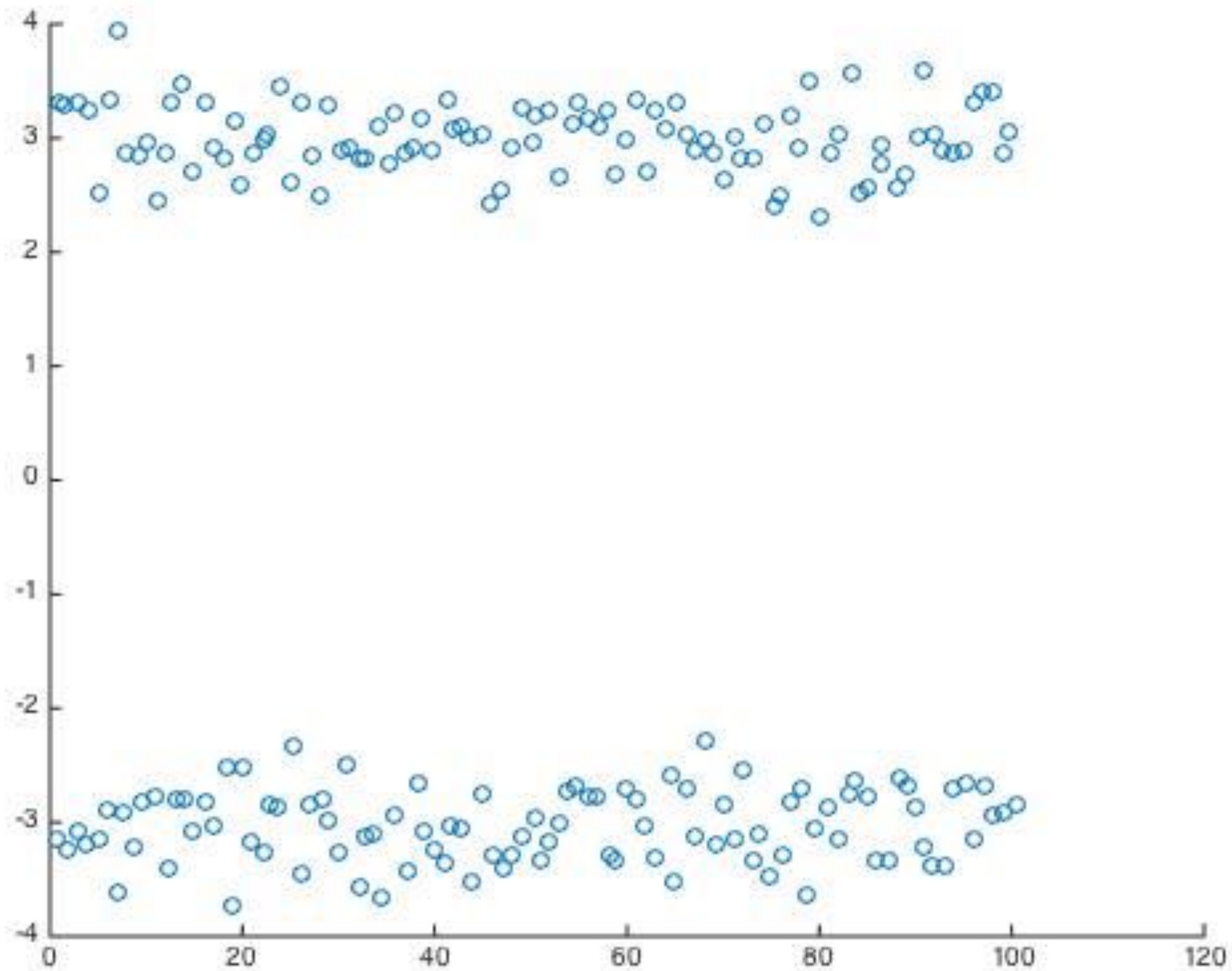
Machine Learning for Data Science (CS4786)
Lecture 5

