

# DD2434 Advanced Machine Learning 2021-2022

# Assignment 2: Probabilistic Graphical Models, Variational Inference and Expectation-Maximization Algorithms

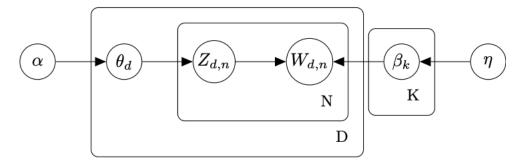
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# 2.1 Dependencies in a Directed Graphical Model

Consider the graphical models shown in Figures 1 and 2. You merely have to answer "yes" or "no" to each question.

Figure 1: Graphical model of smoothed LDA



# Question 2.1.1

In the graphical model of Figure 1, is  $W_{d,n} \perp W_{d,n+1} \mid \theta_d, \beta_{1:K}$ ?

Yes, it holds that  $W_{d,n} \perp W_{d,n+1} \mid \theta_d, \beta_{1:K}$ 

# Question 2.1.2

In the graphical model of Figure 1, is  $\theta_d \perp \theta_{d+1} \mid Z_{d,1:N}$ ?

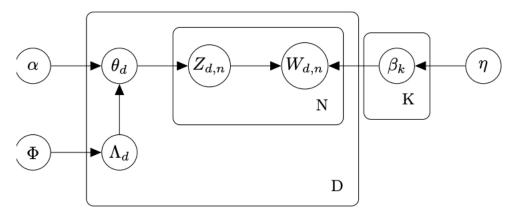
No, it holds that  $\theta_d \not\perp \theta_{d+1} \mid Z_{d,1:N}$ 

# Question 2.1.3

In the graphical model of Figure 1, is  $\theta_d \perp \theta_{d+1} \mid \alpha, Z_{1:D,1:N}$ ?

Yes, it holds that  $\theta_d \perp \theta_{d+1} \mid \alpha, Z_{1:D,1:N}$ 

Figure 2: Graphical model of Labeled LDA



# Question 2.1.4

In the graphical model of Figure 2, is  $W_{d,n} \perp W_{d,n+1} \mid \lambda_d, \beta_{1:K}$ ?

No, it holds that  $W_{d,n} \not\perp W_{d,n+1} \mid \lambda_d, \beta_{1:K}$ 

#### Question 2.1.5

In the graphical model of Figure 2, is  $\theta_d \perp \theta_{d+1} \mid Z_{d,1:N}, Z_{d+1,1:N}$ ?

No, it holds that  $\theta_d \not\perp \theta_{d+1} \mid Z_{d,1:N}, Z_{d+1,1:N}$ 

### Question 2.1.6

In the graphical model of Figure 2, is  $\Lambda_d \perp \Lambda_{d+1} \mid \Phi, Z_{1:D,1:N}$ ?

No, it holds that  $\Lambda_d \not\perp \Lambda_{d+1} \mid \Phi, Z_{1:D,1:N}$ 

# 2.2 Likelihood of a Tree Graphical Model

Let T be a rooted binary tree, with vertex set V(T) and leaf set L(T), and consider the graphical model T,  $\Theta$  described as follows. For each vertex  $v \in V(T)$  there is an associated random variable  $X_v$  that assumes values in [K]. Moreover, for each  $v \in V(T)$ , the CPD  $\theta_v = p(X_v \mid x_{pa(v)})$  is a categorical distribution. Let  $\beta = \{x_l : l \in L(T)\}$  be an assignment of values to all the leaves of T.

#### Question 2.2.7

Implement a dynamic programming algorithm that, for a given  $T, \Theta$  and  $\beta$ , computes  $p(\beta \mid T, \Theta)$ .

To compute  $p(\beta \mid T, \Theta)$  efficiently we need to find an expression of it that allows us to divide the computation in smaller sub-computations, i.e, dynamic programming. Using Bayes' Theorem we can marginalize in the following manner:

$$p(\beta \mid T, \Theta) = \sum_{i} p\left(X_{r \cap \beta}, X_{r} = i \mid T, \Theta\right) = \sum_{i} p\left(X_{r \cap \beta} \mid X_{r} = i, T, \Theta\right) p\left(X_{r} = i\right)$$

where  $X_r$  is the value of the root node. Now, let  $s(v,i) = p\left(X_{O \cap \downarrow v} \mid X_{pa(v)} = i, T, \Theta\right)$  for any vertex v, where  $\{O \cap \downarrow v\}$  are the observed values of the children of node v. Then we have that:

