1 Document Clustering

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Question 1 Expectation Maximisation

Task I

Write mathematical formulations of the optimization functions of maximum likelihood estimation (MLE) for the document clustering model with complete data and incomplete data, respectively. Then briefly describe why MLE with incomplete data is hard to optimize.

Multiple documents MLE (complete data)

For each document d_n, choose a cluster $k \in \{1, \dots, K\}$ by tossing a K-faced dice parameterized by $\boldsymbol{\varphi} = [\varphi_1, \dots, \varphi_K]$:

$$p(z_n = k) = \varphi_k, \quad \sum_{k=1}^{K} \varphi_k = 1$$

where φ_k represents the prior probability that document d_n belongs to cluster k.

Given the selected cluster k, generate each word in the document independently from the word distribution $\boldsymbol{\mu}_k = [\mu_{k,w}]_{w \in \mathcal{A}}$:

$$p(w \mid z_n = k) = \mu_{k,w}, \quad \sum_{w \in \mathcal{A}} \mu_{k,w} = 1$$

Each $\boldsymbol{\mu}_k$ corresponds to the multinomial word distribution for cluster k.

Thus, the joint probability of a document d and its cluster k is:

$$p(d, k) = p(k)\, p(d \mid k) = \varphi_k \prod_{w \in \mathcal{A}} \mu_{k,w}^{c(w,d)}$$

where $c(w,d)$ is the number of times word w appears in document d.

Assume that in addition to the documents $D = \{d_1, d_2, \ldots, d_N\}$, each document d_N has its own topic label $\{k_1, k_2, \ldots, k_N\}$. We can represent the joint probalitity as:

$$p(d_1, k_1, \ldots, d_N, k_N) = p(d_1, k_1) \cdot p(d_2, k_2) \cdot \ldots \cdot p(d_N, k_N) = \prod_{n=1}^{N} p(k_N)\, p(d_N \mid k_N)$$

Therefore, the general form is:

$$p(d_1, z_1, \ldots, d_N, z_N) = \prod_{n=1}^{N} \prod_{k=1}^{K} \left(\varphi_k \prod_{w \in \mathcal{A}} \mu_{k,w}^{c(w,d_n)} \right)^{z_{n,k}}$$

where $z_{n,k} \in \{0, 1\}$ is an indicator variable that equals 1 if document d_n belongs to cluster k, and 0 otherwise.

Multiple documents MLE (incomplete data)

In this case, we can only observe the document d, but we do not know which cluster k it belongs to. The cluster assignment k is therefore a latent variable. Hence, we marginalize over k to eliminate this unobserved variable.

Therefore, we can represent the joint probability of a document d as:

$$p(d) = \sum_k p(d, k) = \sum_k \varphi_k \cdot p(d \mid k) = \sum_k (\varphi_k \prod_{w \in \mathcal{A}} \mu_{k,w}^{c(w,d)})$$

where $c(w,d)$ is the number of times word w appears in document d.

Assume that in addition to the documents $D = \{d_1, d_2, \ldots, d_N\}$, z_n is a latent variable. We can represent the joint probalitity as:

$$p(d_1, \ldots, d_N) = \prod_{n=1}^{N} p(d_n) = \prod_{n=1}^{N} \sum_{k=1}^{K} p(z_{n,k} = 1, d_n)$$

Here, $z_{n,k} = 1$ indicates that document d_n belongs to cluster k, and $z_{n,k} = 0$ otherwise.

Substituting the generative model, we obtain the general form:

$$p(d_1, \ldots, d_N) == \prod_{n=1}^{N} \sum_{k=1}^{K} \left(\varphi_k \prod_{w \in \mathcal{A}} \mu_{k,w}^{c(w,d_n)} \right)$$

Taking the logarithm gives the incomplete-data log-likelihood

$$\ln p(d_1, z_1, \ldots, d_N, z_N) = \sum_{n=1}^{N} \ln p(d_n) = \sum_{n=1}^{N} \ln \sum_{k=1}^{K} \left(\varphi_k \prod_{w \in \mathcal{A}} \mu_{k,w}^{c(w,d_n)} \right)$$

MLE with incomplete data is hard to optimize because the log-likelihood contains a logarithm of a summation over hidden clusters. The latent variables z_n are unobserved, so the parameters φ_k and $\mu_{k,w}$ are coupled inside the logarithm, preventing closed-form analytical updates.

