1 Problem

1.1 Solution

Optimal μ_k is obtained by finding first derivative of D w.r.t μ_k and setting it to zero.

$$D = \sum_{n=1}^{N} \sum_{k=1}^{K} r_{nk} \|\mathbf{x}_n - \mu_k\|_2^2$$
$$\frac{\partial D}{\partial \mu_k} = 0 \Rightarrow \sum_{n=1}^{N} r_{nk} 2(\mu_k - \mathbf{x}_n) = 0$$
$$\Rightarrow \mu_k = \frac{\sum_{n=1}^{N} r_{nk} \mathbf{x}_n}{\sum_{n=1}^{N} r_{nk}}$$

We can also see that the second derivative $(2\sum_{n=1}^{N}r_{nk})$ is positive, so we know that D will be minimized for the above μ_k value.

1.2 Solution

Let us define C_n^t as cluster center that is assigned to data point \mathbf{x}_n at time t i.e.,

$$C_n^t = \mu_k \quad where \quad r_{nk}^t = 1$$

By this definition, our objective function can be written as:

$$D = \sum_{n=1}^{N} \|\mathbf{x}_n - C_n\|_2^2 \quad \text{...introducing time t in this expression}$$

$$D(\mu^t, \mathbf{R}^t) = \sum_{n=1}^{N} \|\mathbf{x}_n - C_n^t\|_2^2$$

Also from the way K-means algorithm is defined, we know that C_n^t is chosen such that it is minimum of distance from data point \mathbf{x}_n to all cluster centers, so we know that:

$$\forall n \in [1, N], \forall k \in [1, K] : \left\| \mathbf{x}_n - C_n^t \right\|_2^2 \le \left\| \mathbf{x}_n - \mu_k \right\|_2^2 \quad \text{...i.e.},$$

$$\forall n \in [1, N] : \left\| \mathbf{x}_n - C_n^t \right\|_2^2 \le \left\| \mathbf{x}_n - C_n^{t-1} \right\|_2^2$$

Combining the above two, we get:

$$D(\mu^{t}, \mathbf{R}^{t}) = \sum_{n=1}^{N} \|\mathbf{x}_{n} - C_{n}^{t}\|_{2}^{2}$$

$$\leq \sum_{n=1}^{N} \|\mathbf{x}_{n} - C_{n}^{t-1}\|_{2}^{2} = D(\mu^{t-1}, \mathbf{R}^{t-1})$$

1.3 Solution

Again, we get the minimum by doing first derivative of objective function and setting it to zero:

$$D = \sum_{n=1}^{N} \sum_{k=1}^{K} r_{nk} \|\mathbf{x}_n - \mu_k\|_{1}$$

In the above, $\mu_k \in \mathbb{R}^d$ i.e., μ_k is a vector of dimension k. Let's consider the derivative of a given μ_k along one dimension value d:

$$\frac{\partial D}{\partial \mu_{kd}} = 0 \Rightarrow \sum_{n=1}^{N} r_{nk} \ sgn(x_{nd} - \mu_{kd}) = 0$$

$$\Rightarrow \sum \mathbb{I}(C_n = \mu_k) \mathbb{I}(x_{nd} > \mu_{kd}) - \sum \mathbb{I}(C_n = \mu_k) \mathbb{I}(x_{nd} \le \mu_{kd}) = 0$$

$$\Rightarrow \sum \mathbb{I}(C_n = \mu_k) \mathbb{I}(x_{nd} > \mu_{kd}) = \sum \mathbb{I}(C_n = \mu_k) \mathbb{I}(x_{nd} \le \mu_{kd})$$

where C_n is the cluster center assigned to data point \mathbf{x}_n and sgn is the sign function. From the above, we can see that along dimension d, from the data points assigned to cluster k, the number of data points where $x_{nd} > \mu_{kd}$ should be equal to points where $x_{nd} \leq \mu_{kd}$ i.e., μ_{kd} is the median of values at dimension d of all data points assigned to cluster k. From this, it follows that μ_k that minimizes D is the element wise median of all data points assigned to cluster k.