1. At the root layer, r:

$$p(\beta \mid T, \Theta) = \sum_{i} s(r, i) p(X_r = i)$$

2. We know that T is a binary tree, i.e, each node has 2 children: w and u. Then, at any node v between root and leaf nodes:

$$s(v,i) = p(X_{O \cap \downarrow v} \mid X_v = i) = p(X_{O \cap \downarrow u} \mid X_v = i) p(X_{O \cap \downarrow w} \mid X_v = i)$$

$$= \left(\sum_{j} s(u,j) p(X_u = j \mid x_v = i)\right) \left(\sum_{j} s(w,j) p(X_w = j \mid x_v = i)\right)$$

3. Finally, we have as base case the leaf nodes l which are the observed ones:

$$s(l,i) = \begin{cases} 1, & X_l = i \\ 0, & \text{otherwise} \end{cases}$$

This manner of expressing  $p(\beta \mid T, \Theta)$  is very convenient since we can calculate it in a dynamic programming fashion by working up the computations from the leaf nodes until the root of the tree. See code in Appendix 2: Tree Code.

#### Question 2.2.8

Report  $p(\beta \mid T, \Theta)$  for each given data, separately. You should report 15 values in total; 5 for small tree, 5 for medium tree and 5 for large tree.

See results in tables 1, 2 and 3.

Sample	Likelihood
0	0.009786075668602368
1	0.015371111945909397
2	0.02429470256988136
3	0.005921848333806081
4	0.016186321212555956

Table 1: Small tree results.

Sample	Likelihood
0	1.7611947348905713e-18
1	2.996933026124685e-18
2	2.891411201505415e-18
3	4.6788419411270006e-18
4	5.664006737201378e-18

Table 2: Medium tree results.

Sample	Likelihood
0	3.63097513075208e-69
1	3.9405421986921234e-67
2	5.549061147187144e-67
3	9.89990102807915e-67
4	3.11420969368965e-72

Table 3: Large tree results.

# 2.3 Simple Variational Inference

Consider the model defined by Equation (10.21)-(10-23) in Bishop. We are here concerned with the VI algorithm for this model covered during the lectures and in the book.

#### Question 2.3.9

Implement the VI algorithm for the variational distribution in Equation (10.24) in Bishop.

We can follow the derivation explained in Bishop, [1]. Given a data set  $D = \{x_1, \ldots, x_N\}$  of observed values x that are drawn from a Gaussian distribution,  $p(D \mid \mu, \tau)$ , we want to infer a posterior distribution,  $p(\mu, \tau \mid D)$ , using variational inference. The likelihood function is:

$$p(D \mid \mu, \tau) = \left(\frac{\tau}{2\pi}\right)^{N/2} \exp\left\{-\frac{\tau}{2} \sum_{n=1}^{N} (x_n - \mu)^2\right\}$$

The prior distributions for  $\mu$  and  $\tau$  are:

$$p(\mu \mid \tau) = \mathcal{N}\left(\mu; \mu_0, (\lambda_0 \tau)^{-1}\right)$$
$$p(\tau) = \Gamma\left(\tau; a_0, b_0\right)$$

where  $\mu_0, \lambda_0, a_0, b_0$  are hyperparameters.

The variational approximation of the posterior is factorized and results in:

$$q(\mu, \tau) = q_{\mu}(\mu)q_{\tau}(\tau)$$

The factorized approximated distributions are computed in Bishop, [1], which result to be:

$$q_{\mu}(\mu) = \mathcal{N}\left(\mu; \mu_N, \lambda_N^{-1}\right)$$
$$q_{\tau}(\tau) = \Gamma\left(\tau; a_N, b_N\right)$$

These approximated distributions are updated and improved by the updates of their parameters, which are updated in the order below until convergence, i.e, change in the parameters update is below a desired threshold.

