

# K-means and Hierarchical Clustering

Schwartz

September 26, 2016

# Best. Music. EVAR

1. Elliott Smith
2. Iron and Wine
3. Damien Rice
4. Sufjan Stevens

1. Kishi Bashi
2. Beirut
3. Christine and the Queens
4. Lyle Lovett

1. Our Lady Peace
2. Oasis
3. Eve Six
4. Better than Ezra

1. Die Antwoord
2. Dan le Sac Vs Scroobius Pip
3. FuntCase & Ry Legit
4. Emalkay

1. Rage Against the Machine
2. System of a Down
3. Smashing Pumpkins
4. Jimmy Eat World

1. Beck
2. Cake
3. Beastie Boys
4. Smash Mouth

# Objectives

- ▶ *Supervised versus Unsupervised*

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- ▶ Expectation-Maximization (EM) algorithm

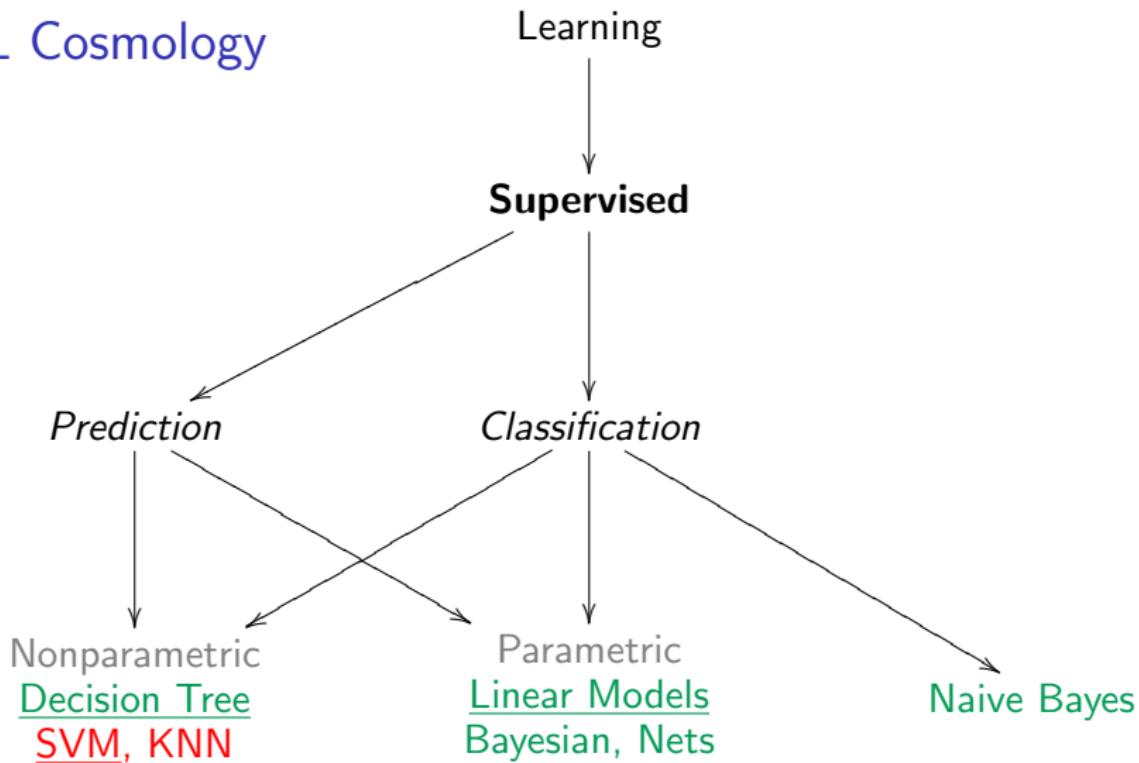
Learning



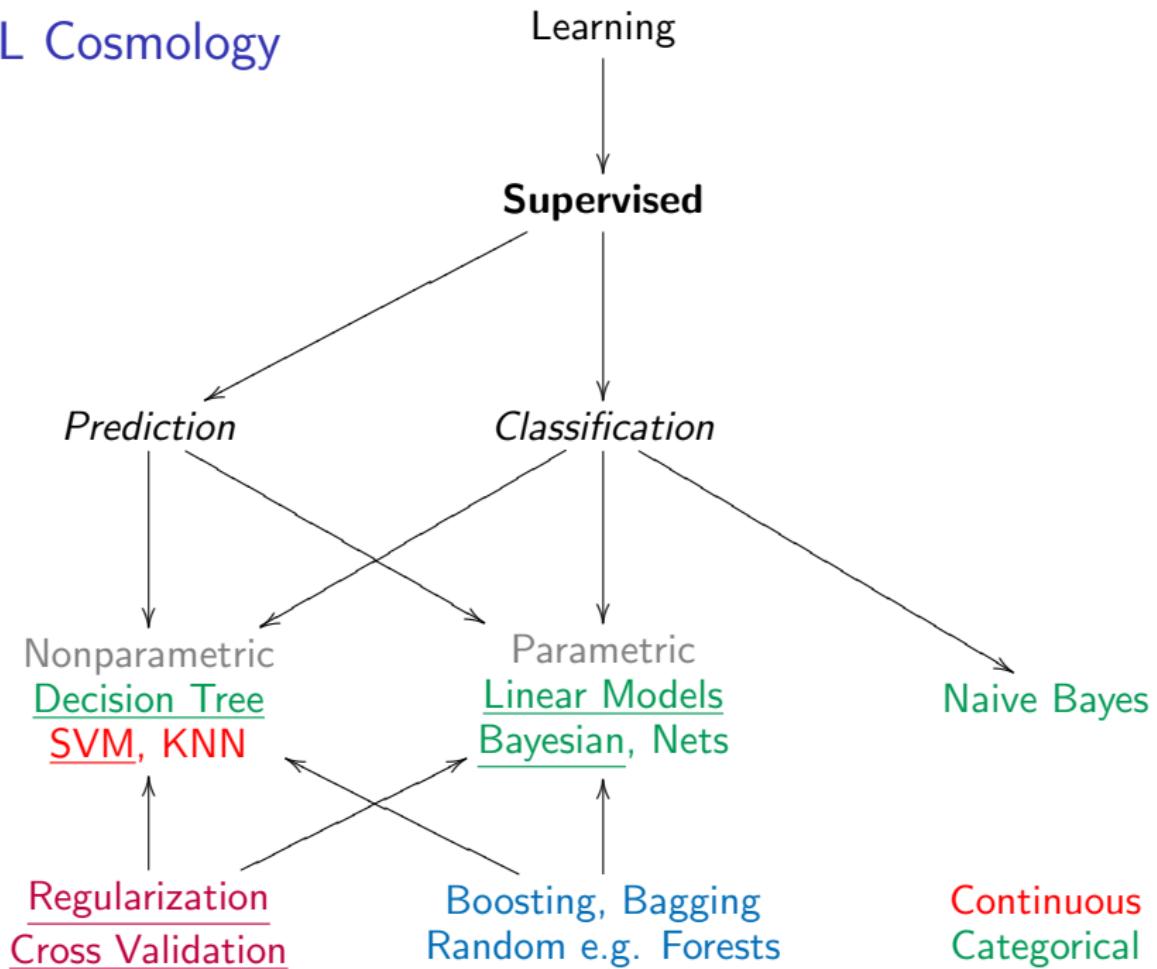
**Supervised**

*Prediction*

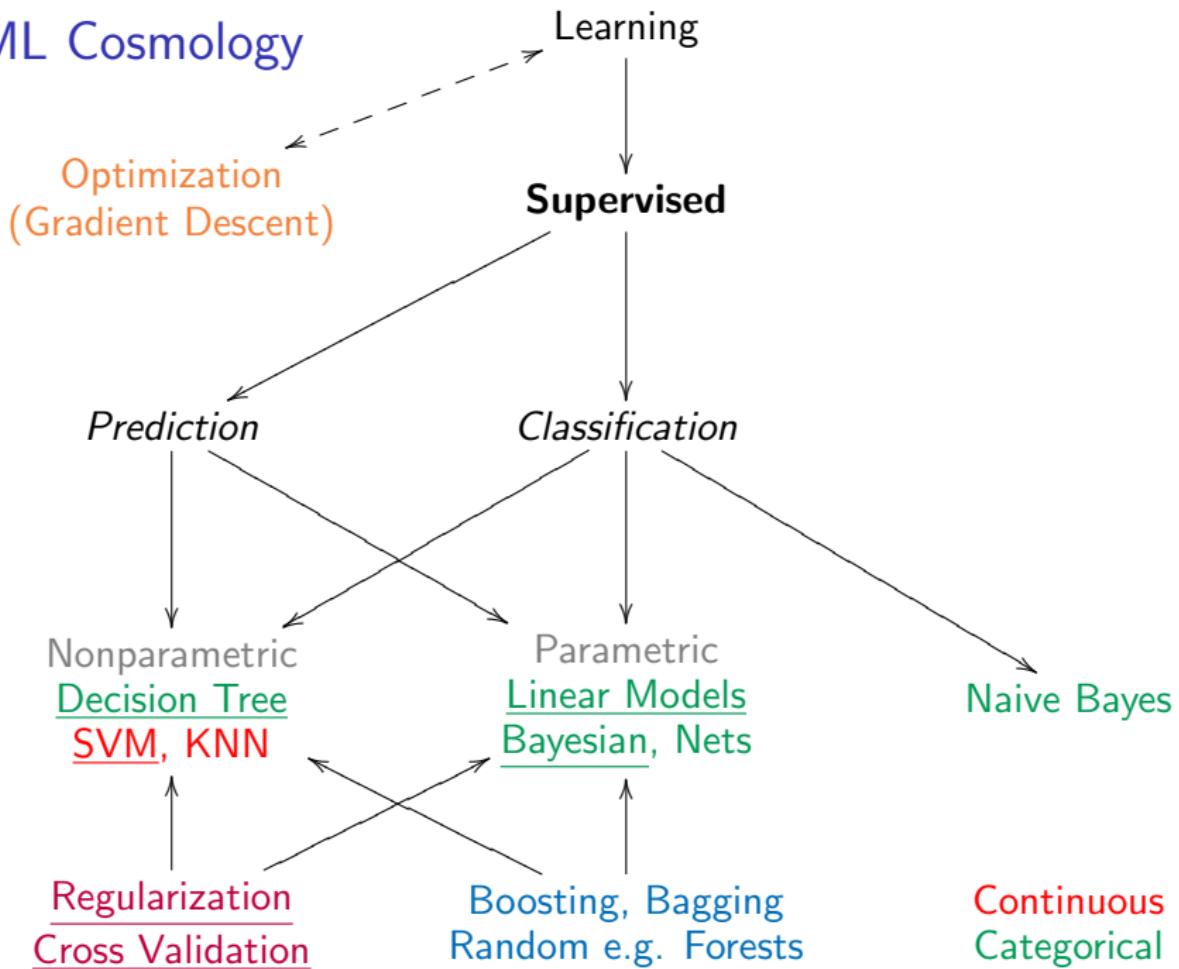
*Classification*



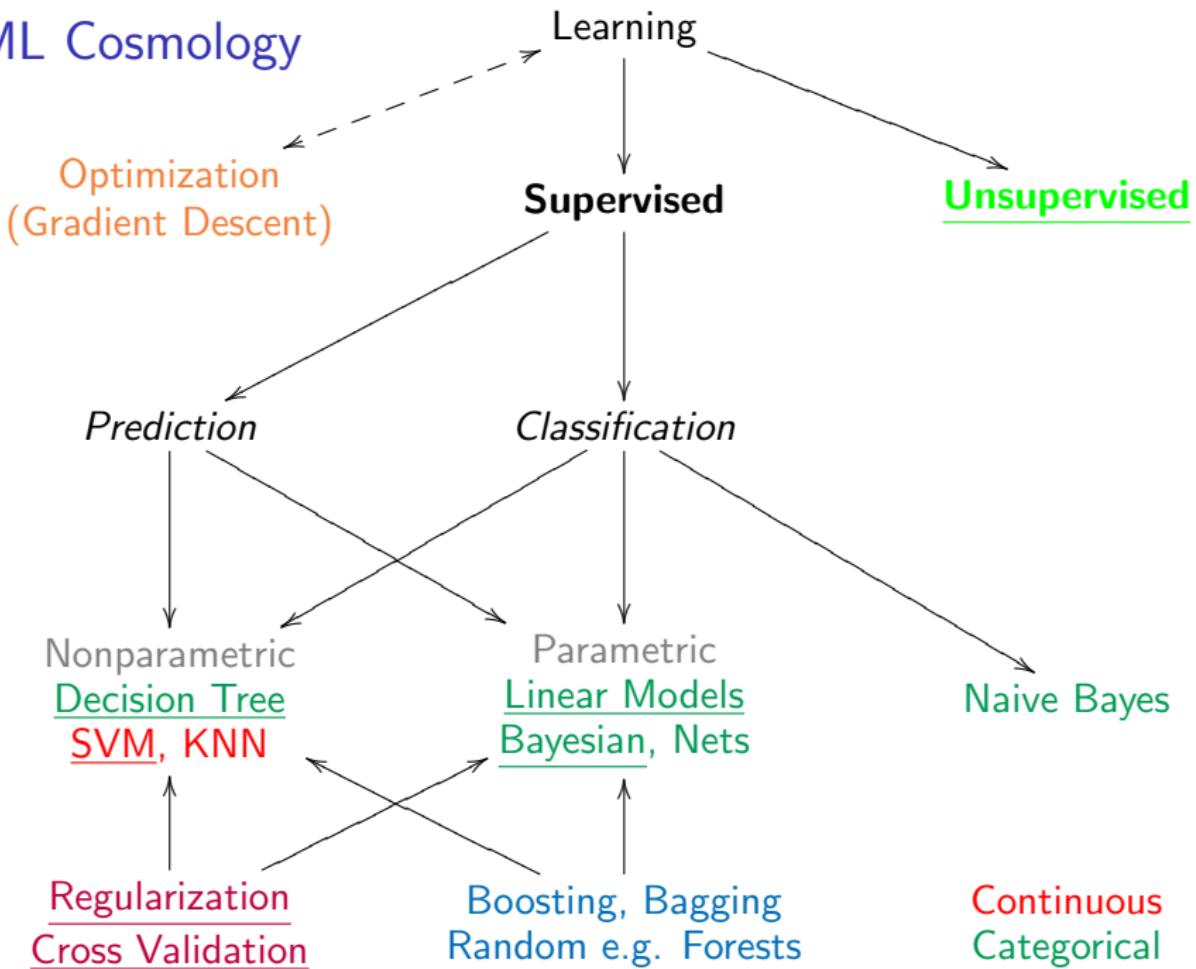
Continuous  
Categorical



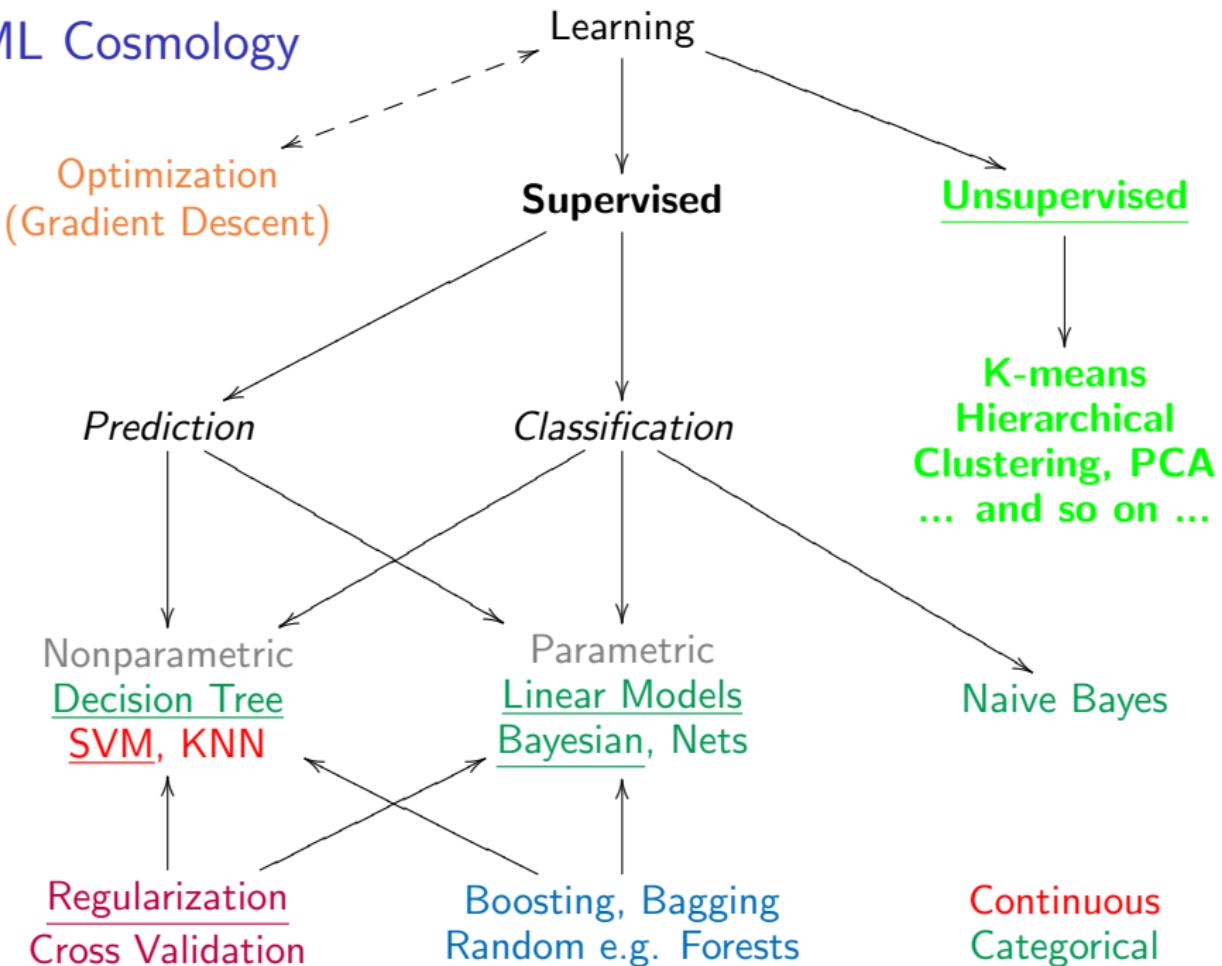
# ML Cosmology



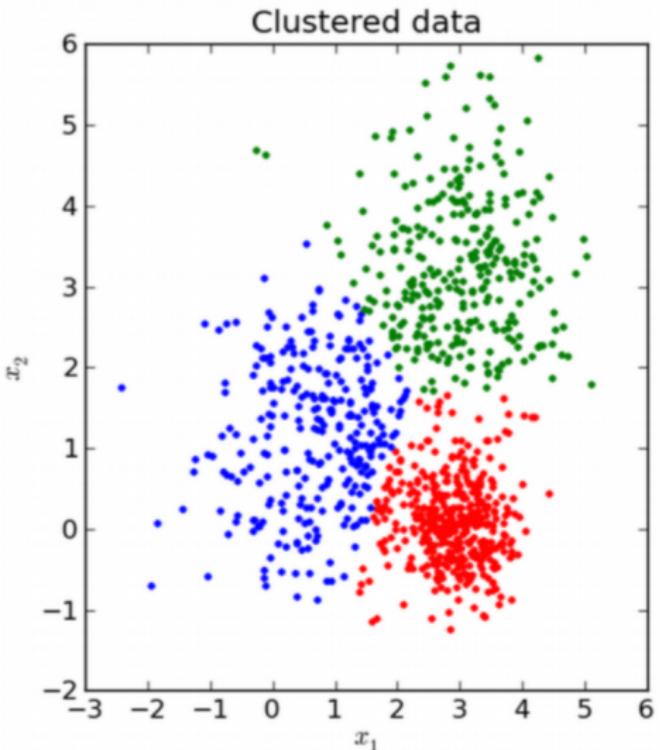
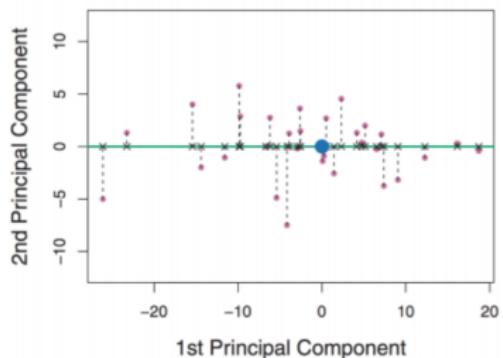
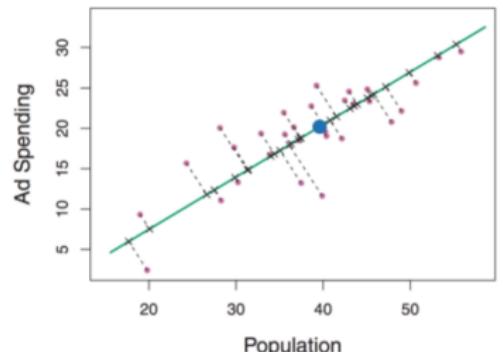
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# Unsupervised learning



