 = \min_{x:||x||=1} \sum_{i,j} w_{ij}(x_i - x_j)^2$$

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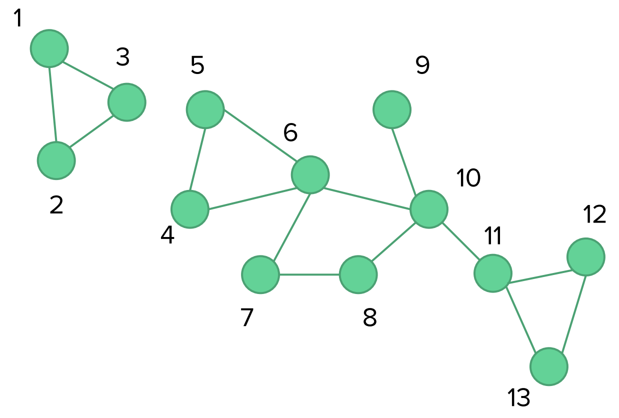

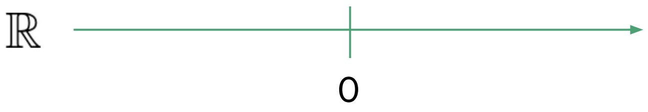

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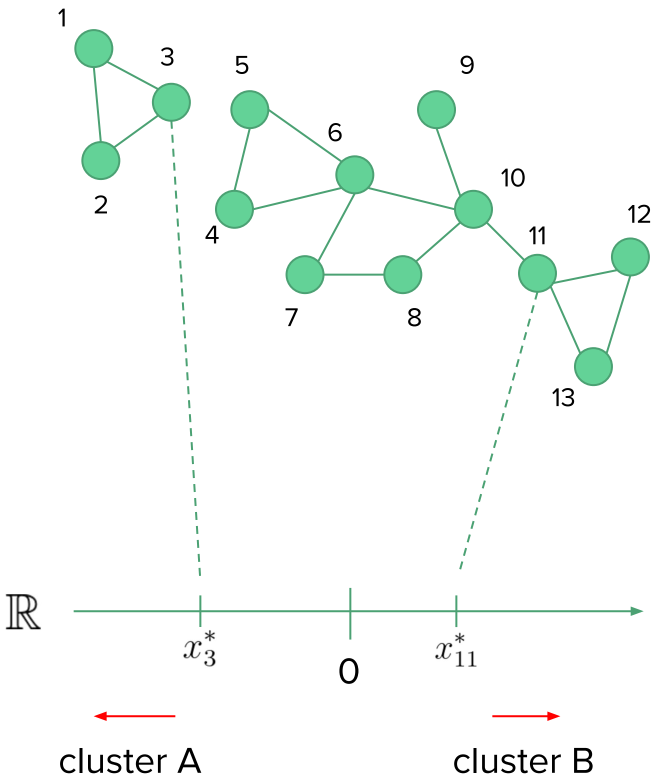

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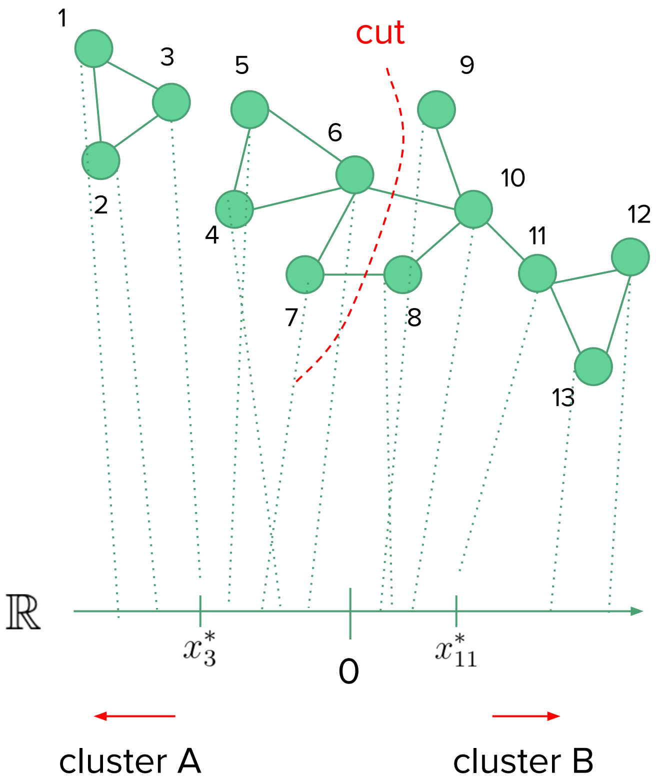
- Another Fact: The eigenvectors with distinct eigenvalues of a real symmetric matrix are orthogonal. $$\sum_{i=1}^{n} x_i^* = 0$$
- Look at where the values of x^* fall on the real line.
- Cut at the point that separates the observations with negative values from those with positive values in x^*