Gaussian Mixture Models

Course Webpage :
http://www.cs.cornell.edu/Courses/cs4786/2017fa/

Clustering demo

Two elongated ellipses



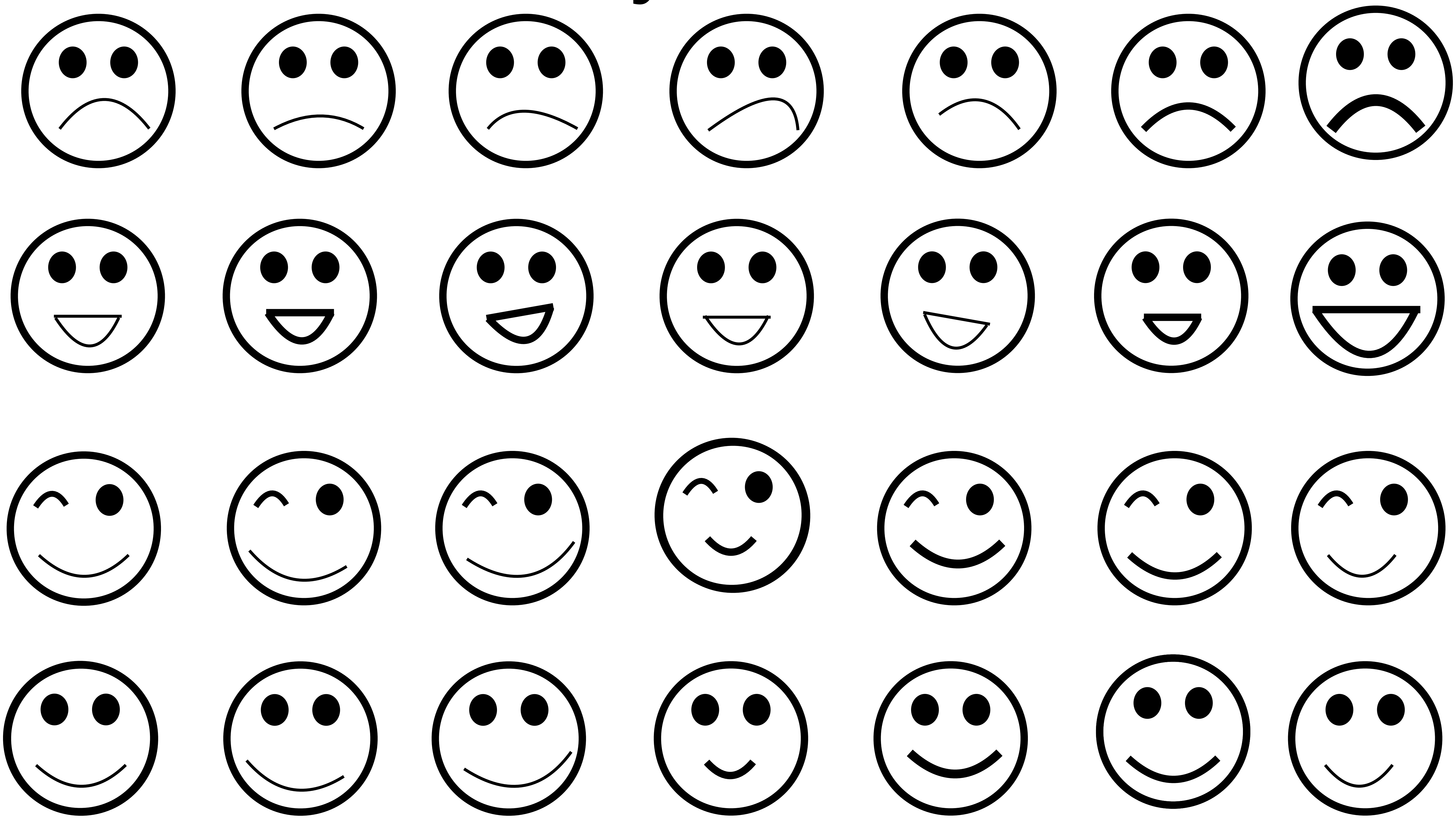
Iris dataset: Flowers

Iris-Setosa

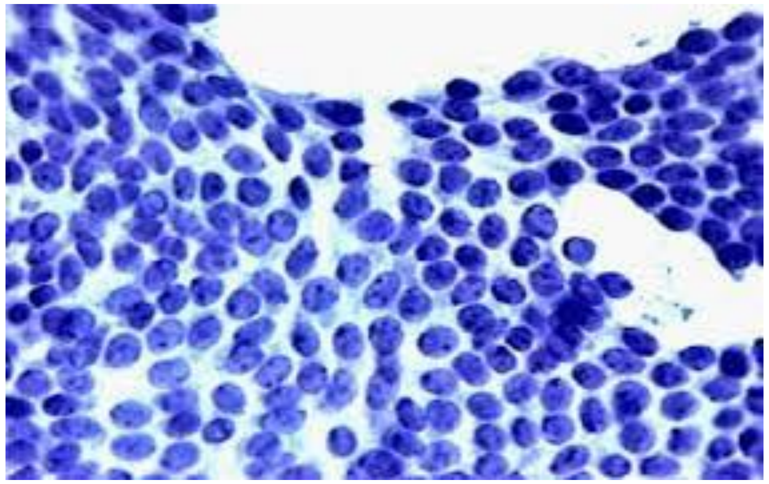