Low dimensional representations  
of data capturing data variation

Homogeneous subgroups  
capturing data substructure

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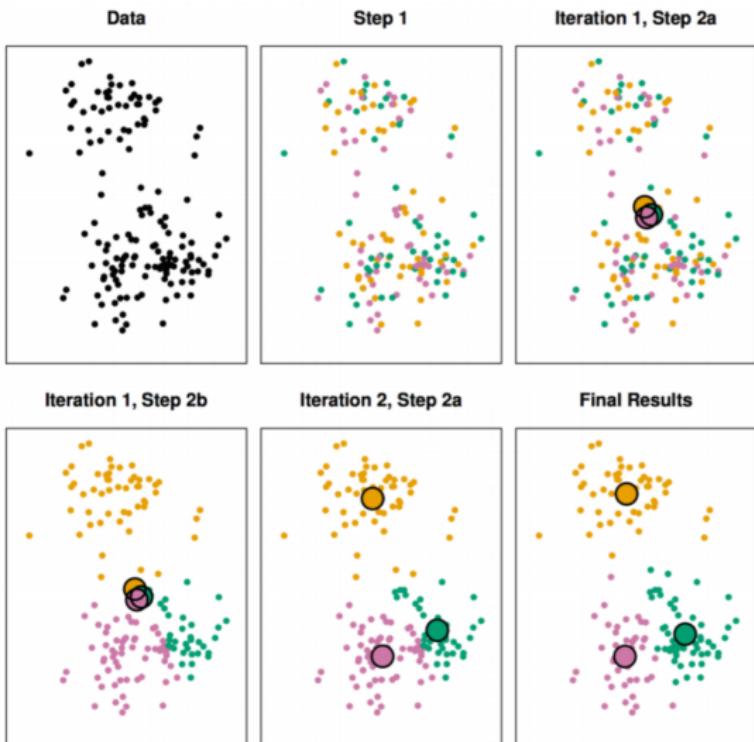
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  - Exploratory data analysis (EDA)
  - Latent data structure discovery
  - Feature engineering/Data reduction
  - Quality control (QC) preprocessing

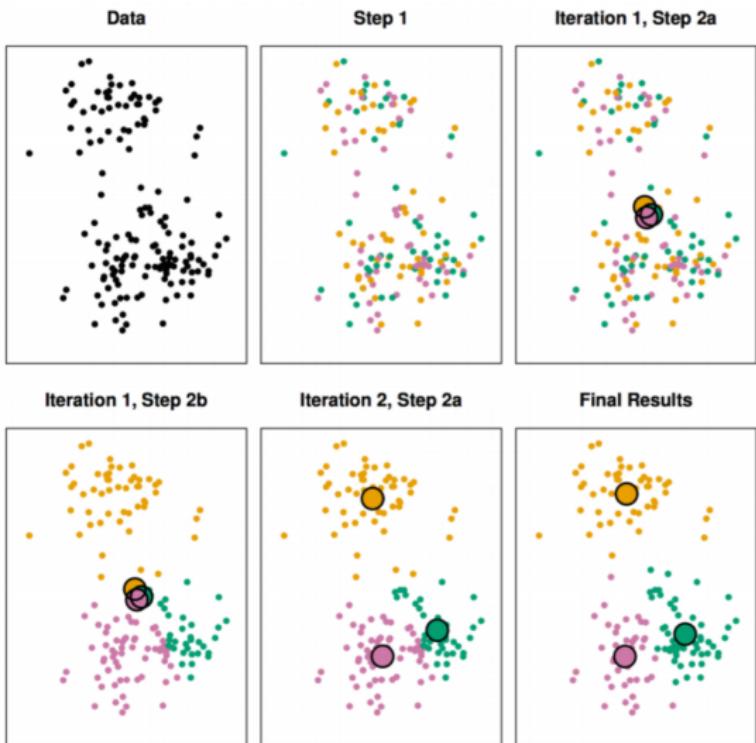
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1. Choose *number of clusters*,  $K$
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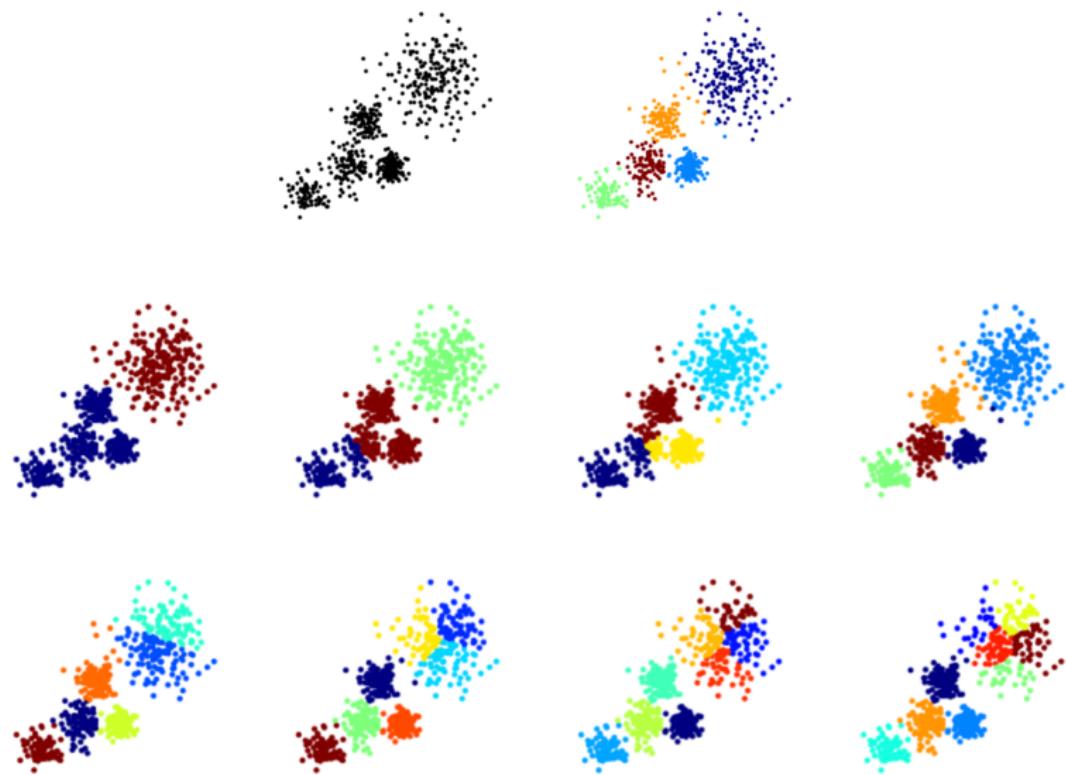
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Any other ideas?

K?