Briefly explain the high-level idea of the EM algorithm to find MLE parameter estimates.

Since the usual MLE on the incomplete-data log-likelihood is hard, EM tackles this by alternating two steps on a current parameter guess.

In the **E-step**, we compute the expected value of the complete-data log-likelihood with respect to the posterior distribution of the latent cluster assignments under the current parameter estimates $\boldsymbol{\theta}^{\text{old}}$.

This gives the **Q function**, which forms the basis of the EM algorithm:

$$Q(\boldsymbol{\theta}, \boldsymbol{\theta}^{\text{old}}) = \sum_{n=1}^{N} \sum_{k=1}^{K} p(z_{n,k} = 1 \mid d_n, \boldsymbol{\theta}^{\text{old}}) \ln p(z_{n,k} = 1, d_n \mid \boldsymbol{\theta})$$

Substituting the generative model of document clustering, we get:

$$Q(\boldsymbol{\theta}, \boldsymbol{\theta}^{\text{old}}) = \sum_{n=1}^{N} \sum_{k=1}^{K} \gamma(z_n, k) \left(\ln \varphi_k + \sum_{w \in \mathcal{A}} c(w, d_n) \ln \mu_{k,w} \right)$$

where

- $\boldsymbol{\theta} = (\boldsymbol{\varphi}, \boldsymbol{\mu}_1, \ldots, \boldsymbol{\mu}_K)$
  is the collection of model parameters.

- $\gamma(z_n, k) = p(z_{n,k} = 1 \mid d_n, \boldsymbol{\theta}^{\text{old}})$
  represents the **responsibility** (posterior probability) that document d_n belongs to cluster k.
- $c(w, d_n)$ is the number of occurrences of word w in document d_n.

In the **M-step**, we maximize this Q function with respect to $\boldsymbol{\theta}$, which yields the updated parameter estimates:

$$\varphi_k^{\text{new}} = \frac{N_k}{N}, \quad N_k = \sum_{n=1}^{N} \gamma(z_n, k)$$

$$\mu_{k,w}^{\text{new}} = \frac{\sum_{n=1}^{N} \gamma(z_n, k) c(w, d_n)}{\sum_{w' \in \mathcal{A}} \sum_{n=1}^{N} \gamma(z_n, k) c(w', d_n)}$$

Each EM iteration alternates between estimating the posterior responsibilities (E-step) and maximizing the expected complete-data log-likelihood (M-step). This process guarantees that the incomplete-data log-likelihood **never decreases** across iterations.

Task II

Problem Setup

Given a collection of documents $D = \{d_1, d_2, \ldots, d_N\}$ with vocabulary $\mathcal{A}$, we want to cluster them into K clusters.

Model Parameters

The parameters to learn are:

$$\boldsymbol{\theta} := (\boldsymbol{\varphi}, \boldsymbol{\mu}_1, \ldots, \boldsymbol{\mu}_K)$$

where:

- **Mixing coefficients:** $\boldsymbol{\varphi} = (\varphi_1, \ldots, \varphi_K)$ with $\sum_{k=1}^{K} \varphi_k = 1$ and $\varphi_k \geq 0$
- **Word distributions:** $\boldsymbol{\mu}_k = (\mu_{k,w})_{w \in \mathcal{A}}$ for cluster k, with $\sum_{w \in \mathcal{A}} \mu_{k,w} = 1$ and $\mu_{k,w} \geq 0$

Latent Variables

$z_n = (z_{n,1}, \ldots, z_{n,K})$ where $z_{n,k} = 1$ if document d_n belongs to cluster k, and 0 otherwise.

Notation

$c(w, d_n) =$ count of word w in document d_n

Derive process

First, random generate initial parameters: μ_{old} and φ_{old}.