$$\begin{split} &\mu_{N} = \frac{\lambda_{0}\mu_{0} + N\bar{x}}{\lambda_{0} + N} \\ &\lambda_{N} = (\lambda_{0} + N) E_{\tau}[\tau] = (\lambda_{0} + N) \frac{a_{N}}{b_{N}} \\ &a_{N} = a_{0} + \frac{N}{2} \\ &b_{N} = b_{0} + \frac{1}{2} E_{\mu} \left[ \sum_{n=1}^{N} (x_{n} - \mu)^{2} + \lambda_{0} (\mu - \mu_{0})^{2} \right] \\ &= b_{0} + \frac{1}{2} \left[ \left( \sum_{n=1}^{N} x_{n}^{2} \right) + N E_{\mu} \left[ \mu^{2} \right] - 2 N \bar{x} E_{\mu}[\mu] + \lambda_{0} \left( E_{\mu} \left[ \mu^{2} \right] + \mu_{0}^{2} - 2 \mu_{0} E_{\mu}[\mu] \right) \right] \\ &= \left\{ E_{\mu}[\mu] = \mu_{N}, E_{\mu} \left[ \mu^{2} \right] = V_{\mu}(\mu) + E_{\mu}[\mu]^{2} = \lambda^{-1} + \mu_{N}^{2} \right\} \\ &= b_{0} + \frac{1}{2} \left[ \left( \sum_{n=1}^{N} x_{n}^{2} \right) + (N + \lambda_{0}) \left( \lambda^{-1} + \mu_{N}^{2} \right) - 2 \mu_{N} \left( N \bar{x} + \mu_{0} \lambda_{0} \right) + \lambda_{0} \mu_{0}^{2} \right] \end{split}$$

See code in Appendix 3: Variational Inference Code.

#### Question 2.3.10

#### What is the exact posterior?

The posterior we are after is  $p(\mu, \tau \mid D)$ . From Bayes' theorem we know that:

$$p(\mu, \tau \mid D) = \frac{p(D \mid \mu, \tau)p(\mu \mid \tau)p(\tau)}{p(D)} \propto p(D \mid \mu, \tau)p(\mu \mid \tau)p(\tau)$$

Both priors  $\mu$  and  $\tau$  are conjugate priors of the likelihood and therefore, will make the posterior

be Gaussian-Gamma distribution [2]:

$$p(\mu, \tau \mid D) \propto p(D \mid \mu, \tau) p(\mu \mid \tau) p(\tau)$$

$$\propto \tau^{\frac{N}{2}} \tau^{\frac{1}{2}} \tau^{a_0 - 1} e^{-b_0 \tau} \exp \left\{ -\frac{\tau}{2} \left[ \sum_{n=1}^{N} (x_n - \mu)^2 + \lambda_0 (\mu - \mu_0)^2 \right] \right\}$$

$$\propto \tau^{\frac{N}{2}} \tau^{\frac{1}{2}} \tau^{a_0 - 1} e^{-b_0 \tau} \exp \left\{ -\frac{1}{2} \tau (N + \lambda_0) \left( \mu - \frac{N\bar{x} + \lambda_0 \mu_0}{N\lambda_0} \right)^2 \right\} \times$$

$$\exp \left\{ -\frac{\tau}{2} \left[ -\frac{(N\bar{x} + \lambda_0 \mu_0)^2}{N + \lambda_0} + \sum_{n=1}^{N} x_n^2 + \lambda_0 \mu_0^2 \right] \right\}$$

$$\propto \tau^{\frac{N}{2}} \tau^{a_0 - 1} e^{-b_0 \tau} \mathcal{N} \left( \mu; \frac{N\bar{x} + \lambda_0 \mu_0}{N\lambda_0}, \frac{1}{\tau (N + \lambda_0)} \right) \times$$

$$\exp \left\{ -\frac{\tau}{2} \left[ -\frac{(N\bar{x} + \lambda_0 \mu_0)^2}{N + \lambda_0} + \sum_{n=1}^{N} x_n^2 + \lambda_0 \mu_0^2 \right] \right\}$$

$$\propto \mathcal{N} (\mu; \mu_{real}, \sigma_{real}) \times \Gamma(\tau; a_{real}, b_{real}))$$

where:

$$\mu_{real} = \frac{N\bar{x} + \lambda_0 \mu_0}{N + \lambda_0}$$

$$\sigma_{real} = \frac{1}{\sqrt{\tau(N + \lambda_0)}}$$

$$a_{real} = a_0 + \frac{N}{2}$$

$$b_{real} = b_0 + \frac{1}{2} \left[ \left( \sum_{n=1}^{N} x_n^2 \right) + \lambda_0 \mu_0^2 - \frac{\left(N\bar{x} + \lambda_0 \mu_0\right)^2}{N + \lambda_0} \right]$$

### Question 2.3.11

Compare the inferred variational distribution with the exact posterior. Run the inference on data points drawn from i.i.d. Gaussians. Do this for three interesting cases and visualize the results. Describe the differences.