## Elbow and Silhouette methods

For some clustering

$$C_K \mapsto \{1, 2, \dots, K\}$$

clustering fit can be measured as

$$W(C_K) = \frac{1}{K} \sum_{C_K(i), C_K(j)=k} ||x_i - x_j||^2$$

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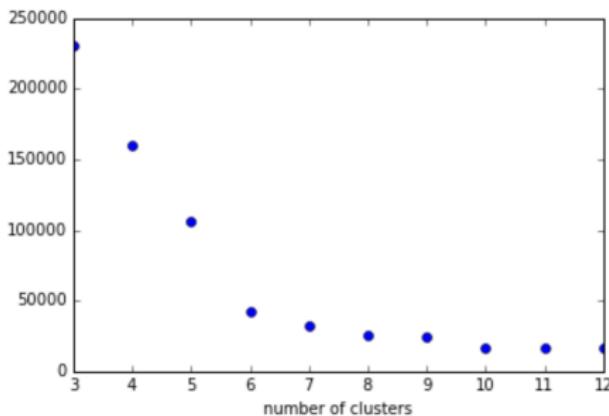
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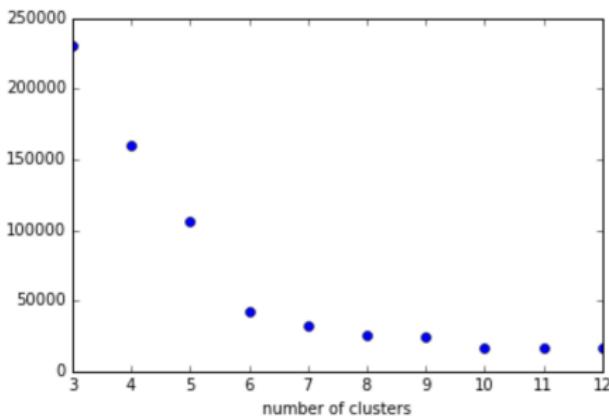
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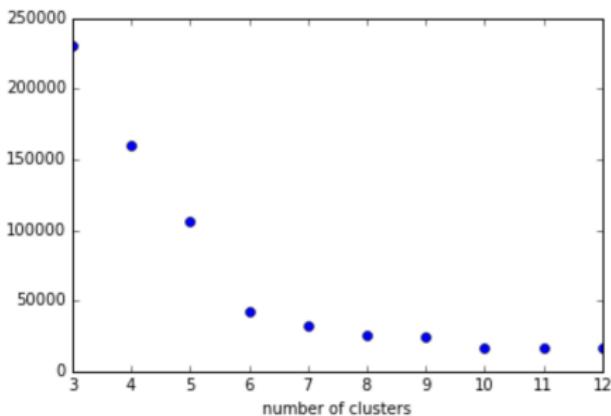
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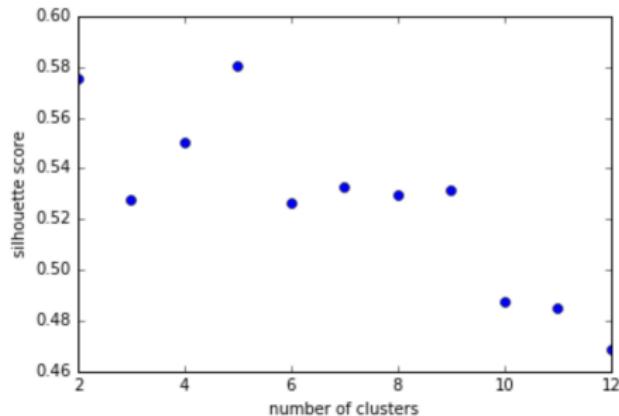
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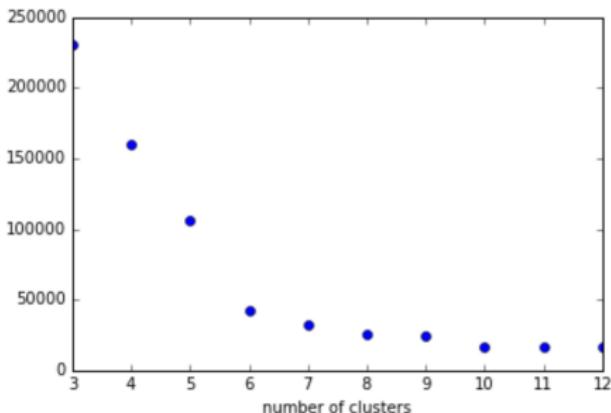
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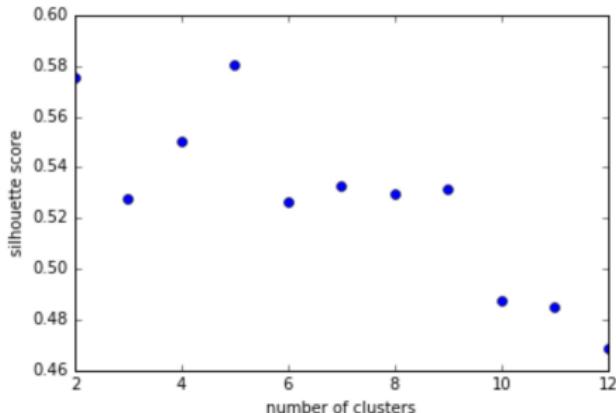
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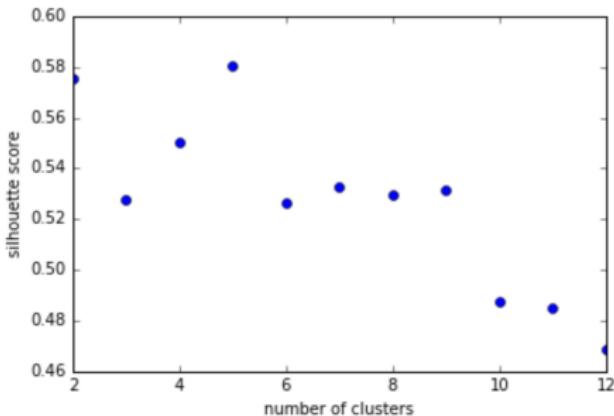
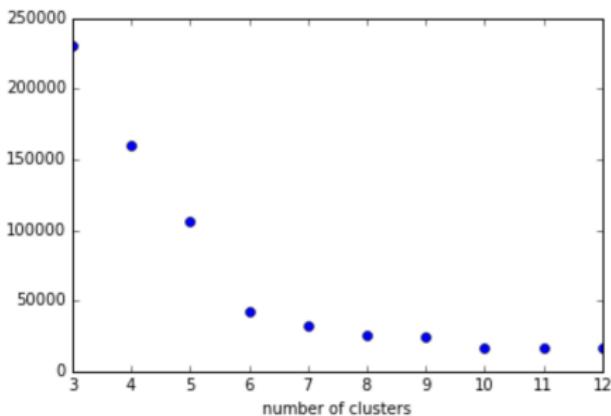
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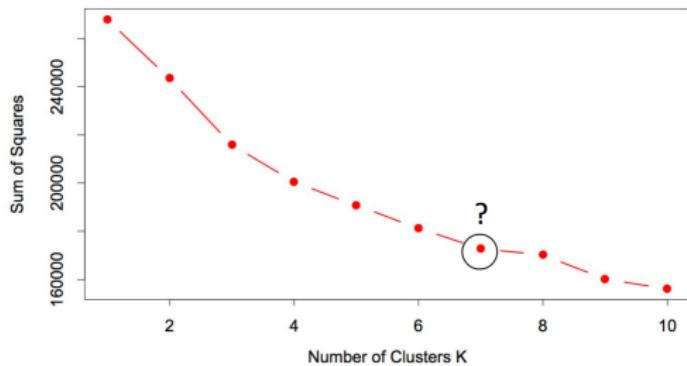
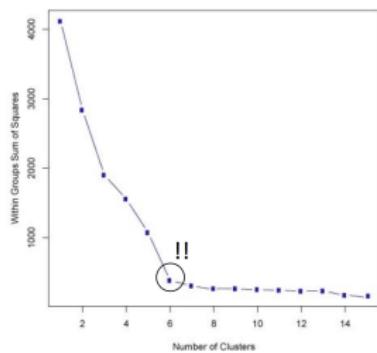
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Interpret silhouette scores?

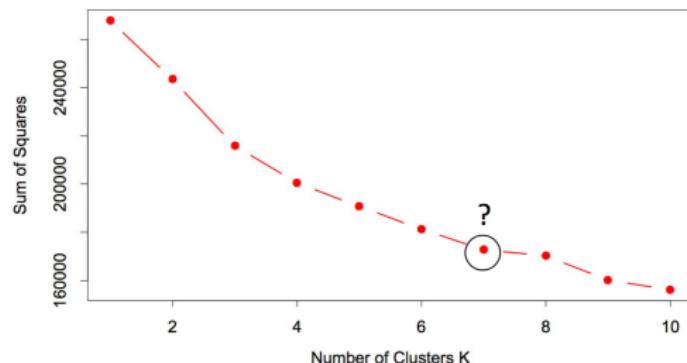
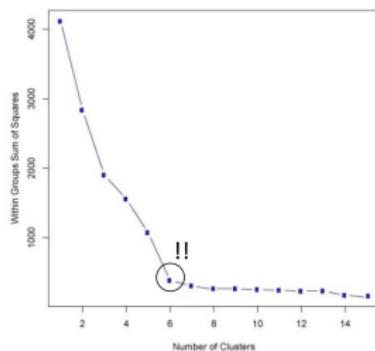
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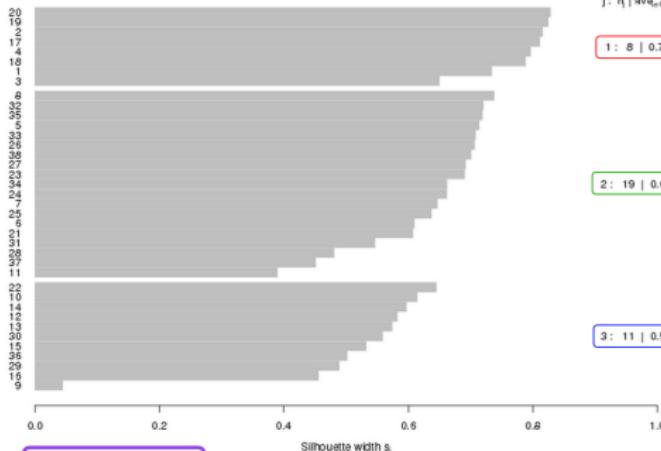


# Elbow and Silhouette methods



Silhouette plot of pam(x = cars.dist, k = 3)

n = 38



Average silhouette width : 0.63

3 clusters  $C_1$   
j: 11 | avg $s_{C_1} s_i$

1: 8 | 0.78

2: 19 | 0.64

3: 11 | 0.51

## Guidelines for Overall Avg Silhouette

Range	Interpretation
0.71 – 1.0	Strong structure found
0.51 – 0.7	Reasonable structure
0.26 – 0.5	Structure weak/artificial
< 0.25	No substantial structure

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How could we test which class is doing better?

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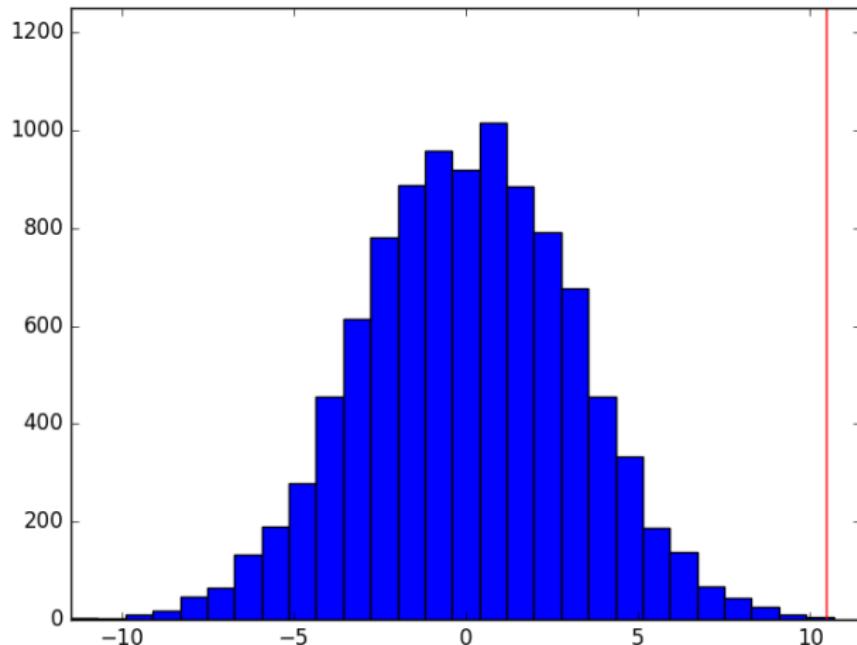
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2. These samples approximate the test statistic distribution under the null
3. Compare the test statistic to this null distribution  
to suggest how "strange" the actual observed test statistic is if the null is true

## The permutation test (*This is Scott S's favorite test!!*)

1. Permute the ids (i.e., believe the null is true: ids don't matter)
2. Recalculate the test statistic each time (under null)
3. See how strange your observed statistic is compared to nulls



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- ▶ What was needed in the permutation test was really the distribution of the test statistic under the null hypothesis
- ▶ We used permutation to get it  
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- ▶ We can test against ANY null distribution we wish to propose

# The Gap statistic

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R. Tibshirani, G. Walther and T. Hastie

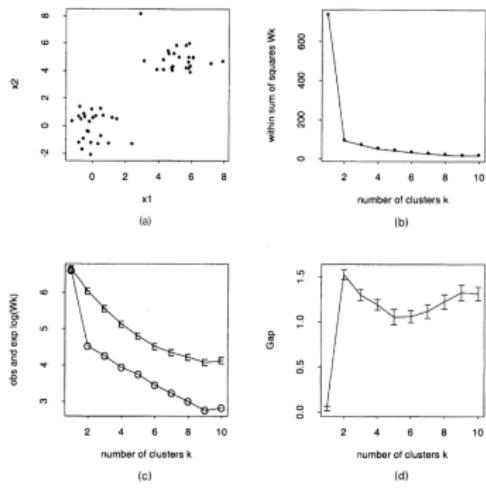


Fig. 1. Results for the two-cluster example: (a) data; (b) within sum of squares function  $W_k$ ; (c) functions  $\log(W_k)$  (O) and  $E(\log(W_k))$  (E); (d) gap curve