Iris-versicolor

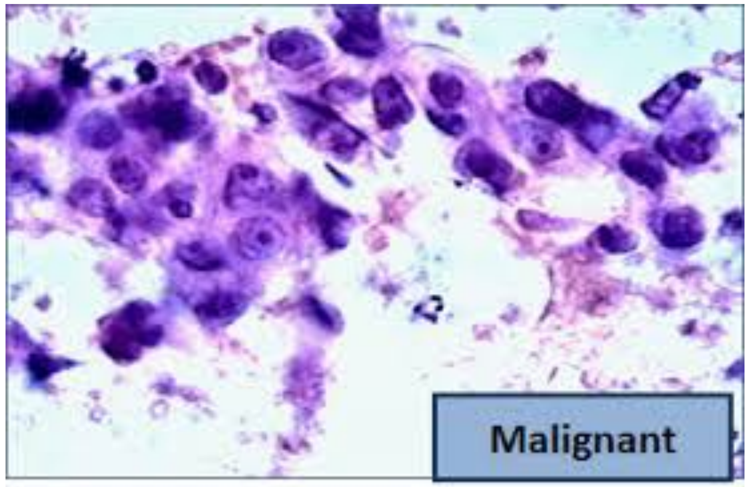
Iris-virginica

Smiley dataset

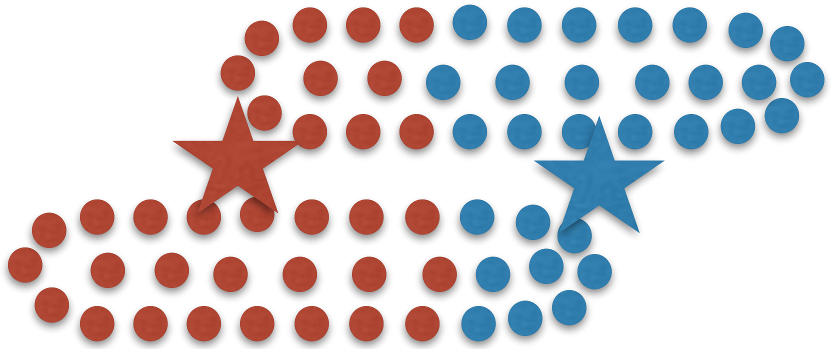


Wisconsin Breast Cancer dataset

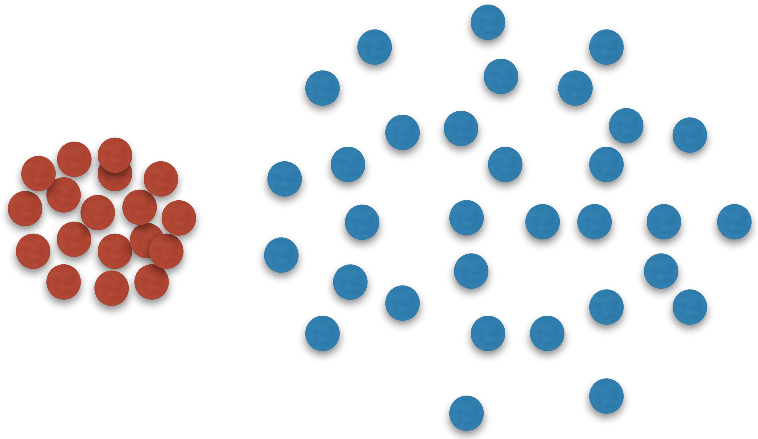




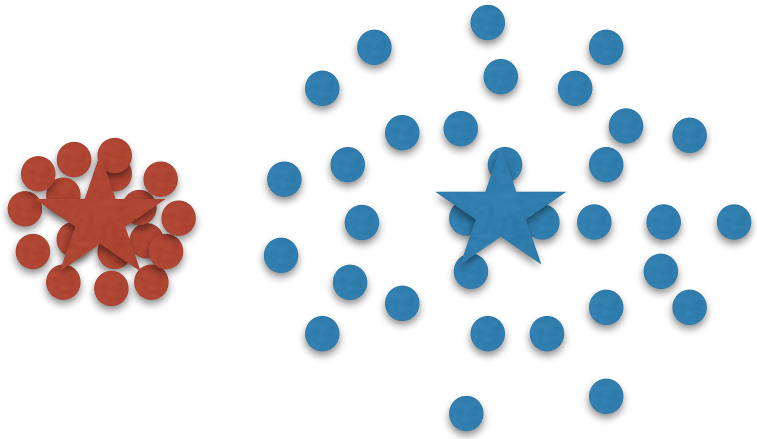
K-means: pitfalls