E-step

In E-step, for every d_n and every cluster k, compute the posterior probability:

$$\gamma(z_n, k) = p(z_{n,k} = 1 \mid d_n, \boldsymbol{\theta}^{\text{old}})$$

According to the Bayes Rules:

$$\gamma(z_n, k) = p(z_{n,k} = 1 \mid d_n, \boldsymbol{\theta}^{\text{old}}) = \frac{p(z_n = k \mid \theta)\, p(d_n \mid z_n = k, \theta)}{\sum_{j=1}^{K} p(z_n = j \mid \theta)\, p(d_n \mid z_n = j, \theta)}$$

Substituting $p(z_n = k \mid \theta) = \mu_k$ and $p(d_n \mid z_n = k, \theta) = \prod_{w \in \mathcal{A}} \mu_{k,w}^{c(w,d_n)}$, we have **E-Step Update Rule**:

$$\gamma(z_n, k) = \frac{\varphi_{old} \prod_{w \in \mathcal{A}} (\mu_{k,w}^{old})^{\,c(w,d_n)}}{\sum_{j=1}^{K} \varphi_j^{old} \prod_{w \in \mathcal{A}} (\mu_{j,w}^{old})^{c(w,d_n)}}$$

In M-Step, we need maximize $Q(\boldsymbol{\theta}, \boldsymbol{\theta}^{\text{old}})$ subject to: $\sum_{k=1}^{K} \varphi_k = 1$ and $\sum_{w \in \mathcal{A}} \mu_{k,w} = 1$.

Form the Lagrangian:

$$\mathcal{L} = Q(\boldsymbol{\theta}, \boldsymbol{\theta}^{\text{old}}) + \lambda \left(\sum_{k=1}^{K} \varphi_k - 1 \right)$$

Taking derivative with respect to φ_k:

$$\frac{\partial \mathcal{L}}{\partial \varphi_k} = \sum_{n=1}^{N} \gamma(z_n, k) \cdot \frac{1}{\varphi_k} + \lambda = 0 \Rightarrow \sum_{n=1}^{N} \gamma(z_n, k) = -\lambda \varphi_k$$

Summing over k:

$$\sum_{k=1}^{K}\sum_{n=1}^{N}\gamma(z_n,k) = -\lambda\sum_{k=1}^{K}\varphi_k = -\lambda$$

Since $\sum_{k=1}^{K}\gamma(z_n,k)=1$, we have $\sum_{k=1}^{K}\sum_{n=1}^{N}\gamma(z_n,k)=N$.

Therefore: $\lambda=-N$. Substituting back we have **M-Step Update Rule for** φ_k:

$$\varphi_k^{\text{new}} = \frac{1}{N}\sum_{n=1}^{N}\gamma(z_n,k) = \frac{N_k}{N}$$

where $N_k := \sum_{n=1}^{N}\gamma(z_n,k)$ is the effective number of documents assigned to cluster k.

M-step

Then we need derive the updating rule of Word Distributions $\mu_{k,w}$:

For each cluster k, form the Lagrangian:

$$\mathcal{L}_k = Q(\boldsymbol{\theta},\boldsymbol{\theta}^{\text{old}}) + \lambda_k\left(\sum_{w\in\mathcal{A}}\mu_{k,w}-1\right)$$

Taking derivative with respect to $\mu_{k,w}$:

$$\frac{\partial\mathcal{L}_k}{\partial\mu_{k,w}} = \sum_{n=1}^{N}\gamma(z_n,k)\cdot\frac{c(w,d_n)}{\mu_{k,w}} + \lambda_k = 0$$

$$\Rightarrow \sum_{n=1}^{N}\gamma(z_n,k)\cdot c(w,d_n) = -\lambda_k\mu_{k,w}$$

Summing over $w\in\mathcal{A}$:

$$\sum_{w\in\mathcal{A}}\sum_{n=1}^{N}\gamma(z_n,k)\cdot c(w,d_n)=-\lambda_k\sum_{w\in\mathcal{A}}\mu_{k,w}=-\lambda_k$$

The left side equals:

$$\sum_{n=1}^{N}\gamma(z_n,k)\sum_{w\in\mathcal{A}}c(w,d_n)=\sum_{n=1}^{N}\gamma(z_n,k)\cdot|d_n|$$

where $|d_n|$ is the total word count in document d_n.