Normalization

- In the simple example above, we used the **unnormalized** graph Laplacian, which solves an approximation of the **RatioCut** objective.
- We could instead use the **normalized** graph Laplacian:

$$L_{sym} = I - D^{-1/2} A D^{-1/2}$$

  - Leads to an approximate solution of the **Ncut** objective
  - This is advised in practice (Sarkar and Bickel, 2015)

Representing your data as a graph

- ε **- neighborhood graph**: connect all points whose pairwise distances are smaller than ε
- k**-nearest neighbors graph**: connect v_i and v_j if they v_j is one of v_i's nearest neighbors
  - Variant: only connect if they are mutually nearest neighbors
- **Fully connected with similarity function**: compute the pairwise similarities or distances between observations
  - Example: Gaussian similarity $\exp\{-\|x_i - x_j\|^2/2\sigma^2\}$

Spectral clustering algorithm

For a given choice of number of clusters K:

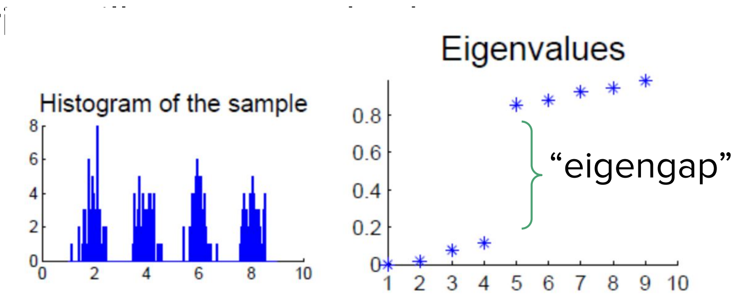
1. Construct a similarity graph and its weighted adjacency matrix W
2. Compute the normalized Laplacian L_{sym}
3. Compute the first K eigenvectors of L_{sym} and collect as the columns of a matrix U
4. Normalized the rows of U to have norm 1
5. Cluster the rows of U using K-means or your preferred “traditional” clustering algorithm

In R: `kernlab::specc()`

Choice of K

- Open area of research

- Method-specific tools:
  - K-means, hierarchical clustering, spectral clusteri
  - NMF: cross-validation / missing data imputation
  - Spectral clustering: Eigengap heuristic



- More general idea/tool: stability
  - Data perturbations (e.g. bootstrap, subsampling)
  - Algorithmic perturbations (e.g., random initialization)

- Still, it’s a tough problem...

But what if we didn’t have to choose K!?

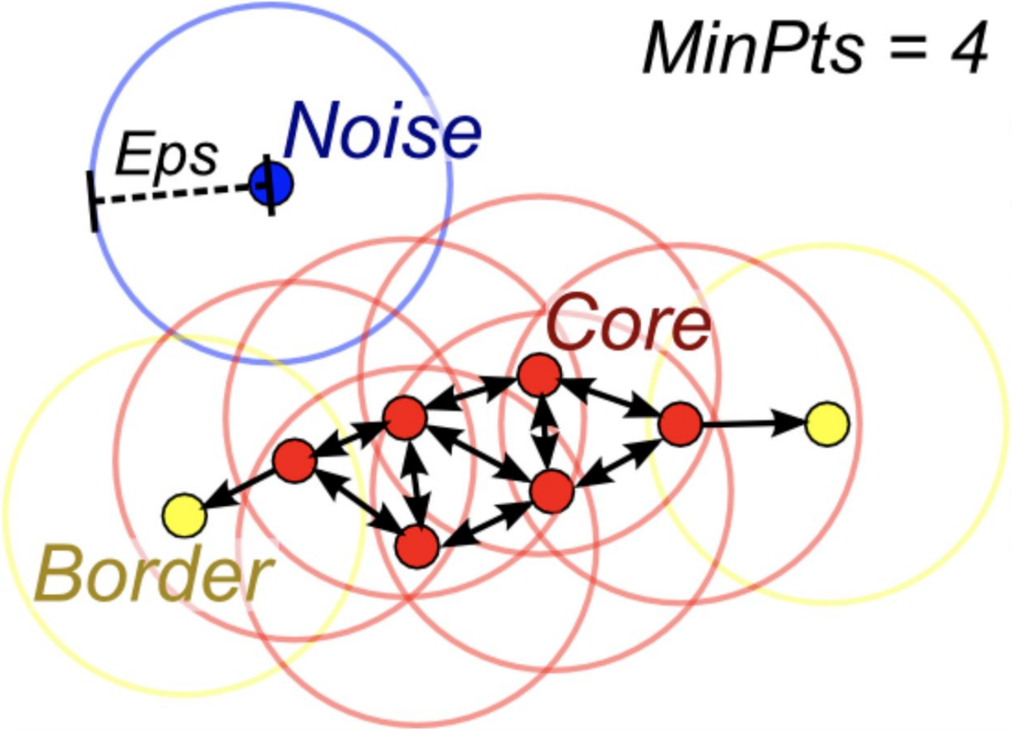
DBSCAN (Ester, Martin, et al. 1996)

- Density-based clustering
- **Idea**: group together points that are closely packed together (points with many nearby neighbors) while marking points that lie in low-density regions as outliers
- Choose (two?) parameters:
  - ε: how close points should be to each other to be in the same cluster (so we need a distance metric)
  - minPts = minimum number of points require to form a dense region

