CSC 411 Lecture 14:Clustering

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K-means Objective

What is actually being optimized?

K-means Objective:
Find cluster centers $\mathbf{m}$ and assignments $\mathbf{r}$ to minimize the sum of squared distances of data points $\{\mathbf{x}^{(n)}\}$ to their assigned cluster centers

$$\min_{\{\mathbf{m}\},\{\mathbf{r}\}} J(\{\mathbf{m}\},\{\mathbf{r}\}) = \min_{\{\mathbf{m}\},\{\mathbf{r}\}} \sum_{n=1}^{N} \sum_{k=1}^{K} r_k^{(n)} ||\mathbf{m}_k - \mathbf{x}^{(n)}||^2$$

$$\text{s.t.} \sum_k r_k^{(n)} = 1, \forall n, \quad \text{where} \qquad r_k^{(n)} \in \{0,1\}, \forall k, n$$

where $r_k^{(n)} = 1$ means that $\mathbf{x}^{(n)}$ is assigned to cluster k (with center $\mathbf{m}_k$)

- Optimization method is a form of coordinate descent ("block coordinate descent")
  - Fix centers, optimize assignments (choose cluster whose mean is closest)
  - Fix assignments, optimize means (average of assigned datapoints)

The K-means Algorithm

- Initialization: Set K cluster means $\mathbf{m}_1, \dots, \mathbf{m}_K$ to random values
- Repeat until convergence (until assignments do not change):
  - Assignment: Each data point $\mathbf{x}^{(n)}$ assigned to nearest mean

    $$\hat{k}^n = arg \min_k d(\mathbf{m}_k, \mathbf{x}^{(n)})$$

    (with, for example, L2 norm: $\hat{k}^n = arg \min_k ||\mathbf{m}_k - \mathbf{x}^{(n)}||^2$)

    and Responsibilities (1-hot encoding)

    $$r_k^{(n)} = 1 \longleftrightarrow \hat{k}^{(n)} = k$$

  - Update: Model parameters, means are adjusted to match sample means of data points they are responsible for:

    $$\mathbf{m}_k = \frac{\sum_n r_k^{(n)} \mathbf{x}^{(n)}}{\sum_n r_k^{(n)}}$$

Soft K-means Algorithm

- Initialization: Set K means $\{\mathbf{m}_k\}$ to random values
- Repeat until convergence (until assignments do not change):
  - Assignment: Each data point n given soft "degree of assignment" to each cluster mean k, based on responsibilities

$$r_k^{(n)} = \frac{\exp[-\beta d(\mathbf{m}_k, \mathbf{x}^{(n)})]}{\sum_j \exp[-\beta d(\mathbf{m}_j, \mathbf{x}^{(n)})]}$$

  - Update: Model parameters, means, are adjusted to match sample means of datapoints they are responsible for:

$$\mathbf{m}_k = \frac{\sum_n r_k^{(n)} \mathbf{x}^{(n)}}{\sum_n r_k^{(n)}}$$