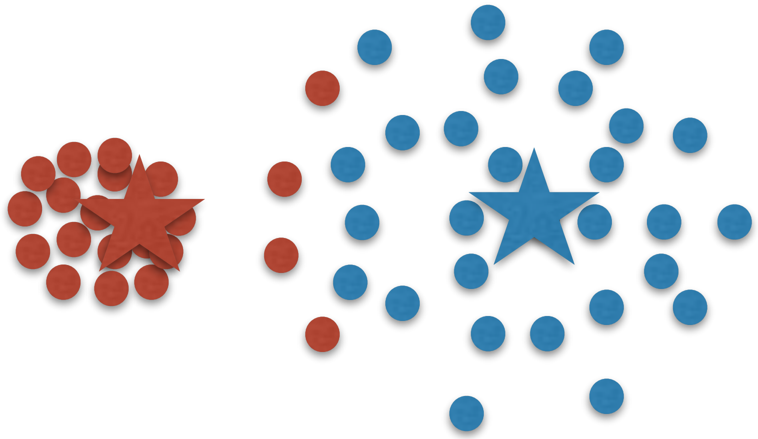
K-means: pitfalls



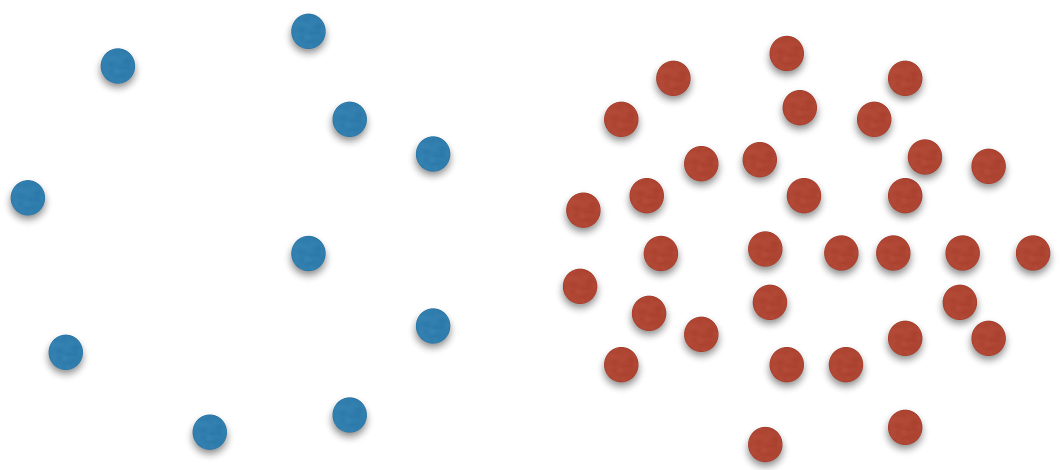
K-means: pitfalls



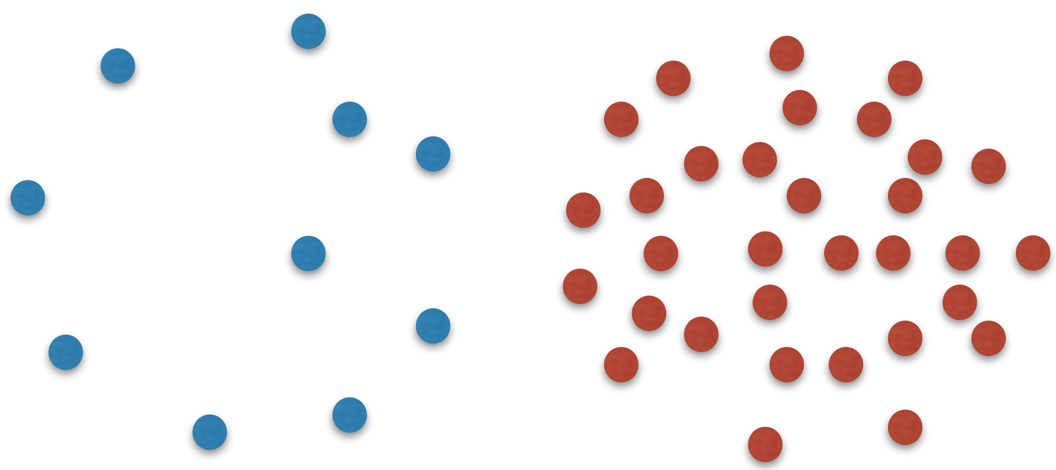
K-means: pitfalls



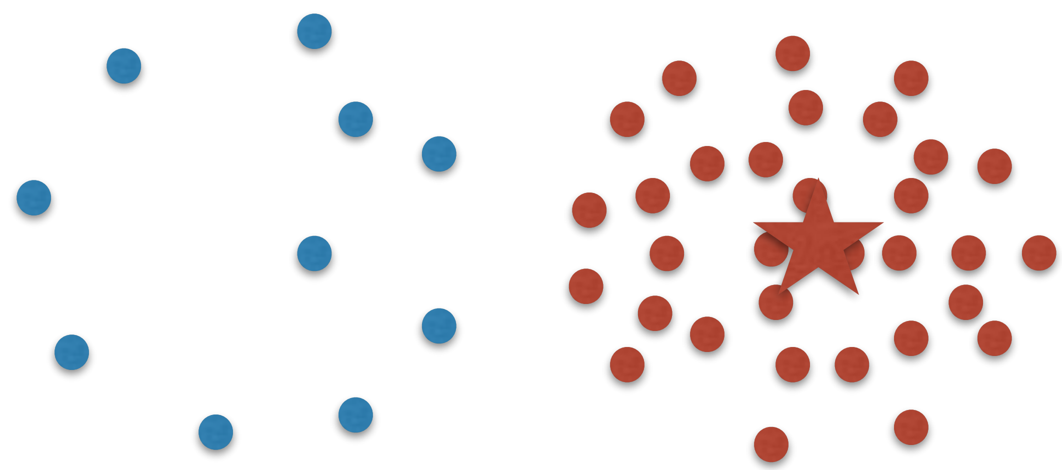
K-means: pitfalls