416

R. Tibshirani, G. Walther and T. Hastie

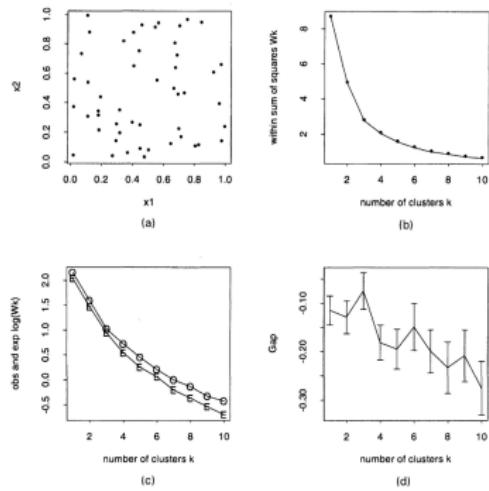


Fig. 2. Results for the uniform data example: (a) data; (b) within sum of squares function  $W_k$ ; (c) functions  $\log(W_k)$  (O) and  $E(\log(W_k))$  (E); (d) gap curve



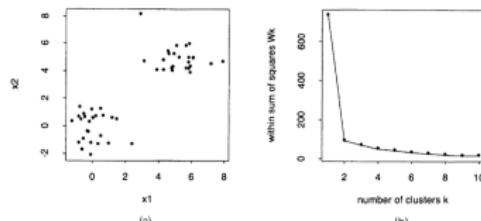
# The Gap statistic

For  $M$  null distribution samples, calculate

$$\text{Gap}(K) = \bar{I} - \log W(C_K) \quad \text{and} \quad s_K = \sqrt{\frac{1}{M} \sum_{j=1}^M (\log W_j(C_K) - \bar{I})^2}$$

$$\text{where } W_j(C_K) = \frac{1}{K} \sum_{C_K(i), C_K(j)=k} \|x_i^{(j)} - x_j^{(j)}\|^2 \quad \text{and} \quad \bar{I} = \frac{1}{M} \sum_{j=1}^M \log W_j(C_K)$$

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416 R. Tibshirani, G. Walther and T. Hastie

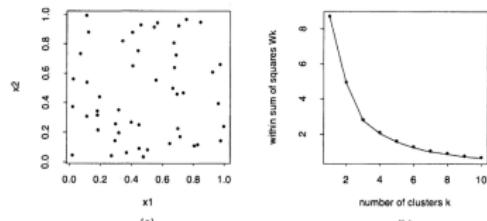


Fig. 1. Results for the two-cluster example: (a) data; (b) within sum of squares function  $W_k$ ; (c) functions  $\log(W_k)$  (O) and  $E_n(\log(W_k))$  (E); (d) gap curve

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Then choose the smallest  $K$  such that  $\text{Gap}(K) \geq \text{Gap}(K+1) - s_{K+1}$

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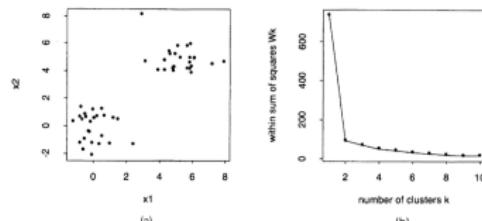


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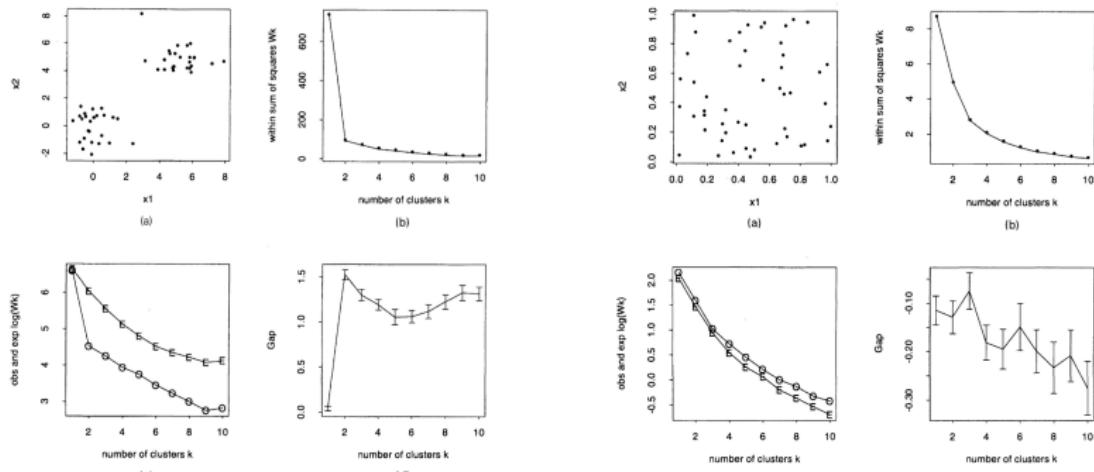


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## Curse of dimensionality

Just as nearest neighbors breaks down in high dimensional space...

Distance based clustering breaks down in high dimensional space...

## Curse of dimensionality

Just as nearest neighbors breaks down in high dimensional space...

Distance based clustering breaks down in high dimensional space...

(Go see Ryan's great slides motivating the curse of dimensionality!)

(They are in the K nearest neighbors (KNN) lecture!!)

# Challange

A

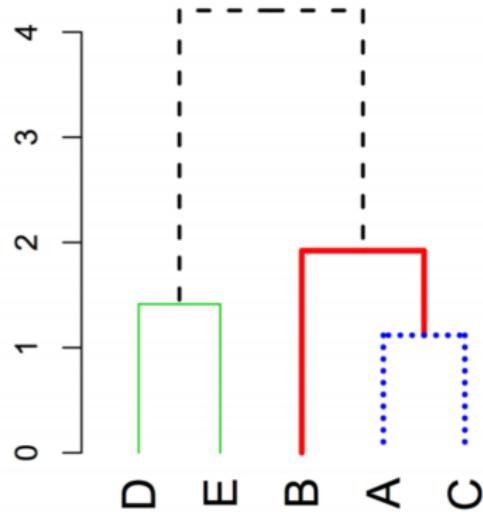
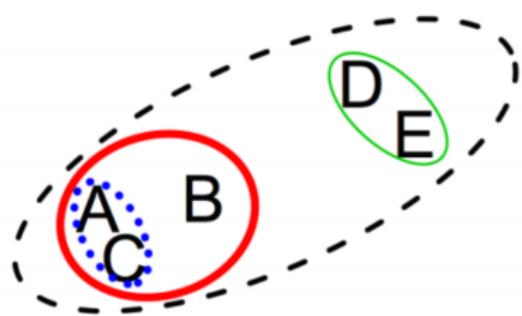
B

C

D

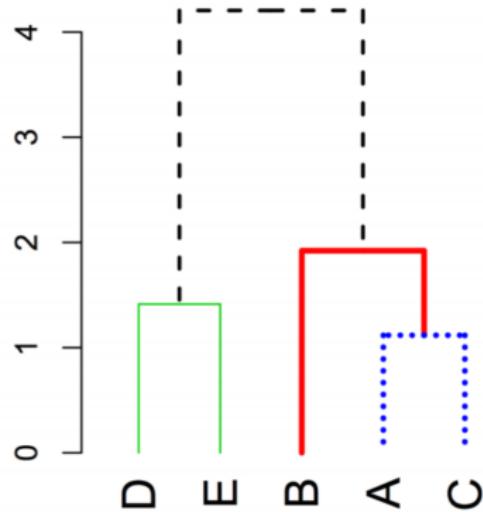
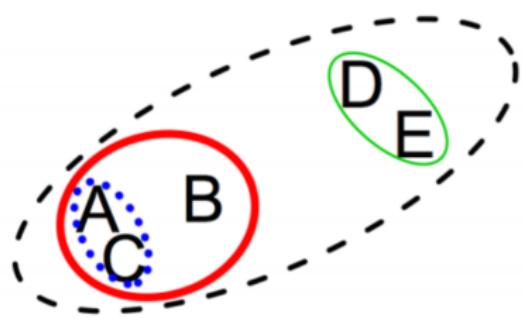
E

# Hierarchical clustering



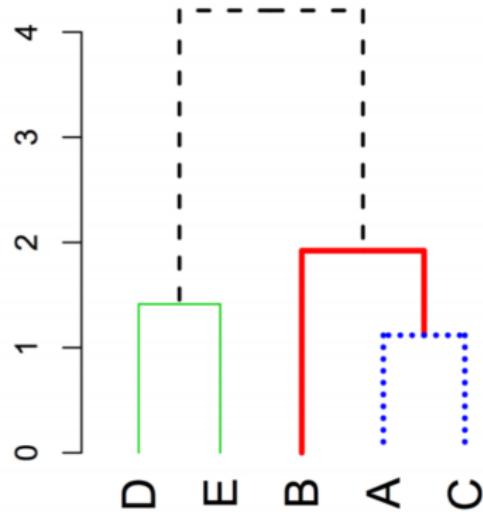
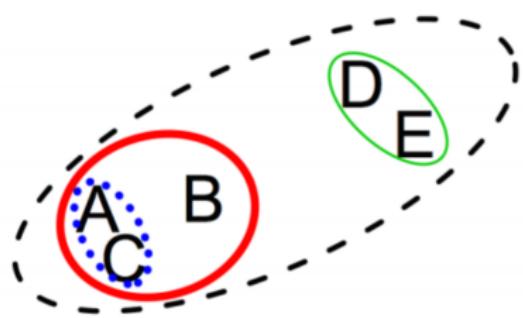
1. Assign each point to a cluster

# Hierarchical clustering



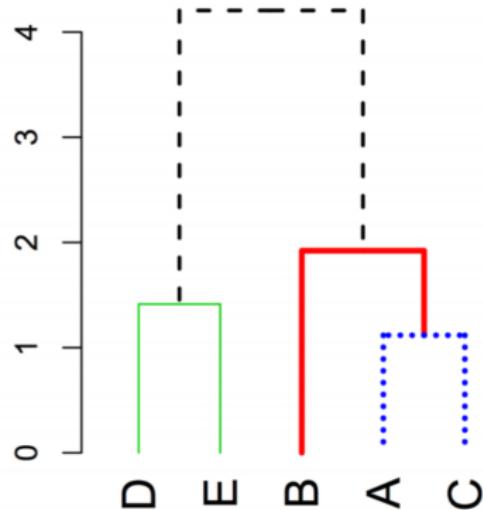
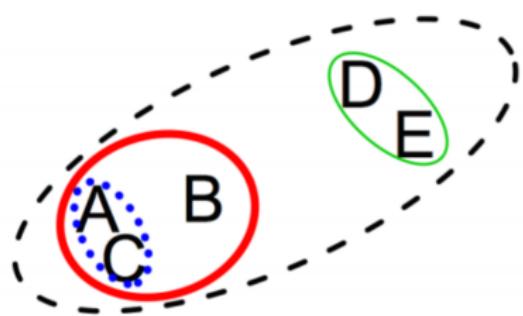
1. Assign each point to a cluster
2. Computer pairwise cluster distances