For simplicity, let:

$$\lambda_k=-\sum_{w'\in\mathcal{A}}\sum_{n=1}^{N}\gamma(z_n,k)\cdot c(w',d_n)$$

Then we get the **M-Step Update Rule for** $\mu_{k,w}$:

$$\mu_{k,w}^{\text{new}}=\frac{\sum_{n=1}^{N}\gamma(z_n,k)\cdot c(w,d_n)}{\sum_{w'\in\mathcal{A}}\sum_{n=1}^{N}\gamma(z_n,k)\cdot c(w',d_n)}$$

Assignment (After Convergence):

Assign document d_n to cluster:

$$k^*=\arg\max_k\gamma(z_n,k)$$

Task III

Load File

In [121…

```
import pandas as pd

with open('/Users/2m/Documents/Monash/FIT5201/Assignment/ML_ASS/ASS2/Dataset_S2_2025/Task2A.txt', 'r') as file:
    text = file.readlines()
```

Data preprocessing

In [122…

```
from sklearn.feature_extraction.text import CountVectorizer

all([length == 2 for length in [len(line.split('\t')) for line in text]])
labels, articles = [line.split('\t')[0].strip() for line in text], [line.split('\t')[1].strip() for line in text]
docs = pd.DataFrame(data = zip(labels,articles), columns=['label', 'article'])
docs.label = docs.label.astype('category')
docs.head()

min_freq = 10
feature_options = []
for i in range(min_freq):
    cv = CountVectorizer(
        lowercase=True, stop_words="english", min_df=i + 1
    )  # min_df: low frequency words
    features = cv.fit_transform(raw_documents=articles)
    feature_options += [features]
    print(len(cv.get_feature_names_out()))

features = feature_options[4]
features.shape
```

```
30288
16806
12153
9724
8094
6986
6182
5562
5063
4593
```