1. Effects of data size: In this case we try to approximate N(0,1) distribution, we leave all parameters set to 1 and vary the sample size to see the effect of the amount of data available on the approximation. We can see on figures 3, 4 and 5 how the more samples we have the better the inferred distribution fits the real distribution of the data. This was expected since its the usual case in machine learning. However, both real and inferred distributions fail to accurately model the data distribution N(0,1) in figure 3, in contrast to the other two cases, due to the extremely low number of points.

# [a0=1 b0=1 mu0=1 lambda0=1] N(0,1) N=10 Inferred Posterior 1.4 True Posterior 1.2 1.0 8.0 <u>a</u> 0.6 0.4 0.2 -0.25 0.00 0.25 0.75 -0.75 0.50 -1.00 -0.50 1.00 Mu

Figure 3: N(0,1) with 10 samples

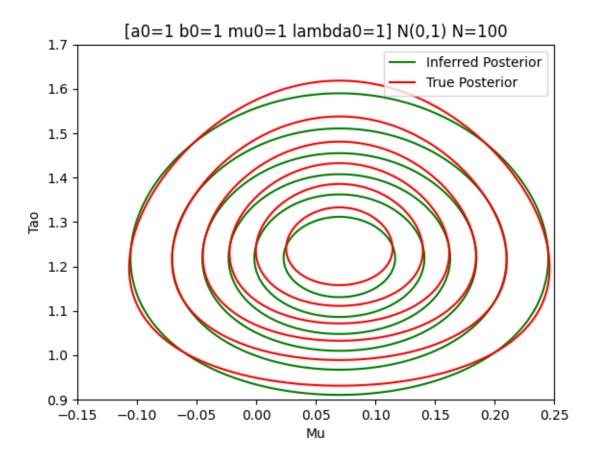


Figure 4: N(0,1) with 100 samples

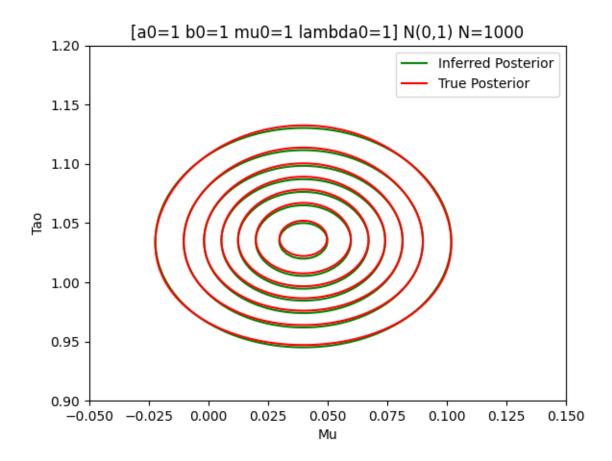


Figure 5: N(0,1) with 1000 samples

2. Effects of model knowledge: In this case we we try to approximate a N(10, 1) distribution and we leave all parameters unchanged like in the previous section. In this section we will see how sometimes even with little data good models can be achieved if we have some knowledge about the model. It can be seen in figure 6 how this initialization of hyperparameters leeds to a good model on  $\mu$  but a very poor one on  $\tau$ .

Now, let say that we learn from some external source that the underlying model has  $\mu = 10$ . Then we will change our initialization of  $\mu_0$  to 10. We can see on figure 7 how this really helped the model on both  $\mu$  and  $\tau$ .

Other parameters like  $\lambda_0$  can be initialized to different values but it seems like for this case is best to keep it unchanged. As we can see in figure 8 the model's  $\tau$  just becomes worse.

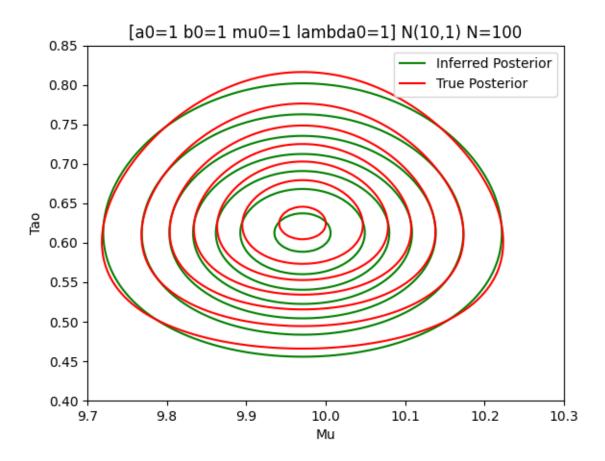


Figure 6: N(10,1) with 100 samples

# [a0=1 b0=1 mu0=10 lambda0=1] N(10,1) N=100 Inferred Posterior 1.6 True Posterior 1.5 1.4 <u>ල</u> 1.3 1.2 1.1 1.0 0.9 <del>+</del> 9.7 9.9 9.8 10.2 10.1 10.0 10.3 Mu

