# HEART: Statistics and Data Science with Networks 

Joshua Agterberg

Johns Hopkins University

## Outline

(1) Data Science
(2) Clustering

3 Dimensionality Reduction


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

## Crash Course on Data Science and Machine Learning

- Broadly speaking, there are two areas of machine learning


## Crash Course on Data Science and Machine Learning

- Broadly speaking, there are two areas of machine learning
- Supervised learning:
- Regression (continuous response)


## Crash Course on Data Science and Machine Learning

- Broadly speaking, there are two areas of machine learning
- Supervised learning:
- Regression (continuous response)
- Classification (categorical response variable)


## Crash Course on Data Science and Machine Learning

- Broadly speaking, there are two areas of machine learning
- Supervised learning:
- Regression (continuous response)
- Classification (categorical response variable)
- Unsupervised learning:
- No specific response variable


## Crash Course on Data Science and Machine Learning

- Broadly speaking, there are two areas of machine learning
- Supervised learning:
- Regression (continuous response)
- Classification (categorical response variable)
- Unsupervised learning:
- No specific response variable
- Dimensionality Reduction


## Crash Course on Data Science and Machine Learning

- Broadly speaking, there are two areas of machine learning
- Supervised learning:
- Regression (continuous response)
- Classification (categorical response variable)
- Unsupervised learning:
- No specific response variable
- Dimensionality Reduction
- Clustering


## Crash Course on Data Science and Machine Learning

- Broadly speaking, there are two areas of machine learning
- Supervised learning:
- Regression (continuous response)
- Classification (categorical response variable)
- Unsupervised learning:
- No specific response variable
- Dimensionality Reduction
- Clustering
- Manifold Learning


## Crash Course on Data Science and Machine Learning

- Broadly speaking, there are two areas of machine learning
- Supervised learning:
- Regression (continuous response)
- Classification (categorical response variable)
- Unsupervised learning:
- No specific response variable
- Dimensionality Reduction
- Clustering
- Manifold Learning


## Crash Course on Data Science and Machine Learning

- Broadly speaking, there are two areas of machine learning
- Supervised learning:
- Regression (continuous response)
- Classification (categorical response variable)
- Unsupervised learning:
- No specific response variable
- Dimensionality Reduction
- Clustering
- Manifold Learning
- In either case, the resulting inference task may still be hypothesis testing, estimation, or prediction


## Crash Course on Data Science and Machine Learning

- Broadly speaking, there are two areas of machine learning
- Supervised learning:
- Regression (continuous response)
- Classification (categorical response variable)
- Unsupervised learning:
- No specific response variable
- Dimensionality Reduction
- Clustering
- Manifold Learning
- In either case, the resulting inference task may still be hypothesis testing, estimation, or prediction
- Textbooks often focus on estimation and prediction


## Crash Course on Data Science and Machine Learning

- Machine Learning can be closer to engineering or closer to statistics


## Crash Course on Data Science and Machine Learning

- Machine Learning can be closer to engineering or closer to statistics
- I believe machine learning should be principled, but many just believe it should do well on real problems


## Crash Course on Data Science and Machine Learning

- Machine Learning can be closer to engineering or closer to statistics
- I believe machine learning should be principled, but many just believe it should do well on real problems
- Linear regression is principled, and neural networks work on real problems


## Crash Course on Data Science and Machine Learning

- Machine Learning can be closer to engineering or closer to statistics
- I believe machine learning should be principled, but many just believe it should do well on real problems
- Linear regression is principled, and neural networks work on real problems
- Even still, we do not understand everything about linear regression!