1.4 Solution

Given $\tilde{\mu}_k$ is the center of cluster in feature space:

$$\begin{split} \tilde{\mu}_k &= \frac{\sum_n r_{nk} \phi(\mathbf{x}_n)}{\sum_n r_{nk}} = \frac{\sum_n r_{nk} \phi(\mathbf{x}_n)}{N_k} \quad \text{...where } N_k = \sum_n r_{nk} \\ \tilde{D} &= \sum_n \sum_k r_{nk} \|\phi(\mathbf{x}_n) - \tilde{\mu}_k\|_2^2 \\ &= \sum_k \sum_n r_{nk} (\phi(\mathbf{x}_n) - \tilde{\mu}_k)^T (\phi(\mathbf{x}_n) - \tilde{\mu}_k) \\ &= \sum_k \sum_n r_{nk} [\phi(\mathbf{x}_n)^T \phi(\mathbf{x}_n) - \phi(\mathbf{x}_n)^T \tilde{\mu}_k - \tilde{\mu}_k^T \phi(\mathbf{x}_n) + \tilde{\mu}_k^T \tilde{\mu}_k] \\ &= \sum_k \sum_n r_{nk} [f(\mathbf{x}_n, \mathbf{x}_n) - 2\phi(\mathbf{x}_n)^T \frac{\sum_m r_{mk} \phi(\mathbf{x}_m)}{N_k} + \frac{\sum_l r_{lk} \phi(\mathbf{x}_l)^T \sum_m r_{mk} \phi(\mathbf{x}_m)}{N_k}] \\ &= \sum_k \sum_n r_{nk} [f(\mathbf{x}_n, \mathbf{x}_n) - 2\frac{\sum_m r_{mk} f(\mathbf{x}_n, \mathbf{x}_m)}{N_k} + \frac{\sum_l \sum_m r_{lk} r_{mk} f(\mathbf{x}_l, \mathbf{x}_m)}{N_k^2}] \\ &= \sum_k \sum_n r_{nk} [f(\mathbf{x}_n, \mathbf{x}_n) - 2\frac{\sum_m r_{mk} f(\mathbf{x}_n, \mathbf{x}_m)}{N_k} + \frac{\sum_l \sum_m r_{lk} r_{mk} f(\mathbf{x}_l, \mathbf{x}_m)}{N_k^2}] \\ &= \sum_n f(\mathbf{x}_n, \mathbf{x}_n) \sum_k r_{nk} - \sum_k 2\frac{\sum_n \sum_m r_{nk} r_{mk} f(\mathbf{x}_n, \mathbf{x}_m)}{N_k} + \sum_k \frac{\sum_l \sum_m r_{lk} r_{mk} f(\mathbf{x}_l, \mathbf{x}_m)}{N_k^2} \sum_n r_{nk} \\ &= \sum_n f(\mathbf{x}_n, \mathbf{x}_n) - \sum_k \frac{\sum_l \sum_m r_{lk} r_{mk} f(\mathbf{x}_l, \mathbf{x}_m)}{N_k} \end{split}$$

2 Problem

2.1 Solution

If k is the index where $z_k = 1$, the probability of X is given by distribution θ_k i.e.,

$$P(X = \mathbf{x} | z_k = 1) = \prod_{i=1}^d \theta_{ki}^{x_i} (1 - \theta_{ki})^{(1-x_i)} \quad \text{...can also be expressed as}$$
$$= \prod_{i=1}^d \theta_{ki}^{z_k x_i} (1 - \theta_{ki})^{z_k (1-x_i)} \quad \text{...since } z_k = 1$$