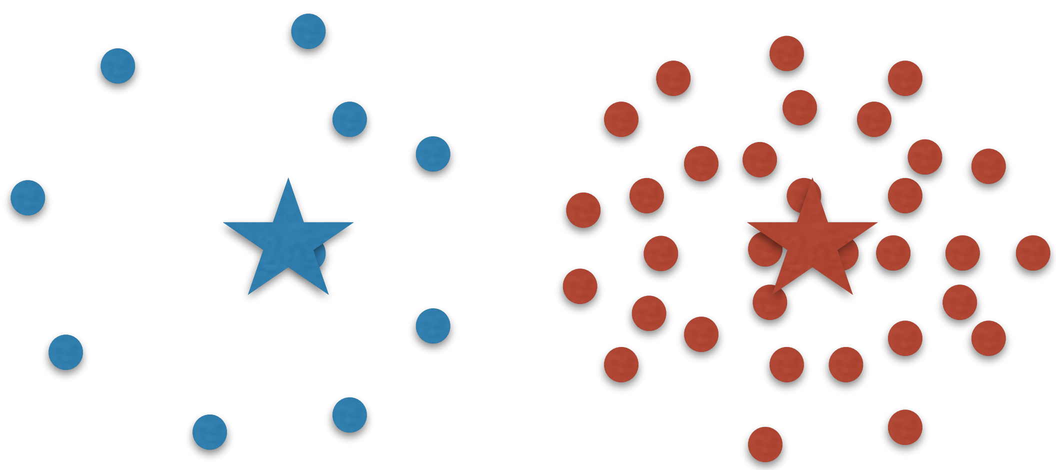
K-means: pitfalls



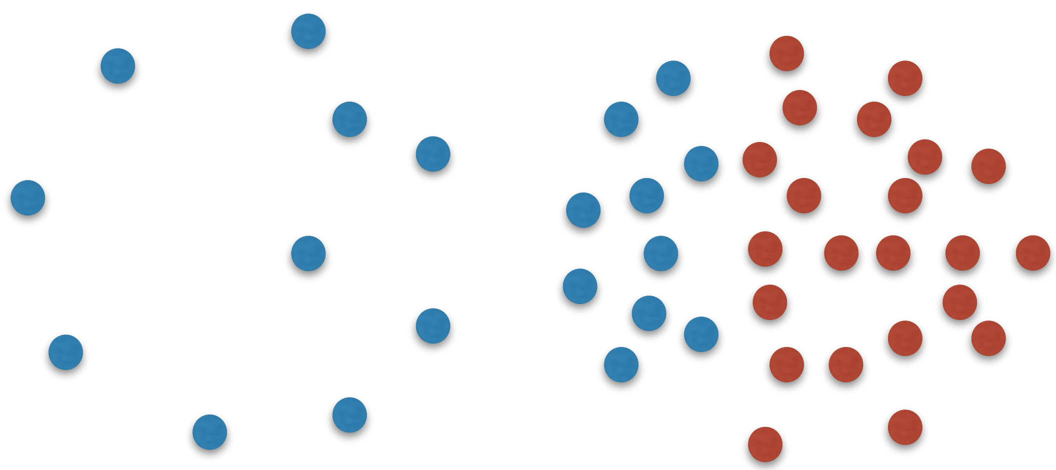
K-means: pitfalls



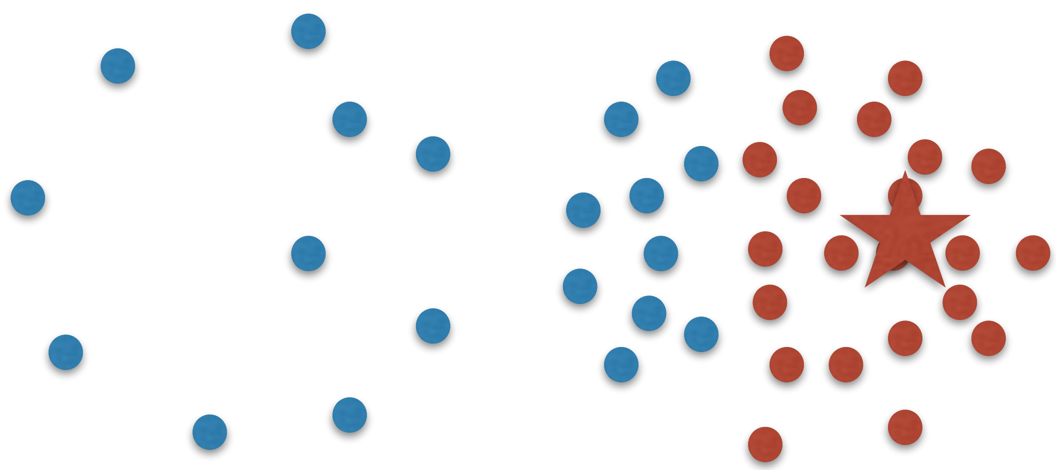
K-means: pitfalls



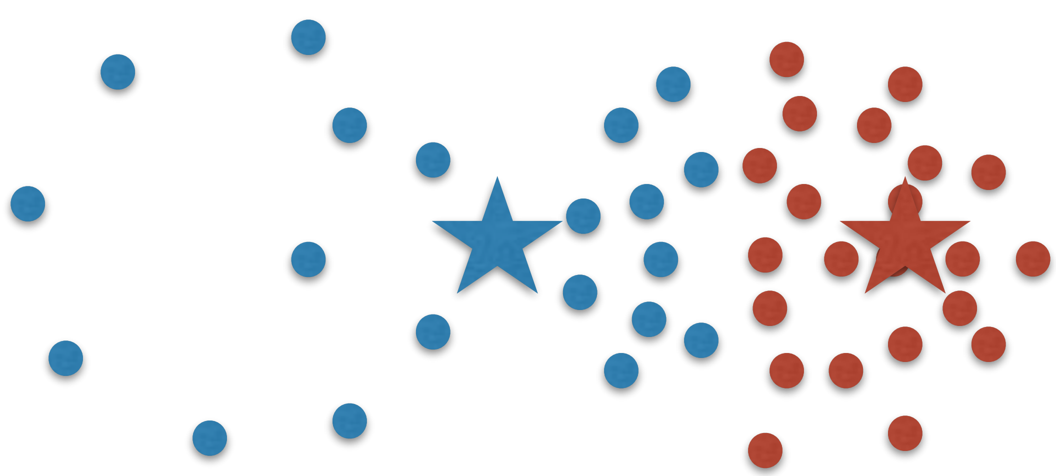
K-means: pitfalls



K-means: pitfalls