## Crash Course on Data Science and Machine Learning

- Machine Learning can be closer to engineering or closer to statistics
- I believe machine learning should be principled, but many just believe it should do well on real problems
- 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


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

## Clustering

- Clustering assumes data come from a mixture and seeks to estimate the clusters


## Clustering

- 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/

## Dimensionality Reduction

- Goal: start with some complex, high-dimensional data and want to obtain representations of each data point in a smaller dimension


## Dimensionality Reduction

- 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


## Dimensionality Reduction

- 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 $n \times n$ Adjacency matrix


## Dimensionality Reduction for Graphs

- Start with $n \times n$ 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)


## Dimensionality Reduction for Graphs

How to do dimensionality reduction for graphs?
(1) Let $S$ be a similarity matrix (e.g. adjacency matrix or Laplacian matrix)

## Dimensionality Reduction for Graphs

How to do dimensionality reduction for graphs?
(1) Let $S$ be a similarity matrix (e.g. adjacency matrix or Laplacian matrix)
(2) Compute biggest $d$ eigenvalues and corresponding eigenvectors of $S$, call them $\hat{u}_{1}, \ldots, \hat{u}_{d}$ and $\hat{\lambda}_{1}, \ldots, \hat{\lambda}_{d}$

## Dimensionality Reduction for Graphs

How to do dimensionality reduction for graphs?
(1) Let $S$ be a similarity matrix (e.g. adjacency matrix or Laplacian matrix)
(2) Compute biggest $d$ eigenvalues and corresponding eigenvectors of $S$, call them $\hat{u}_{1}, \ldots, \hat{u}_{d}$ and $\hat{\lambda}_{1}, \ldots, \hat{\lambda}_{d}$
(3) Set either $\hat{U}$ or $\hat{X}$ as the graph embedding where $\hat{U}$ is the $n \times d$ matrix whose columns are $\hat{u}_{i}$ or $\hat{X}$ as the $n \times d$ matrix

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

## Dimensionality Reduction for Graphs

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)


## Spectral Clustering and Community Detection

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
- Principal Components Analysis assumes data are linear combination of underlying variables
- Lots of theory exists in fixed-dimension, high-dimension, and more
- Principal Components Analysis assumes data are linear combination of underlying variables
- Lots of theory exists in fixed-dimension, high-dimension, and more
- Highly intuitive explanation in terms of covariances and singular value decompositions
- Principal Components Analysis assumes data are linear combination of underlying variables
- Lots of theory exists in fixed-dimension, high-dimension, and more
- Highly intuitive explanation in terms of covariances and singular value decompositions
- First component of PCA maximizes the variance along that direction


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

## Manifold Learning

- Assume we observe $X_{i} \in \mathbb{R}^{D}$, where $D$ is very large


## Manifold Learning

- Assume we observe $X_{i} \in \mathbb{R}^{D}$, where $D$ is very large
- Idea is $X_{i}$ are noisy observations of a manifold $\mathcal{M} \subset \mathbb{R}^{D}$, where $\mathcal{M}$ is of dimension $d<D$


## Manifold Learning

- Assume we observe $X_{i} \in \mathbb{R}^{D}$, where $D$ is very large
- Idea is $X_{i}$ are noisy observations of a manifold $\mathcal{M} \subset \mathbb{R}^{D}$, where $\mathcal{M}$ is of dimension $d<D$
- Example: $X_{i}$ are from the unit sphere in $\mathbb{R}^{D}$, then $\mathcal{M}$ is of dimension $d=D-1$


## Manifold Learning

- Assume we observe $X_{i} \in \mathbb{R}^{D}$, where $D$ is very large
- Idea is $X_{i}$ are noisy observations of a manifold $\mathcal{M} \subset \mathbb{R}^{D}$, where $\mathcal{M}$ is of dimension $d<D$
- Example: $X_{i}$ are from the unit sphere in $\mathbb{R}^{D}$, then $\mathcal{M}$ is of dimension $d=D-1$
- Manifold Learning seeks to uncover this manifold structure


## Manifold Learning

- Assume we observe $X_{i} \in \mathbb{R}^{D}$, where $D$ is very large
- Idea is $X_{i}$ are noisy observations of a manifold $\mathcal{M} \subset \mathbb{R}^{D}$, where $\mathcal{M}$ is of dimension $d<D$
- Example: $X_{i}$ are from the unit sphere in $\mathbb{R}^{D}$, then $\mathcal{M}$ 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/Algorithms-for-manifold-learningCayton/100dcf6aa83ac559c83518c8a41676b1a3a55fc0/figure/0