Also, we can see that when $z_{k'} = 0$ (all other dimension values for \mathbf{z}), the term $\pi_{k'}^{z'_k} = 1$ and $\forall i \in [1, d], \theta_{k'i}^{z'_k x_i} (1 - \theta_{k'i})^{z'_k (1 - x_i)} = 1$ as well. So multiplying any value with these terms

won't change the value. We will write the joint probability from this observation as:

$$P(X = \mathbf{x}, Z = \mathbf{z} | \Theta, \pi) = \prod_{k=1}^{K} \pi_k^{z_k} \prod_{i=1}^{d} \theta_{ki}^{z_k x_i} (1 - \theta_{ki})^{z_k (1 - x_i)}$$

The marginal probability can be written as below...

$$P(X = \mathbf{x} | \Theta, \pi) = \sum_{k=1}^{K} \pi_k \prod_{i=1}^{d} \theta_{ki}^{x_i} (1 - \theta_{ki})^{(1-x_i)}$$

Note that if we know a specific k for which $z_k = 1$ in \mathbf{z} , the expression for $P(X = \mathbf{x}, Z = \mathbf{z} | \Theta, \pi)$ can be simplified greatly (which is the case for next solution).

2.2 Solution

$$\gamma_{nk} = P(z_k = 1 | X = \mathbf{x}_n, \Theta, \pi) = \frac{P(z_k = 1, X = \mathbf{x}_n | \Theta, \pi)}{P(X = \mathbf{x}_n | \Theta, \pi)}$$
$$= \frac{\pi_k \prod_{i=1}^d \theta_{ki}^{x_{ni}} (1 - \theta_{ki})^{(1 - x_{ni})}}{\sum_{k=1}^K \pi_k \prod_{i=1}^d \theta_{ki}^{x_{ni}} (1 - \theta_{ki})^{(1 - x_{ni})}}$$

2.3 Solution

The expression that we need to maximize w.r.t Θ and π is given by:

$$Q = \sum_{n=1}^{N} \sum_{k=1}^{K} \gamma_{nk} \ln P(\mathbf{x}_{n}, z_{k} = 1 | \Theta, \pi)$$

$$= \sum_{n=1}^{N} \sum_{k=1}^{K} \gamma_{nk} \ln \left[\pi_{k} \prod_{i=1}^{d} \theta_{ki}^{x_{ni}} (1 - \theta_{ki})^{(1 - x_{ni})} \right]$$

$$= \sum_{n=1}^{N} \sum_{k=1}^{K} \gamma_{nk} \ln(\pi_{k}) + \sum_{n=1}^{N} \sum_{k=1}^{K} \gamma_{nk} \sum_{i=1}^{d} \left[x_{ni} \ln(\theta_{ki}) + (1 - x_{ni}) \ln(1 - \theta_{ki}) \right]$$

We can consider only the first term for deriving updates for π and second term for deriving updates for Θ since other terms would be constants in each derivation.

Update for π is solved using the lagrangian with constraints and applying KKT conditions:

Constraints:
$$\pi_k \ge 0 \ \forall k$$
; $\sum_{k=1}^K \pi_k = 1$

$$L = \sum_{n=1}^N \sum_{k=1}^K \gamma_{nk} \ ln(\pi_k) + \mu(1 - \sum_{k=1}^K \pi_k) - \sum_{k=1}^K \lambda_k \pi_k$$

$$\lambda_k = 0 \ \forall k \qquad \text{...from complimentary slackness}$$

$$\frac{\partial L}{\partial \pi_k} = 0 \Rightarrow \sum_{n=1}^N \frac{\gamma_{nk}}{\pi_k} - \mu - \lambda_k = 0$$

$$\Rightarrow \pi_k = \frac{\sum_{n=1}^N \gamma_{nk}}{\mu} \quad \text{...putting this back in constraint}$$

$$\sum_{k=1}^K \frac{\sum_{n=1}^N \gamma_{nk}}{\mu} = 1 \Rightarrow \mu = \sum_{k=1}^K \sum_{n=1}^N \gamma_{nk} = \sum_{n=1}^N \sum_{k=1}^K \gamma_{nk} = \sum_{n=1}^N 1 = N$$