K-means: pitfalls



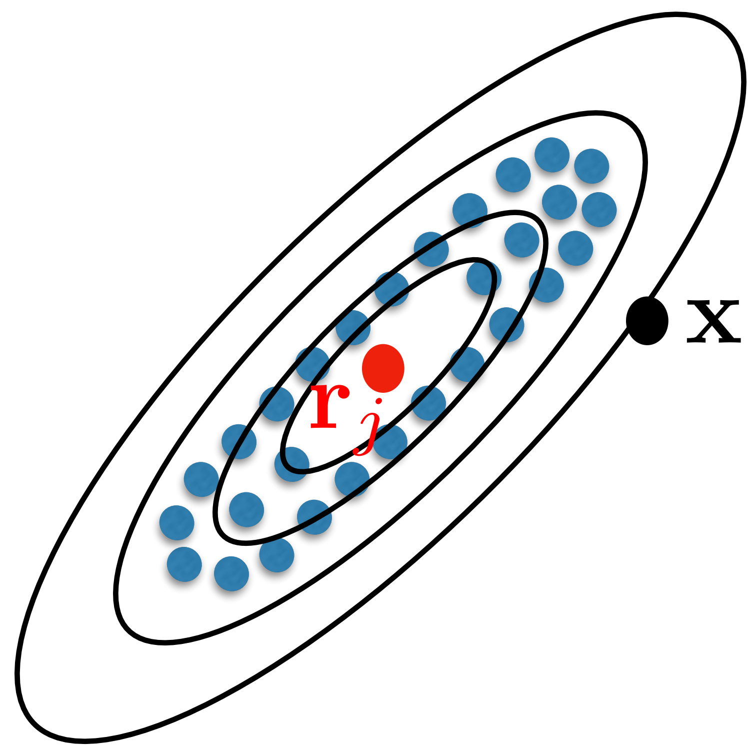
K-means: pitfalls

- Looks for spherical clusters
- Of same radius
- And with roughly equal number of points

K-means: pitfalls

- Can we design algorithm that can address these shortcomings?