Out[122]:

```
(2373, 8094)
```

Task IV

In [ ]:

```
import numpy as np
from scipy.special import logsumexp
```

```python
class EM:
    def __init__(self, K, tau_max=200, epsilon=0.01, random_state=None, hardEM=False):
        self.K = K  # number of EM clusters
        self.tau_max = tau_max  # max number of iterations
        self.epsilon = epsilon  # minimum acceptable error rate
        self.random_state = random_state
        self.hardEM = hardEM
        np.random.seed(self.random_state)

    def get_params(self, deep=False):
        return {
            "K": self.K,
            "tau_max": self.tau_max,
            "epsilon": self.epsilon,
            "random_state": self.random_state,
            "hardEM": self.hardEM,
        }

    def __str__(self):
        params = self.get_params()
        return "EM({0})".format(
            ",".join(["=".join([key, str(params[key])]) for key in params.keys()])
        )

    def __repr__(self):
        return self.__str__()

    def compute_gamma(self, X, phi, mu):
        """
        Compute the posterior probability (responsibility) using log-sum-exp.
        """
        X = X.toarray()
        N, V = X.shape
        K = self.K
        r = np.zeros((N, K))

        for n in range(N):  # for each document
            doc = X[n]
            scores = np.zeros(K)
            for k in range(K):  # for each cluster
                # Compute log p
                log_prob = np.log(phi[k] + 1e-12)  # avoid log 0
                for w in range(V):
                    if doc[w] > 0:
```

```
                log_prob += doc[w] * np.log(mu[k, w] + 1e-12)
            scores[k] = log_prob

        # LSE
        log_sum = logsumexp(scores)

        # normalized
        r[n] = np.exp(scores - log_sum)

    return r  # shape: (N, K)

def update_phi(self, gamma, phi, N):
    """
    Update the mixing coefficients
    """
    for k in range(self.K):
        total = 0.0
        for n in range(N):
            total += gamma[n][k]
        phi[k] = total / N
    return phi

def update_mu(self, X, gamma, N, V):
    """
    Update the word distributions
    """
    documents = X.toarray()
    new_mu = np.zeros((self.K, V))  # new mu for each cluster
    for k in range(self.K):  # for each cluster
        total = 0.0
        for n in range(N):  # for each document
            doc = documents[n]
            for w in range(V):  # for each word
                count = doc[w]
                new_mu[k][w] += gamma[n][k] * count
                total += (
                    gamma[n][k] * count
                )  # accumulate the total count of words in cluster k
        # normalize
        for w in range(V):
            if total > 0:
                new_mu[k][w] /= total

    return new_mu
```

```python
    def fit(self, X, verbose=False):
        N, V = X.shape  # N is the number of documents, V is the number of words

        # initialize phi with equal probability
        self.phi = np.full(self.K, 1 / self.K)

        # initialize mu randomly and normalize
        self.mu = np.random.rand(self.K, V)
        self.mu /= np.sum(self.mu, axis=1, keepdims=True)

        # initialize gamma as 0, calculate in E-step
        r = np.zeros((N, self.K))

        terminate = False
        tau = 0

        # fitting loop
        Mu_hat_old = self.mu  # store the last iteration value for mu_hat
        while not terminate:
            if tau % 10 == 0 and verbose:
                print("iteration {0}".format(tau))
            # E step:
            r = self.compute_gamma(X, self.phi, self.mu)

            # if hardEM, set r to 0 or 1
            if self.hardEM:
                max_vals = r.max(axis=1, keepdims=True)
                r_hard = (r == max_vals).astype(int)
                r = r_hard

            # M step
            self.phi = self.update_phi(r, self.phi, N)
            self.mu = self.update_mu(X, r, N, V)

            # increase iteration counter
            tau += 1

            # check termination condition
            if tau >= self.tau_max:
                terminate = True
            if np.allclose(self.mu, Mu_hat_old, rtol=self.epsilon):
                terminate = True
```

```python
            # record the means
            Mu_hat_old = self.mu

        if verbose:
            print(f"Converged in {tau} iterations")

        return self

    def predict_proba(self, x):
        r = self.compute_gamma(x, self.phi, self.mu)
        return r

    def predict(self, x):
        probs = self.predict_proba(x)
        preds = np.argmax(probs, axis=1)
        return preds
```

Task V

Set the number of clusters K=4, and run the hard clustering (using hard-EM) and soft clustering (using soft-EM) on the provided data

In [124…

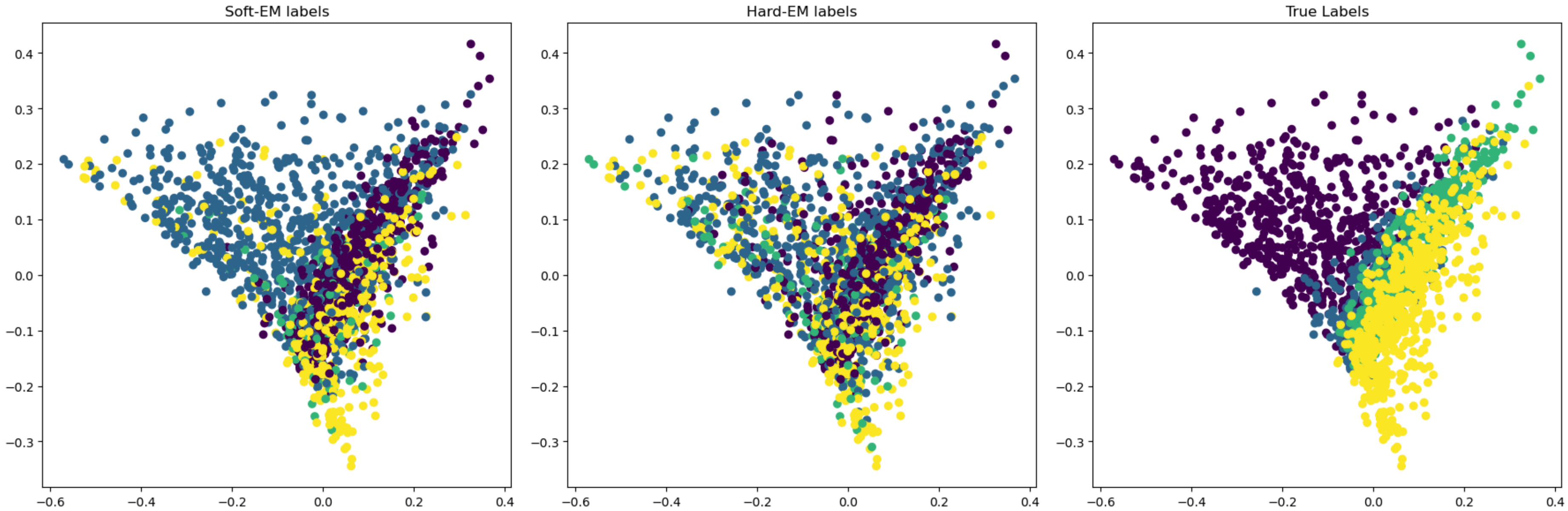
```python
print("======== Trainning and predicting using hard-EM: ========")
hardEM = EM(K=4, hardEM=True, random_state=1234)
hardEM.fit(features, verbose=True)
preds_hard = hardEM.predict(features)
# preds_hard

print("======== Trainning and predicting using soft-EM: ========")
softEM = EM(K=4, random_state=1234)
softEM.fit(features, verbose=True)
preds_soft = softEM.predict(features)
# preds_soft
```

```
======== Trainning and predicting using hard-EM: ========
iteration 0
Converged in 9 iterations
======== Trainning and predicting using soft-EM: ========
iteration 0
iteration 10
iteration 20
iteration 30
iteration 40
iteration 50
Converged in 59 iterations
```

