Machine Learning for Data Science (CS4786)
Lecture 13

Clustering

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

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

  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. $m \leftarrow m + 1$

Clustering Criterion

- Minimize within cluster average dissimilarity

$$M_6 = \sum_{j=1}^{K} \sum_{s \in C_j} \mathrm{dissimilarity}\left(\mathbf{x}_s, C_j\right)$$

$$= \sum_{j=1}^{K} \sum_{s \in C_j} \left(\frac{1}{|C_j|} \sum_{t \in C_j, t \neq s} \mathrm{dissimilarity}\left(\mathbf{x}_s, \mathbf{x}_t\right) \right)$$

$$= \sum_{j=1}^{K} \frac{1}{|C_j|} \sum_{s \in C_j} \left(\sum_{t \in C_j, t \neq s} \|\mathbf{x}_s - \mathbf{x}_t\|_2^2 \right)$$

- Minimize within-cluster variance: $\mathbf{r}_j = \frac{1}{n_j} \sum_{\mathbf{x} \in C_j} \mathbf{x}$

$$M_5 = \sum_{j=1}^{K} \sum_{t \in C_j} \|\mathbf{x}_t - \mathbf{r}_j\|_2^2$$

Clustering Criterion

- minimizing $M_5 \equiv$ minimizing M_6

K-means objective

$$\sum_{j=1}^{K}\sum_{t\in C_j}\left\|\mathbf{x}_t-\frac{1}{|C_j|}\sum_{s\in C_j}\mathbf{x}_s\right\|^2=\min_{\mathbf{r}_1,\ldots,\mathbf{r}_K}\sum_{j=1}^{K}\sum_{t\in C_j}\|\mathbf{x}_t-\mathbf{r}_j\|^2$$

$$\|\qquad\qquad\qquad\qquad\|$$

$$M_5=\min_{\mathbf{r}_1,\ldots,\mathbf{r}_K}O(c;\mathbf{r}_1,\ldots,\mathbf{r}_K)$$

$$O\left(c;\mathbf{r}_1,\ldots,\mathbf{r}_K\right)=\sum_{j=1}^{K}\sum_{c(\mathbf{x}_t)=j}\|\mathbf{x}_t-\mathbf{r}_j\|_2^2$$

Minimize above objective over c and $\mathbf{r}_1,\ldots,\mathbf{r}_K$

Fact: Centroid is Minimizer

$$\forall \mathbf{r}_j, \quad \sum_{t \in C_j} \left\| \mathbf{x}_t - \frac{1}{|C_j|} \sum_{s \in C_j} \mathbf{x}_s \right\|^2 \leq \sum_{t \in C_j} \|\mathbf{x}_t - \mathbf{r}_j\|^2$$

Proof

$$\sum_{t \in C_j} \|\mathbf{x}_t - \mathbf{r}_j\|^2$$

$$\mu_j = \frac{1}{|C_j|} \sum_{t \in C_j} \mathbf{x}_t$$

$$= \sum_{t \in C_j} \|\mathbf{x}_t - \mu_j + \mu_j - \mathbf{r}_j\|^2$$

$$= \sum_{t \in C_j} \|\mathbf{x}_t - \mu_j\|^2 + \sum_{t \in C_j} \|\mu_j - \mathbf{r}_j\|^2 + 2 \sum_{t \in C_j} (\mathbf{x}_t - \mu_j)^\top (\mu_j - \mathbf{r}_j)$$

$$= \sum_{t \in C_j} \|\mathbf{x}_t - \mu_j\|^2 + \sum_{t \in C_j} \|\mu_j - \mathbf{r}_j\|^2 + 2 \left(\cancel{\sum_{t \in C_j} \mathbf{x}_t} - \cancel{|C_j| \mu_j} \right)^\top (\mu_j - \mathbf{r}_j)$$

$$= \sum_{t \in C_j} \|\mathbf{x}_t - \mu_j\|^2 + \sum_{t \in C_j} \|\mu_j - \mathbf{r}_j\|^2$$

$$\geq \sum_{t \in C_j} \|\mathbf{x}_t - \mu_j\|^2$$

K-MEANS CONVERGENCE

- K-means algorithm converges to local minima of objective

$$O\left(c; \mathbf{r}_1, \ldots, \mathbf{r}_K\right) = \sum_{j=1}^{K} \sum_{c(\mathbf{x}_t)=j} \|\mathbf{x}_t - \mathbf{r}_j\|_2^2$$

- Proof:
  Clustering assignment improves objective:

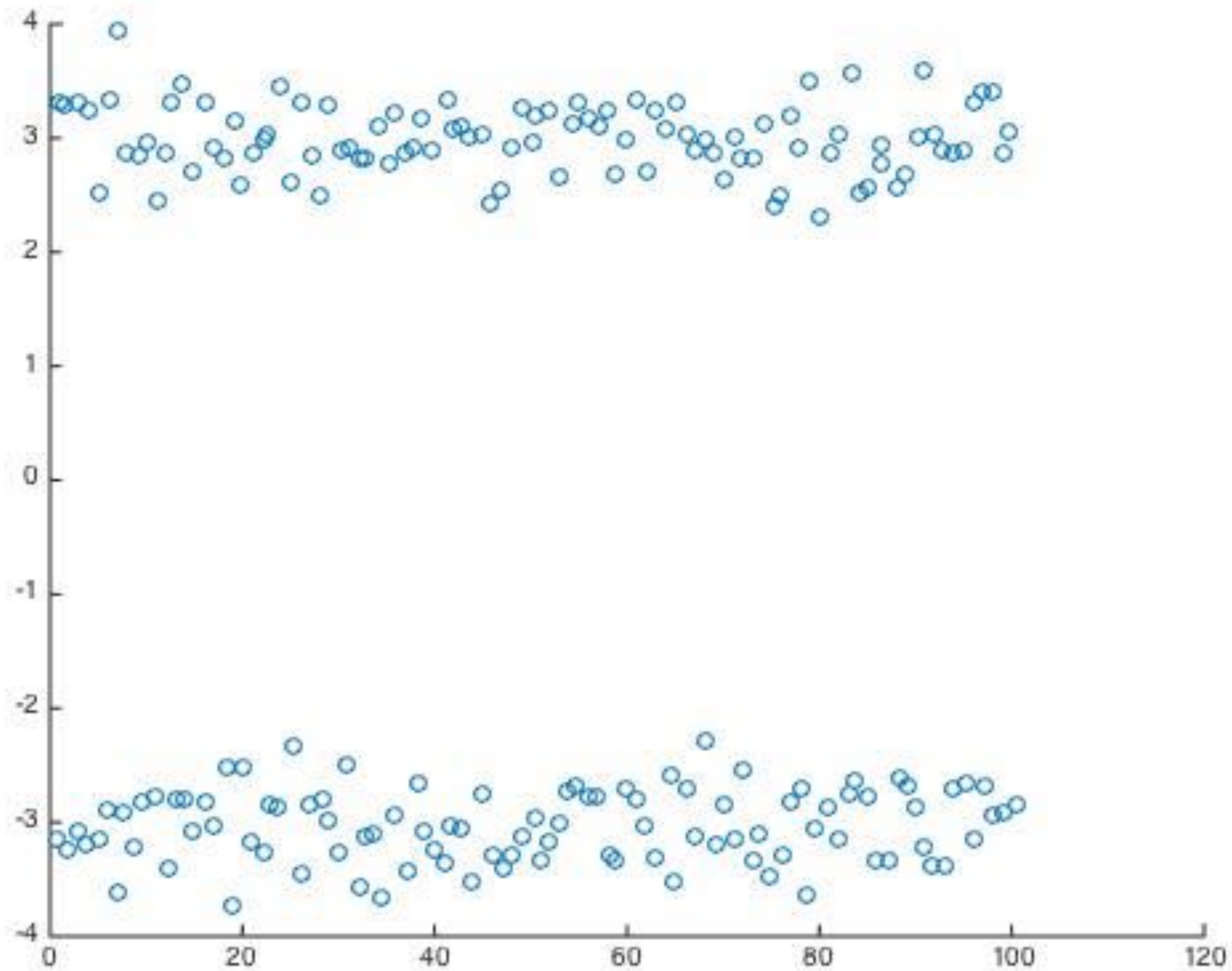
$$O\left(\hat{c}^{m-1}; \mathbf{r}_1^{m-1}, \ldots, \mathbf{r}_K^{m-1}\right) \geq O\left(\hat{c}^{m}; \mathbf{r}_1^{m-1}, \ldots, \mathbf{r}_K^{m-1}\right)$$

  (By definition of $\hat{c}^m(\mathbf{x}_t)$)
  Computing centroids improves objective:

$$O\left(\hat{c}^{m}; \mathbf{r}_1^{m-1}, \ldots, \mathbf{r}_K^{m-1}\right) \geq O\left(\hat{c}^{m}; \mathbf{r}_1^{m}, \ldots, \mathbf{r}_K^{m}\right)$$

  (By the fact about centroid)

Two elongated ellipses



Iris dataset: Flowers

Iris-Setosa

Iris-versicolor

Iris-virginica

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?