Source: https://medium.com/@elutins/dbscan-what-is-it-when-to-use-it-how-to-use-it-8bd506293818

The slides on DBSCAN thanks to Tiffany Tang

DBSCAN



Red: Core Points

Yellow: Border points. Still part of the cluster because it's within epsilon of a core point, but not does not meet the min_points criteria

Blue: Noise point. Not assigned to a cluster

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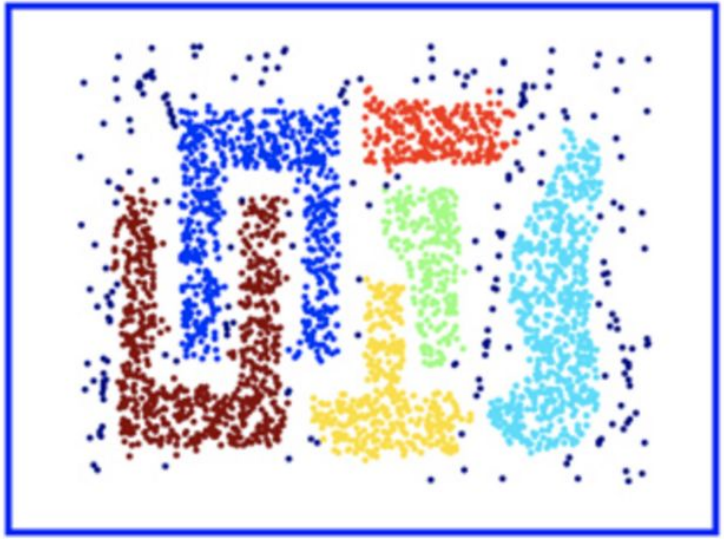
DBSCAN



In R: `dbscan::dbscan()`

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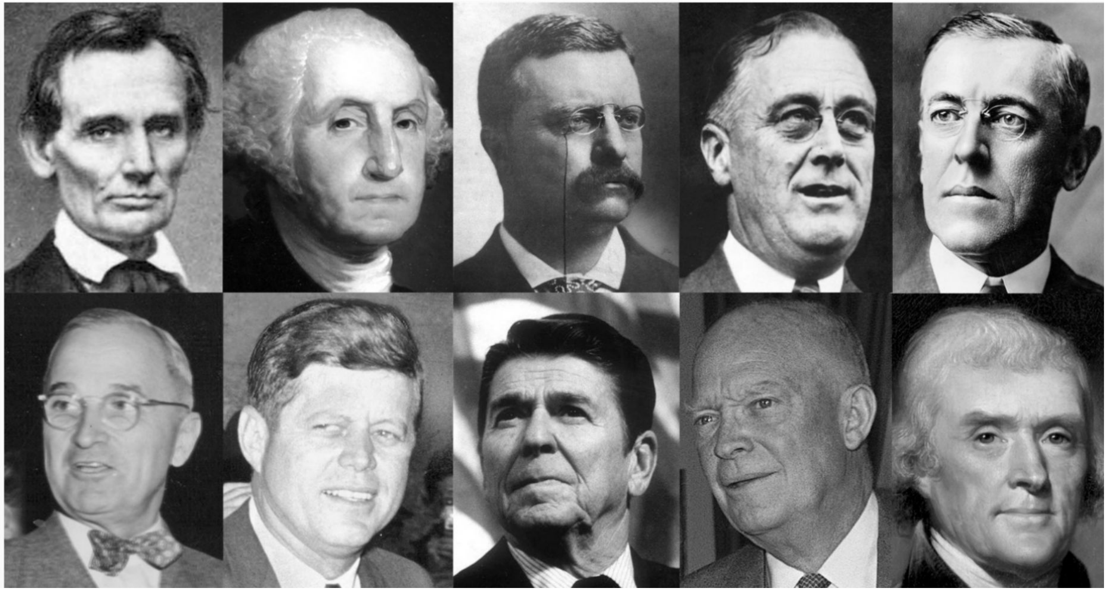
Presidential speech dataset

See quick example in `clustering_demo.R` in the week6 folder



DBSCAN

Advantages:

- Don’t have to choose K (but depends on choice of ε and minPts)
- Great for spatial data
- Great at separating clusters of similar densities that are well separated
- Robust to outliers
- Flexible to arbitrarily-shaped clusters

Disadvantages

- If the data and scale are not well understood, choosing a meaningful distance threshold ε and minPts can be difficult
- Struggles when clusters are of varying densities since (ε , minPts) cannot be chosen appropriately for all clusters
- Curse of dimensionality when distance metric is Euclidean distance
- Algorithm depends on ordering of points; border points that are reachable from more than one cluster can be part of either cluster, depending on the order the data are processed

In-class labs

- **Week 1**: tidyverse basics
- **Week 2**: ggplot + Rmd tips and tricks
- **Week 3**: more ggplot + additional plotting tools (pair plots, heatmaps, etc.)
- **Week 4**: PCA
- **Week 5**: K-means, hierarchical clustering NMF