Task VI

In [125…

```python
## perform pca
import matplotlib.pyplot as plt
from sklearn.decomposition import PCA
from sklearn.preprocessing import Normalizer

l2_norm = Normalizer(norm='l2')
features_normalised = l2_norm.fit_transform(features.toarray())

pca = PCA(n_components=2)
_2D_features = pca.fit_transform(features_normalised)

_, axs = plt.subplots(1, 3, figsize=(18, 6), tight_layout=True)
## plot the soft-EM outcome
axs[0].scatter(x=_2D_features[:,0],y=_2D_features[:,1], c=preds_soft)
axs[0].set_title('Soft-EM labels')

## plot the hard-EM outcome
axs[1].scatter(x=_2D_features[:,0],y=_2D_features[:,1], c=preds_hard)
axs[1].set_title('Hard-EM labels')

## plot the original data
axs[2].scatter(x=_2D_features[:,0],y=_2D_features[:,1], c=docs.label.cat.codes)
axs[2].set_title('True Labels')
plt.show()
```



Discussion: Soft-EM vs Hard-EM

From the plots, the **Soft-EM** and **Hard-EM** results look quite similar in overall structure and where the clusters appear. Both models produce four main fan-shaped clusters roughly in the same positions. That’s because, in the Soft-EM visualization, I used the argmax of the responsibility values to assign a single label to each sample. In other words, the soft probabilities were converted into hard labels, which makes the colors look discrete instead of showing a smooth gradient.

When comparing Soft-EM with the True Labels, the overall cluster patterns line up pretty well. Soft-EM clearly captures the global structure of the data better — even if some boundaries are a bit fuzzy, it still aligns with the true grouping. This happens because Soft-EM updates its parameters using probability-weighted expectations (the responsibilities), which makes the learning process smoother, more stable, and less sensitive to noise. In contrast, Hard-EM uses discrete assignments in each step, which can make it a bit more sensitive to small boundary changes.

The Hard-EM result, on the other hand, shows a much larger mismatch with the ground truth. Some clusters are noticeably shifted or overlapping, and quite a few samples end up in the wrong regions. That’s because Hard-EM does “hard assignments” during the E-step — each data point is forced into the single cluster with the highest probability, losing the uncertainty information that Soft-EM keeps. As a result, Hard-EM tends to be more sensitive to initialization and can easily get stuck in a suboptimal solution, where the cluster centers don’t match the real data structure.