# HEART: Statistics and Data Science with Networks

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2 Clustering

Oimensionality Reduction



Figure: Source: https://towardsdatascience.com/no-machine-learning-is-not-just-glorified-statistics-26d3952234e3

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- Textbooks often focus on estimation and prediction

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- Linear regression is principled, and neural networks work on real problems
- Even still, we do not understand everything about linear regression!
- I am happy to discuss this more with anyone

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Figure: Source: https://xkcd.com/1838/

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- Clustering assumes data come from a mixture and seeks to estimate the clusters
- Examples of Clustering Algorithms:
  - K-Means (uses only means)
  - Expectation Maximization Algorithm (Mixtures of Gaussians)
  - K-Medoids
  - and more!



Figure: Source: https://www.geeksforgeeks.org/clustering-in-machine-learning/

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- Goal: start with some complex, high-dimensional data and want to obtain representations of each data point in a smaller dimension
- Examples:
  - Manifold Learning
  - Principal Components Analysis
  - Spectral Embeddings
- Why would we want to do this?

## **Dimensionality Reduction for Graphs**

• Start with *n* × *n* Adjacency matrix

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- Start with *n* × *n* Adjacency matrix
- Obtain a graph embedding of dimension  $n \times d$
- Idea is *d* is small (e.g. for SBM it is the rank of the SBM)

How to do dimensionality reduction for graphs?

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- Set either Û or X as the graph embedding where Û is the n × d matrix whose columns are û<sub>i</sub> or X as the n × d matrix

$$\hat{X} := \hat{U}\hat{\Lambda}^{1/2}$$

Practical considerations:

- This requires knowing d in advance but we know how to choose d now
- For large graphs, computing eigenvectors and eigenvalues can be computationally intensive, so may want to use irlba or randomized SVD algorithms that reduce computation time
- For this class, the SVD and eigendecomposition are essentially the same (SVD works on rectangular matrices, but eigendecompositions only work on square matrices)
- Can be modified to obtain a general procedure for general data by computing a similarity matrix *S* between data points (e.g. using a Gaussian kernel or other method)

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Now we get to spectral clustering:

- Starting with a graph, obtain  $n \times d$  graph embedding matrix  $\hat{X}$  or  $\hat{U}$  whose rows are vertex representations
- Cluster the rows of this matrix using K-means or other clustering method



 Principal Components Analysis assumes data are linear combination of underlying variables

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- Lots of theory exists in fixed-dimension, high-dimension, and more

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- First component of PCA maximizes the variance along that direction

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Figure: Source: https://towardsdatascience.com/pca-is-not-feature-selection-3344fb764ae6

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## Manifold Learning

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- Example: X<sub>i</sub> are from the unit sphere in ℝ<sup>D</sup>, then M is of dimension d = D − 1
- Manifold Learning seeks to uncover this manifold structure
- Lots of algorithms exist (see Wiki on nonlinear dimensionality reduction)



Figure: Source: https://www.semanticscholar.org/paper/Algorithmsfor-manifold-learning-

Cayton/100dcf6aa83ac559c83518c8a41676b1a3a55fc0/figure/0