# Hierarchical clustering



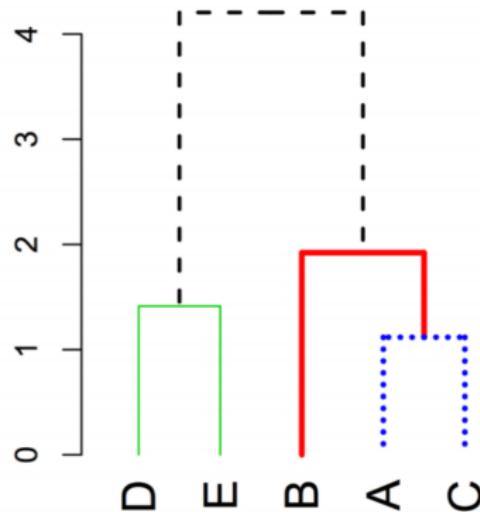
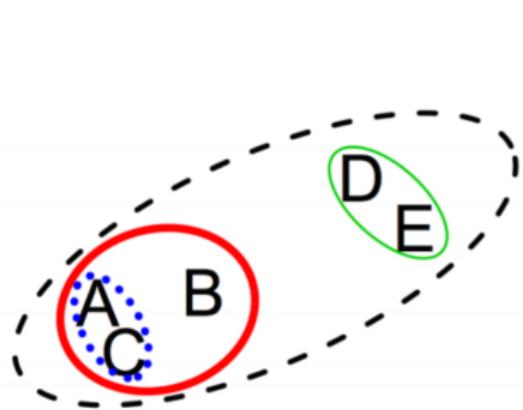
1. Assign each point to a cluster
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3. Merge *closest* two clusters

# Hierarchical clustering



1. Assign each point to a cluster
2. Computer pairwise cluster distances
3. Merge *closest two* clusters
4. Return to 2 until all clusters merged

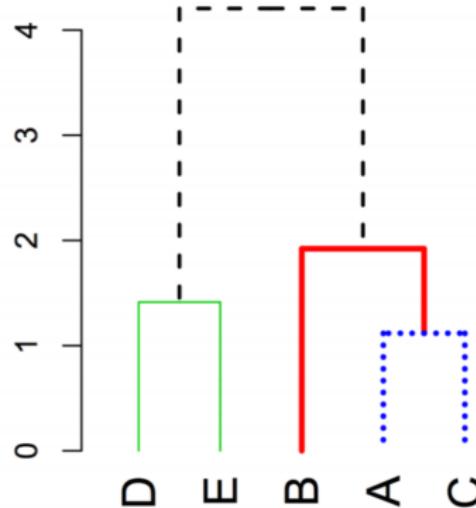
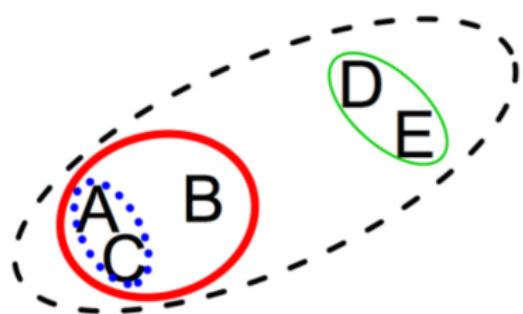
# Hierarchical clustering



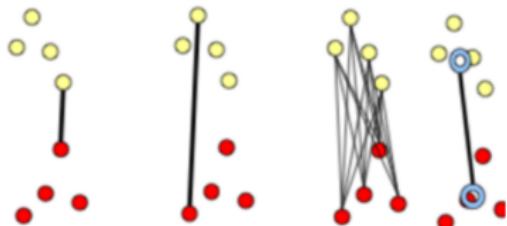
1. Assign each point to a cluster
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3. Merge *closest two clusters*
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- ▶ Single: minimum pairwise point dissimilarity
- ▶ Complete: maximum pairwise point dissimilarity
- ▶ Average: average pairwise point dissimilarity
- ▶ Centroid: centroid dissimilarity

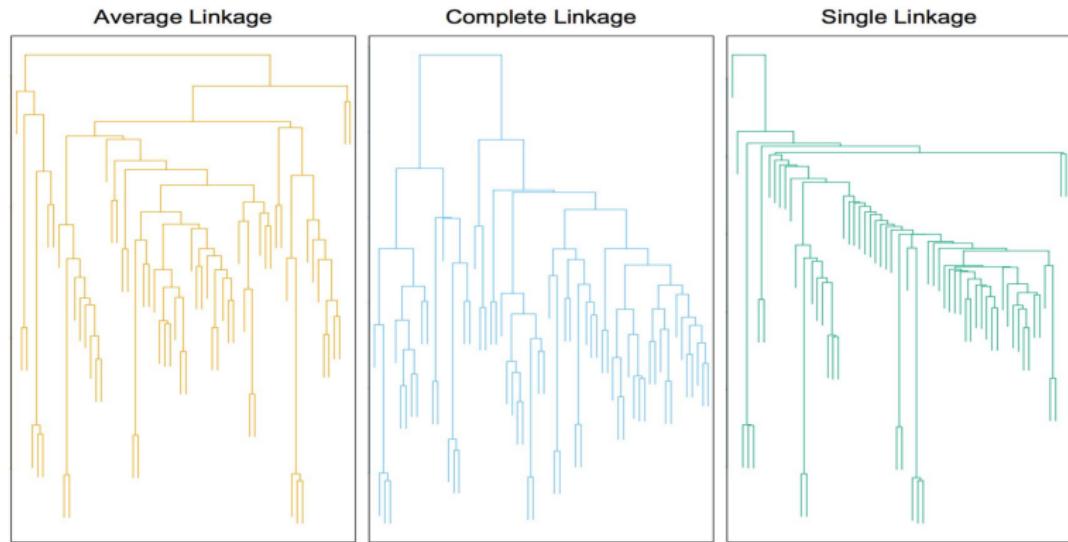
# Hierarchical clustering



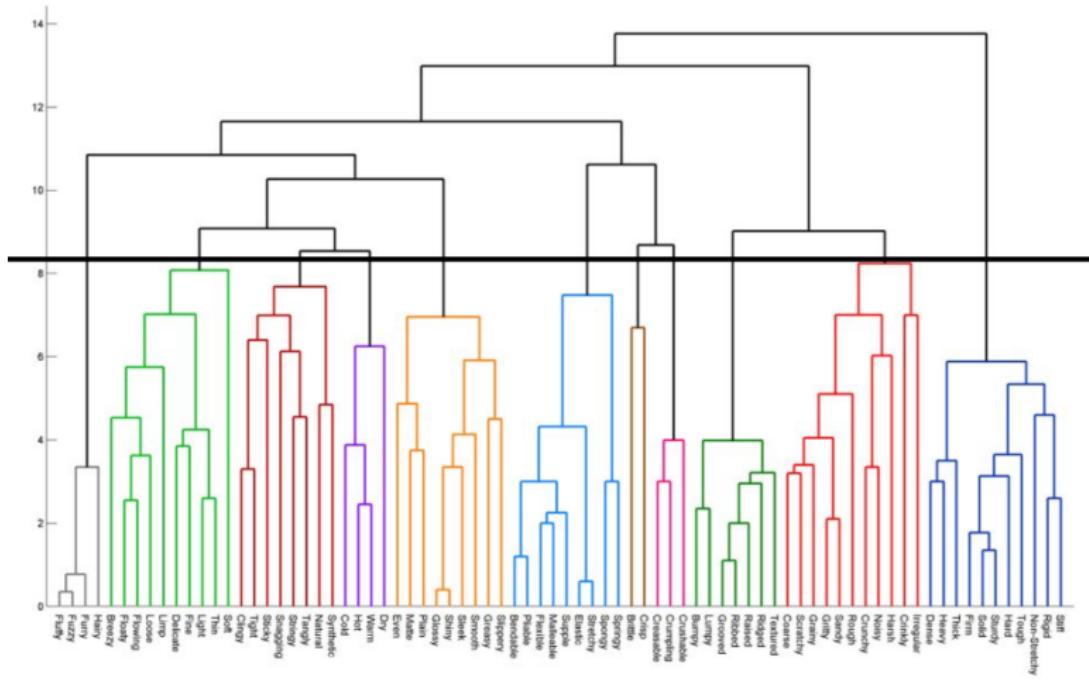
1. Assign each point to a cluster
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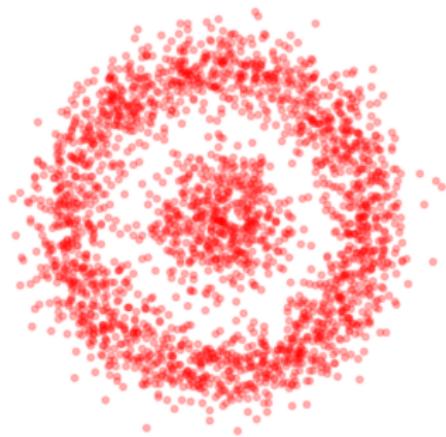
# Hierarchical clustering *distance characteristics*



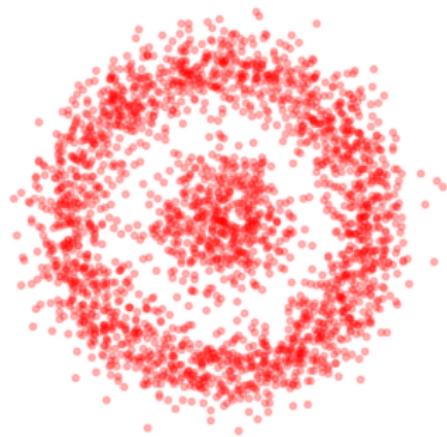
# Hierarchical clustering *cluster count*



# DBSCAN

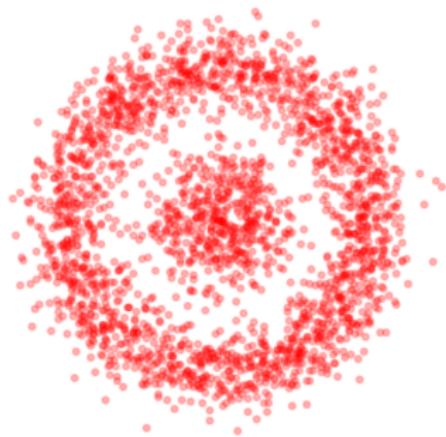


# DBSCAN



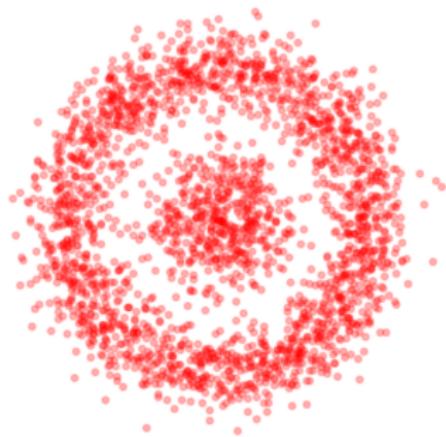
- ▶ Specify connection distance  $\epsilon$  and minimum number of points for core  $m$