Ellipsoid



$$(\mathbf{x} - \mathbf{r}_j)^\top \Sigma^{-1} (\mathbf{x} - \mathbf{r}_j)$$

$$\Sigma = \frac{1}{|C_j|} \sum_{t \in C_j} (\mathbf{x}_t - \mathbf{r}_j)(\mathbf{x}_t - \mathbf{r}_j)^\top$$

K-MEANS CLUSTERING

- For all $j \in [K]$, initialize cluster centroids $\hat{\mathbf{r}}_j^0$ randomly and set $m = 1$
- Repeat until convergence (or until patience runs out)
  1. For each $t \in \{1, \ldots, n\}$, set cluster identity of the point

$$\hat{c}^m(\mathbf{x}_t) = \underset{j \in [K]}{\operatorname{argmin}} \|\mathbf{x}_t - \hat{\mathbf{r}}_j^{m-1}\|$$

  2. For each $j \in [K]$, set new representative as

$$\hat{\mathbf{r}}_j^m = \frac{1}{|\hat{C}_j^m|} \sum_{\mathbf{x}_t \in \hat{C}_j^m} \mathbf{x}_t$$

  3. $m \leftarrow m + 1$

Ellipsoidal Clustering

- For all $j \in [K]$, initialize cluster centroids $\hat{\mathbf{r}}_j^0$ and ellipsoids $\hat{\Sigma}_j^0$ randomly and set $m = 1$
- Repeat until convergence (or until patience runs out)
  1. For each $t \in \{1, \ldots, n\}$, set cluster identity of the point

$$\hat{c}^m(\mathbf{x}_t) = \underset{j \in [K]}{\operatorname{argmin}} \; (\mathbf{x}_t - \hat{\mathbf{r}}_j^{m-1})^\top \left(\hat{\Sigma}^{m-1}\right)^{-1} (\mathbf{x}_t - \hat{\mathbf{r}}_j^{m-1})$$

  2. For each $j \in [K]$, set new representative as

$$\hat{\mathbf{r}}_j^m = \frac{1}{|\hat{C}_j^m|} \sum_{\mathbf{x}_t \in \hat{C}_j^m} \mathbf{x}_t \qquad \hat{\Sigma}^m = \frac{1}{|C_j|} \sum_{t \in C_j} (\mathbf{x}_t - \hat{\mathbf{r}}_j^m)(\mathbf{x}_t - \hat{\mathbf{r}}_j^m)^\top$$

  3. $m \leftarrow m + 1$

K-means: pitfalls

- Looks for spherical clusters ✓
- Of same radius ✓
- And with roughly equal number of points ✗

Hard Gaussian Mixture Model

- For all $j \in [K]$, initialize cluster centroids $\hat{\mathbf{r}}_j^0$, ellipsoids $\hat{\Sigma}_j^0$ and initial proportions π^0 randomly and set $m = 1$
- Repeat until convergence (or until patience runs out)
  1. For each $t \in \{1, \ldots, n\}$, set cluster identity of the point

$$\hat{c}^m(\mathbf{x}_t) = \underset{j \in [K]}{\operatorname{argmin}} \ (\mathbf{x}_t - \hat{\mathbf{r}}_j^{m-1})^\top \left(\hat{\Sigma}^{m-1}\right)^{-1} (\mathbf{x}_t - \hat{\mathbf{r}}_j^{m-1}) - \log(\pi_j^{m-1})$$

  2. For each $j \in [K]$, set new representative as

$$\hat{\mathbf{r}}_j^m = \frac{1}{|\hat{C}_j^m|} \sum_{\mathbf{x}_t \in \hat{C}_j^m} \mathbf{x}_t \qquad \hat{\Sigma}^m = \frac{1}{|C_j|} \sum_{t \in C_j} (\mathbf{x}_t - \hat{\mathbf{r}}_j^m)(\mathbf{x}_t - \hat{\mathbf{r}}_j^m)^\top \qquad \pi_j^m = \frac{|C_j^m|}{n}$$