Putting this back in expression for π_k , we have:

$$\pi_k = \frac{\sum_{n=1}^N \gamma_{nk}}{N}$$

Update for each θ_{ki} can be obtained by equating the first derivative of corresponding term to zero:

$$\frac{\partial Q}{\partial \theta_{ki}} = 0 \Rightarrow \sum_{n=1}^{N} \gamma_{nk} \left[\frac{x_{ni}}{\theta_{ki}} - \frac{1 - x_{ni}}{1 - \theta_{ki}} \right] = 0$$

$$\Rightarrow \frac{1 - \theta_{ki}}{\theta_{ki}} = \frac{\sum_{n=1}^{N} \gamma_{nk} (1 - x_{ni})}{\sum_{n=1}^{N} \gamma_{nk} x_{ni}}$$

$$\Rightarrow \frac{1}{\theta_{ki}} = 1 + \frac{\sum_{n=1}^{N} \gamma_{nk} (1 - x_{ni})}{\sum_{n=1}^{N} \gamma_{nk} x_{ni}} = \frac{\sum_{n=1}^{N} \gamma_{nk}}{\sum_{n=1}^{N} \gamma_{nk} x_{ni}}$$

From the above, we can write the expression for θ_{ki} as:

$$\theta_{ki} = \frac{\sum_{n=1}^{N} \gamma_{nk} x_{ni}}{\sum_{n=1}^{N} \gamma_{nk}}$$

Same thing can be expressed in vector form as:

$$\theta_k = \frac{\sum_{n=1}^{N} \gamma_{nk} \mathbf{x}_n}{\sum_{n=1}^{N} \gamma_{nk}}$$

3 Problem

3.1 Solution

From the class (not showing the proof again), we know the value for sequence probability:

$$\begin{split} P(X_{1:T} = x_{1:T}) &= \sum_{s'} \alpha_{s'}(T) \quad ... \text{so} \\ P(Z_{T+1} = s | X_{1:T} = x_{1:T}) &= \sum_{s'} P(Z_{T+1} = s, Z_T = s' | X_{1:T} = x_{1:T}) \quad ... \text{from marginal probability} \\ &= \frac{\sum_{s'} P(Z_{T+1} = s, Z_T = s', X_{1:T} = x_{1:T})}{P(X_{1:T} = x_{1:T})} \quad ... \text{from conditional probability} \\ &= \frac{\sum_{s'} P(Z_{T+1} = s | Z_T = s', X_{1:T} = x_{1:T}) P(Z_T = s', X_{1:T} = x_{1:T})}{P(X_{1:T} = x_{1:T})} \quad ... \text{chain rul} \\ &= \frac{\sum_{s'} P(Z_{T+1} = s | Z_T = s') P(Z_T = s', X_{1:T} = x_{1:T})}{P(X_{1:T} = x_{1:T})} \quad ... \text{markov property} \\ &= \frac{\sum_{s'} a_{s',s} \alpha_{s'}(T)}{\sum_{s'} \alpha_{s'}(T)} \quad ... \text{substituting values} \end{split}$$

3.2 Solution

$$\begin{split} P(Z_{T+k} = s | X_{1:T} = x_{1:T}) &= \sum_{s'} P(Z_{T+k} = s, Z_{T+k-1} = s' | X_{1:T} = x_{1:T}) \quad \text{...marginal probability} \\ &= \sum_{s'} P(Z_{T+k} = s | Z_{T+k-1} = s', X_{1:T} = x_{1:T}) P(Z_{T+k-1} = s' | X_{1:T} = x_{1:T}) \quad \text{...chain rule} \\ &= \sum_{s'} P(Z_{T+k} = s | Z_{T+k-1} = s') P(Z_{T+k-1} = s' | X_{1:T} = x_{1:T}) \quad \text{...markov property} \\ &= \sum_{s'} a_{s',s} P(Z_{T+k-1} = s' | X_{1:T} = x_{1:T}) \quad \text{...substituting value} \end{split}$$