# DBSCAN



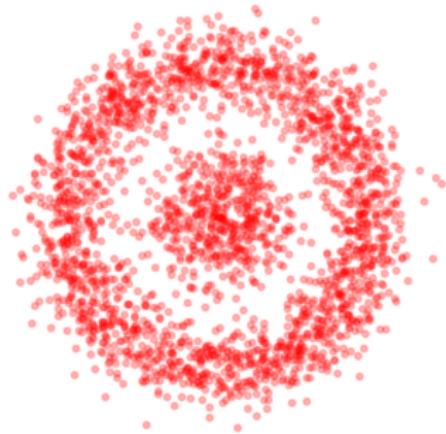
- ▶ Specify connection distance  $\epsilon$  and minimum number of points for core  $m$
- ▶ A cluster is all connected *core points*

# DBSCAN

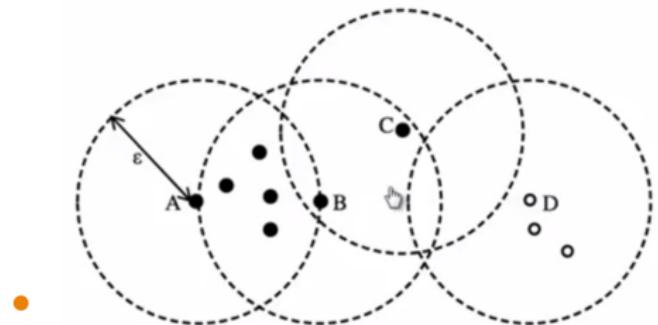


- ▶ Specify connection distance  $\epsilon$  and minimum number of points for core  $m$
- ▶ A cluster is all connected *core points*
- ▶ All other points are *noise*

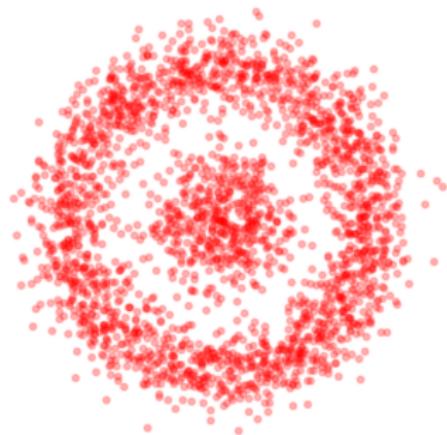
# DBSCAN



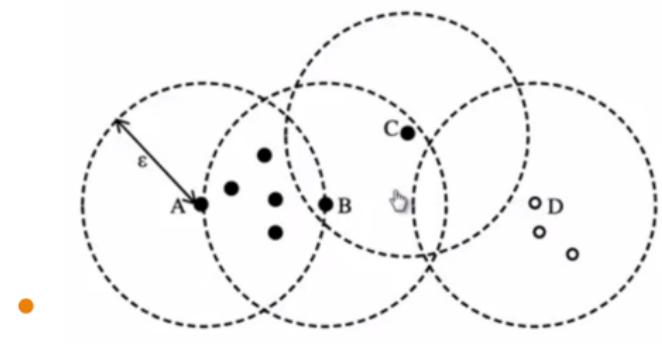
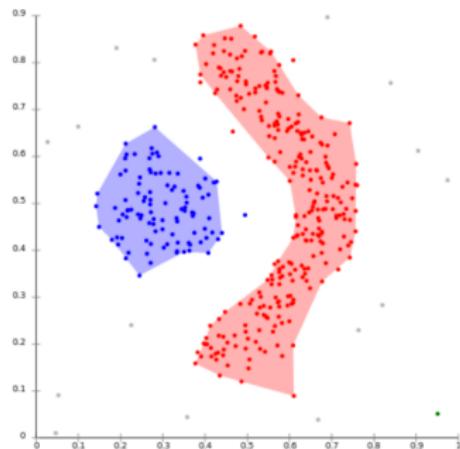
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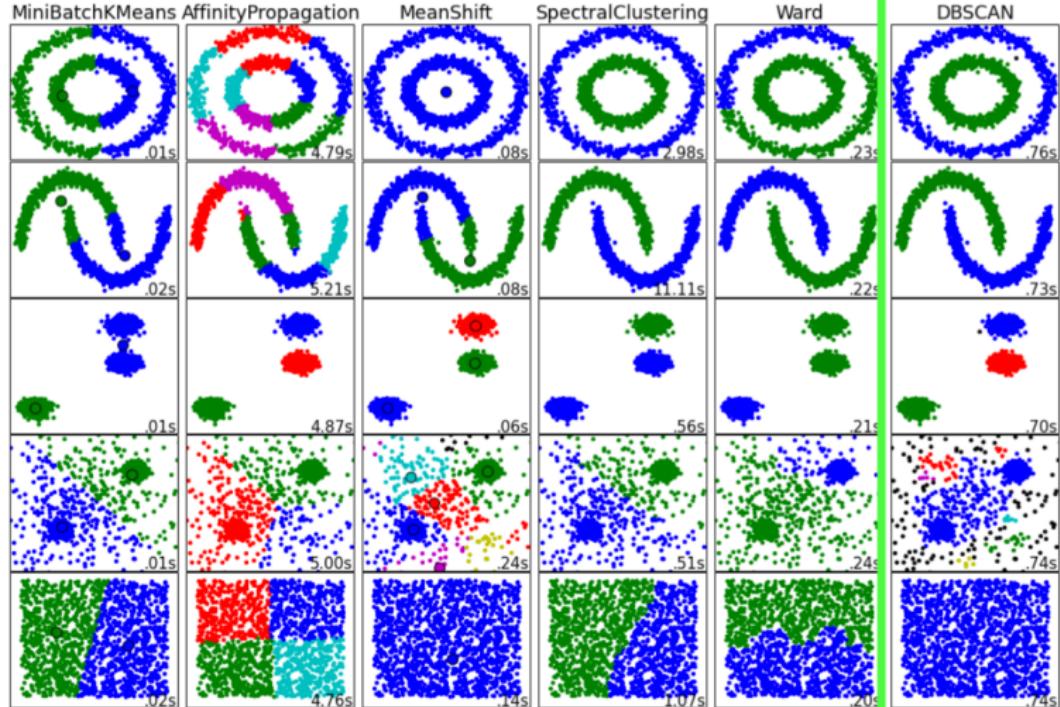
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# DBSCAN



# Bayesian Mixture Models (*xtra: Scott S's grad school jam*)

$$f(X_i|\boldsymbol{\mu}, \sigma^2, \pi, \boldsymbol{\pi}) = \sum_{k=1}^K \pi_k N(\mu_k, \sigma_k^2)$$

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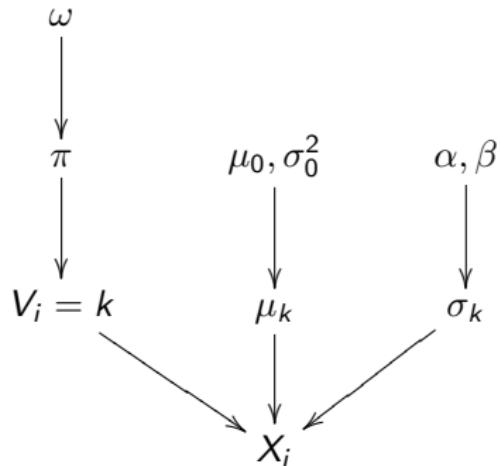
$$f(X_i|V_i, \mu, \sigma^2, \pi) = N(\mu_k, \sigma_k^2)$$

$$\Pr(V_i) = \text{Multinomial}(\pi, n=1)$$

$$f(\pi) = \text{Dirichlet}(\omega)$$

$$f(\mu_k) = N(\mu_0, \sigma_0^2)$$

$$f(\sigma_k^{-2}) = \text{Gamma}(\alpha, \beta)$$



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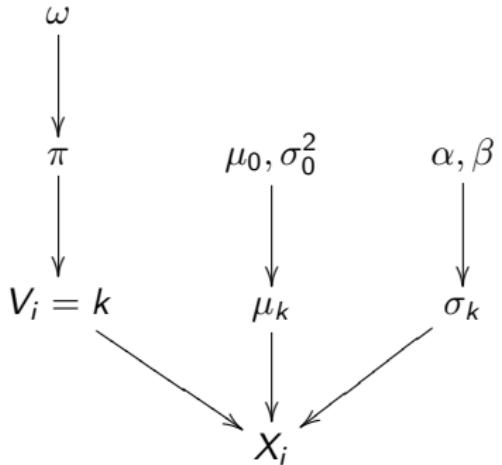
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$$f(\mathbf{X}, \mathbf{V}, \boldsymbol{\mu}, \sigma^2, \boldsymbol{\pi} | \boldsymbol{\mu}_0, \sigma_0^2, \boldsymbol{\alpha}, \boldsymbol{\beta}, \boldsymbol{\omega}) =$$

$$\prod_{i=1}^n \left[ \left( \sum_{k=1}^K 1_{[V_{ik}=1]} \frac{1}{\sqrt{2\pi}\sigma_k} e^{-\frac{1}{2}\left(\frac{X_i - \mu_k}{\sigma_k}\right)^2} \right) \left( \prod_{k=1}^K \pi_k^{V_{ik}} \right) \right]$$

$$\times \left( \prod_{k=1}^K \frac{1}{\sqrt{2\pi}\sigma_0} e^{-\frac{1}{2}\left(\frac{\mu_k - \mu_0}{\sigma_0}\right)^2} \frac{\beta^\alpha}{\Gamma(\alpha)} \left(\frac{1}{\sigma^2}\right)^{\alpha-1} e^{-\beta \frac{1}{\sigma^2}} \right) \left( \frac{1}{\mathbf{B}(\omega)} \prod_{k=1}^K \pi_k^{\omega_k - 1} \right)$$

## Markov Chain Monte Carlo (MCMC) posterior sampling

A Gibbs sampler for the posterior

$$f(\mathbf{V}, \boldsymbol{\mu}, \sigma^2, \boldsymbol{\pi} | \mathbf{X}, \mu_0, \sigma_0^2, \alpha, \beta, \boldsymbol{\omega})$$