Figure 7: Effect of  $\mu_0$  on N(10,1) with 100 samples

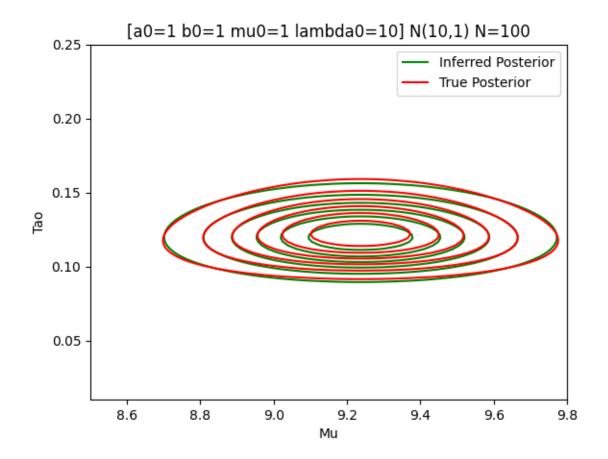


Figure 8: Effect of  $\lambda_0$  on N(10,1) with 100 samples

3. Other hyperparameter effects: In this section we tune  $a_0$  and  $b_0$  and experiment with how their changes affect the distributions N(0,1). In order to do so we fix the data to have a 1000 samples and fix the other hyperparameters to be 0. As we can see in all of the cases (see figures 9, 10 and 11) the inferred posterior fits extremely well the true posterior due to the high number of data points. However, it can be seen in figure 9 how a high value of  $b_0$  leads to an down shifted  $\tau$ , in contrast, in figure 10 we see an up shifted  $\tau$  do to the high value of the hyper parameter  $a_0$ . Finally, in figure 11 we can observe how, interestingly, when setting both  $a_0$  and  $b_0$  to the same value regardless of how high this value is, we obtain a almost perfect model for N(0,1).

# 

Figure 9: Effect of  $b_0$  on N(0,1) with 1000 samples

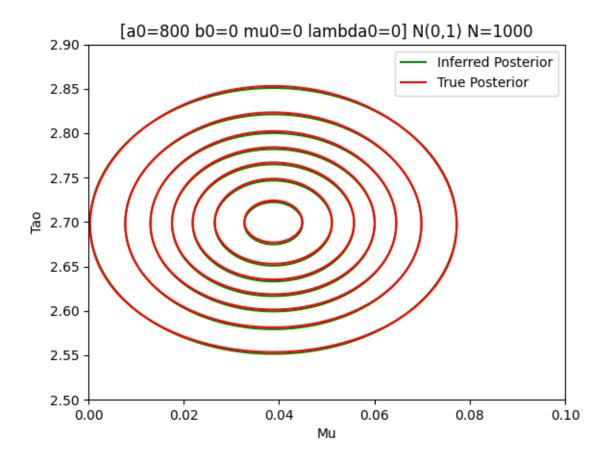


Figure 10: Effect of  $a_0$  on N(0,1) with 1000 samples

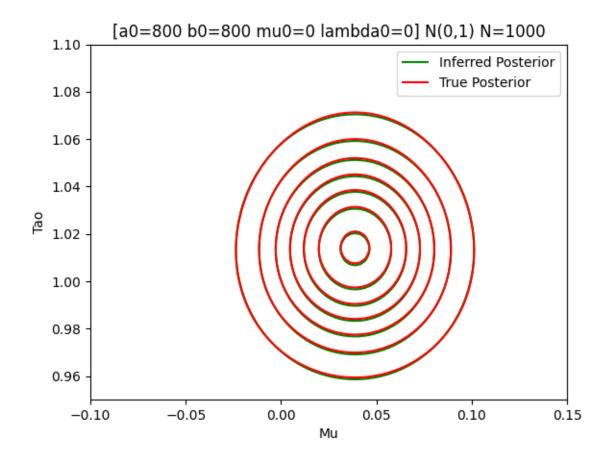
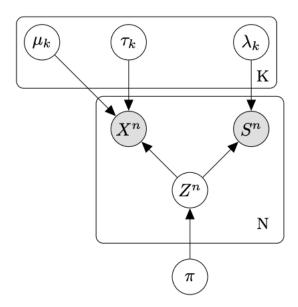