  3. $m \leftarrow m + 1$

Multivariate Gaussian

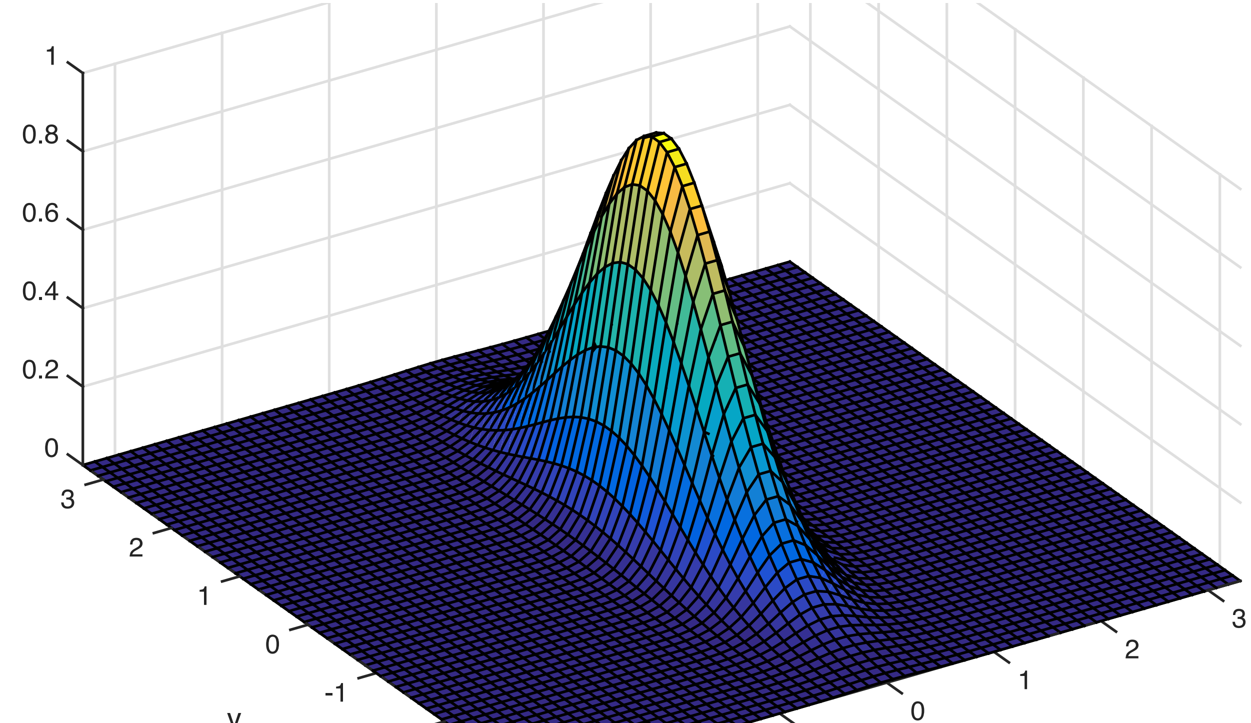
- Two parameters:
  - Mean $\mu \in \mathbb{R}^d$
  - Covariance matrix Σ of size dxd

$$p(x; \mu, \Sigma) = (2\pi)^{d/2} \det(\Sigma)^{-1/2} \exp\left(-\frac{1}{2}(x-\mu)^\top \Sigma^{-1}(x-\mu)\right)$$

Multivariate Gaussian

- Two parameters:
  - Mean $\mu \in \mathbb{R}^d$
  - Covariance matrix Σ of size dxd

$$p(x;\mu,\Sigma) = (2\pi)^{d/2}\det(\Sigma)^{-1/2}\exp\left(-\frac{1}{2}(x-\mu)^\top\Sigma^{-1}(x-\mu)\right)$$



Hard Gaussian Mixture Model

- For all $j \in [K]$, initialize cluster centroids $\hat{\mathbf{r}}_j^0$, ellipsoids $\hat{\Sigma}_j^0$ and initial proportions π^0 randomly and set $m = 1$
- Repeat until convergence (or until patience runs out)
  1. For each $t \in \{1, \ldots, n\}$, set cluster identity of the point

$$\hat{c}^m(\mathbf{x}_t) = \underset{j \in [K]}{\operatorname{argmin}} \; p(\mathbf{x}_t, \hat{\mathbf{r}}_j^{m-1}, \hat{\Sigma}^{m-1}) \times \pi^m(j)$$

  2. For each $j \in [K]$, set new representative as

$$\hat{\mathbf{r}}_j^m = \frac{1}{|\hat{C}_j^m|} \sum_{\mathbf{x}_t \in \hat{C}_j^m} \mathbf{x}_t \qquad \hat{\Sigma}^m = \frac{1}{|C_j|} \sum_{t \in C_j} (\mathbf{x}_t - \hat{\mathbf{r}}_j^m)(\mathbf{x}_t - \hat{\mathbf{r}}_j^m)^\top \qquad \pi_j^m = \frac{|C_j^m|}{n}$$

  3. $m \leftarrow m + 1$

(Soft) Gaussian Mixture Model

- For all $j \in [K]$, initialize cluster centroids $\hat{\mathbf{r}}_j^0$ and ellipsoids $\hat{\Sigma}_j^0$ randomly and set $m = 1$
- Repeat until convergence (or until patience runs out)
  1. For each $t \in \{1, \dots, n\}$, set cluster identity of the point

$$Q_t^m(j) = p(\mathbf{x}_t, \hat{\mathbf{r}}_j^{m-1}, \hat{\Sigma}^{m-1}) \times \pi^m(j)$$

  2. For each $j \in [K]$, set new representative as

$$\hat{\mathbf{r}}_j^m = \frac{\sum_{t=1}^n Q_t(j)\mathbf{x}_t}{\sum_{t=1}^n Q_t(j)} \qquad \hat{\Sigma}^m = \frac{\sum_{t=1}^n Q_t(j)(\mathbf{x}_t - \hat{\mathbf{r}}_j^m)(\mathbf{x}_t - \hat{\mathbf{r}}_j^m)^\top}{\sum_{t=1}^n Q_t(j)}$$

$$\pi_j^m = \frac{\sum_{t=1}^n Q_t(j)}{n}$$

  3. $m \leftarrow m + 1$