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Is made by cycling through the *full conditional distributions*

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$$\Pr(\pi | \mathbf{X}, \mathbf{V}, \boldsymbol{\mu}, \sigma^2, \mu_0, \sigma_0^2, \alpha, \beta, \boldsymbol{\omega})$$

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## Markov Chain Monte Carlo (MCMC) *full conditionals*

$$\Pr(V_{ik} = 1 | \mathbf{X}, \boldsymbol{\mu}, \boldsymbol{\sigma}^2, \boldsymbol{\pi}, \mu_0, \sigma_0^2, \alpha, \beta, \boldsymbol{\omega}) \propto \pi_k \frac{1}{\sqrt{2\pi}\sigma_k} e^{-\frac{1}{2} \left( \frac{X_i - \mu_k}{\sigma_k} \right)^2}$$

$$f(\pi | \mathbf{V}, \boldsymbol{m\mu}, \boldsymbol{\sigma}^2, \mathbf{X}, \mu_0, \sigma_0^2, \alpha, \beta, \boldsymbol{\omega}) = Dirichlet(\{\omega_k + n_k : k = 1, \dots, K\})$$

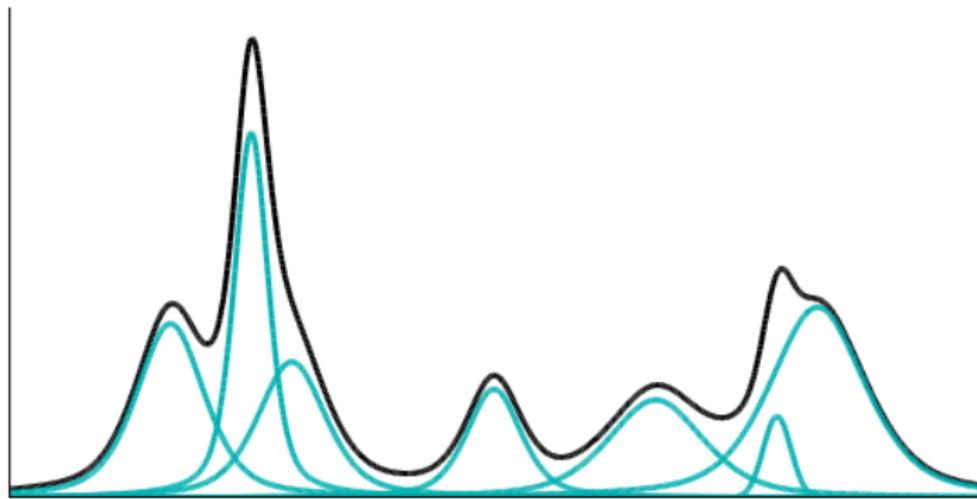
$$n_k = \sum_{V_{ik}=1} 1$$

$$f(\sigma_k^2 | \mathbf{V}, \boldsymbol{\mu}, \mathbf{X}, \mu_0, \sigma_0^2, \alpha, \beta, \boldsymbol{\omega}) = Gamma \left( \frac{n_k}{2} + \alpha, \frac{1}{2} \sum_{V_{ik}=1} (X_i - \mu_k)^2 + \beta \right)$$

$$f(\mu_k | \mathbf{V}, \boldsymbol{\sigma}^2, \mathbf{X}, \mu_0, \sigma_0^2, \alpha, \beta, \boldsymbol{\omega}) =$$

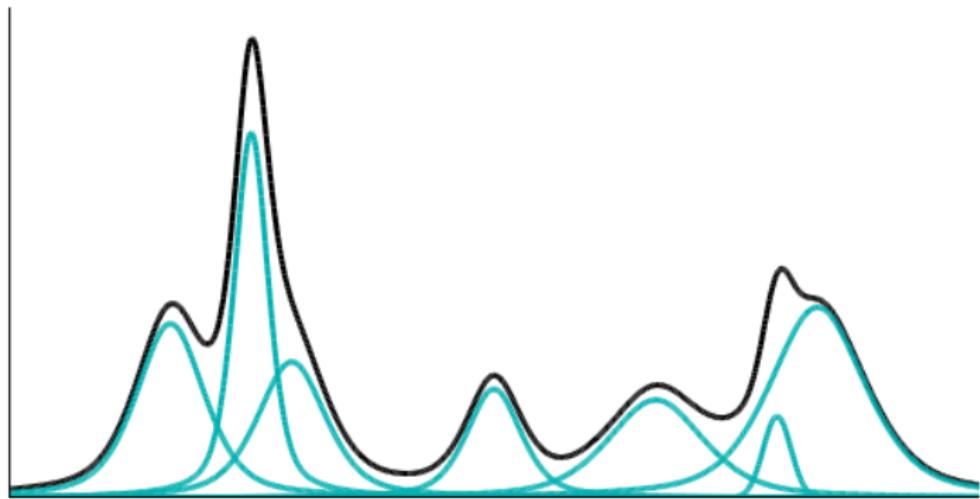
$$N \left( \hat{\sigma}_k^2 \left( \frac{\sum_{V_{ik}=1} X_i}{\sigma_k^2} + \frac{\mu_0}{\sigma_0^2} \right), \hat{\sigma}_k^2 = \left( \frac{n_k}{\sigma_k^2} + \frac{1}{\sigma_0^2} \right)^{-1} \right)$$

# Mixture Models!



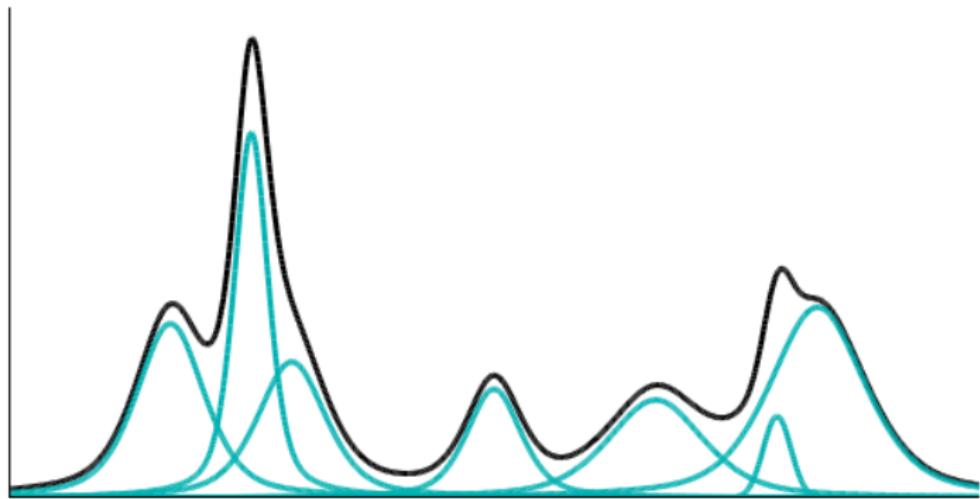
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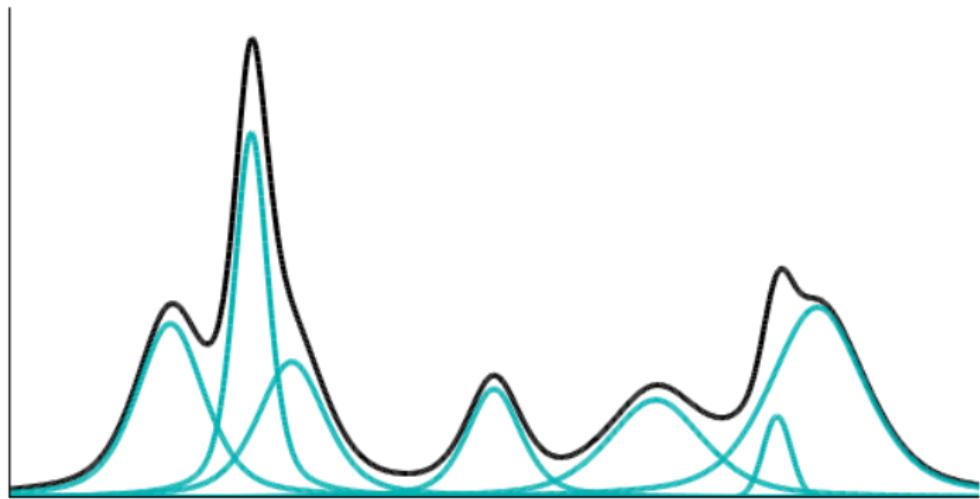
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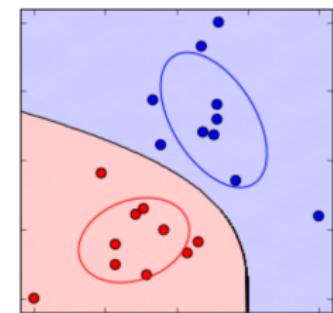
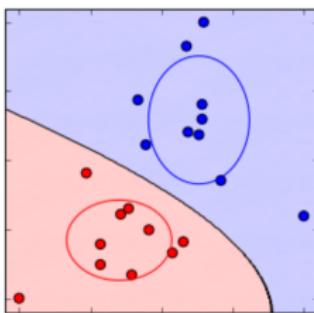
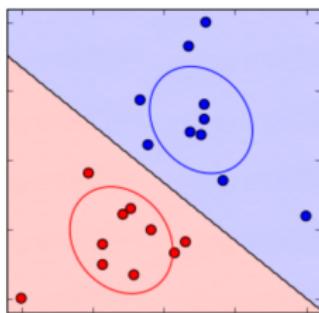
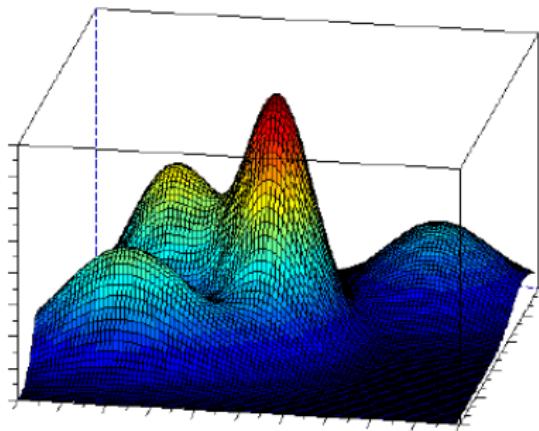
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- ▶ Can be used to model “subpopulations”
- ▶ Or simply complex distributional shapes
- ▶ It’s *almost nonparametric* like kernel density estimation
- ▶ Also can be fit with Expectation-Maximization (EM) alg.

# Mixture Models!



Byee!!

# Scott's Last Lecture Party!!

<Party Dance, Party Dance>