Figure 11: Effect of  $a_0, b_0$  on N(0,1) with 1000 samples

# 2.4 Super Epicentra - Expectation-Maximization

We have seismographic from an area with frequent earthquakes emanating from K super epicentra. Each super epicentra is modeled by a 2-dimensional Gaussian determining the location of an earthquake and a Poisson distribution determining its strength. As shown in Figure 12 the entire model is a mixture of K such components. The variable  $Z^n$  is a class variable that follows a categorical distribution  $\pi$  and determines the super epicentra of the nth observation, i.e., the parameters of the Gaussian distribution that  $X^n$  is sampled from,  $\mu_k = (\mu_{k,1}, \mu_{k,2})$  and  $\tau_k = (\tau_{k,1}, \tau_{k,2})$  where  $\tau_{k,1}$  and  $\tau_{k,2}$  are diagonal elements of the diagonal precision matrix, as well as the intensity of the Poisson distribution that  $S^n$  is sampled from,  $\lambda_k$ .

Figure 12: Mixture of components modeling location and strengths of earthquakes associated with a super-epicentra. In the figure,  $\mu_k = (\mu_{k,1}, \mu_{k,2})$  and  $\tau_k = (\tau_{k,1}, \tau_{k,2})$ 



#### Question 2.4.12

#### Derive an EM algorithm for the model

The objective of EM algorithm is to maximize this likelihood [1]:

$$p(\boldsymbol{X} \mid \boldsymbol{\theta}) = \prod_{\boldsymbol{Z}} p(\boldsymbol{X}, \boldsymbol{Z} \mid \boldsymbol{\theta})$$

where X represents the observed variables  $X^n$  and  $S^n$ .  $X^n$  follows a  $Normal(\mu_k, \tau_k)$  and  $S^n$  follows a  $Poisson(\lambda_k)$ . Z are the unobserved variables  $Z^n$  which follow a  $Categorical(\pi_k)$ .  $\theta$  concerns all parameters  $\pi_k, \mu_k, \tau_k, \lambda_k$  which are what we actually need to find. We will define  $\theta_k = (\mu_k, \tau_k, \lambda_k)$  and  $\theta = (\pi, \theta_1, ..., \theta_k)$ . Since it is more convenient for computations we will use the log-likelihood:

$$\ln(p(X^n, S^n \mid \boldsymbol{\theta})) = \left\{ \sum_{Z} \ln(p(X^n, S^n, Z^n \mid \boldsymbol{\theta})) \right\}$$

From the given graphical model, we can see  $X^n$  and  $S^n$  are conditionally independent given the latent variable  $Z^n$  and hence we can rewrite it as this:

$$P(X^{n}, S^{n}, Z^{n} \mid \theta) = p(Z^{n} \mid \theta) p(X^{n} \mid Z^{n}, \theta) p(S^{n} \mid Z^{n}, \theta)$$

Now, using all the information given, we can rewrite as:

$$p\left(X^{n},S^{n}\right) = \sum_{Z} p\left(Z^{n}\right) p\left(X^{n} \mid Z^{n}\right) p\left(S^{n} \mid Z^{n}\right) = \sum_{k=1}^{K} \pi_{k} Normal\left(\boldsymbol{x}_{n} \mid \boldsymbol{\mu}_{k}, \boldsymbol{\tau}_{k}^{-1}I\right) Poisson\left(S_{n} \mid \lambda_{k}\right)$$

Finally, from Bishop [1], the algorithm we must follow is:

- 1. Initalize  $\pi_k, \mu_k, \tau_k, \lambda_k$
- 2. Compute Expectation [1]:

$$r_{nk} = \frac{\pi_k Normal\left(\boldsymbol{x}_n \mid \boldsymbol{\mu}_k, \boldsymbol{\tau}_k^{-1} I\right) Poisson\left(\lambda_k\right)}{\sum_{k=1}^K \pi_k N\left(\boldsymbol{x}_n \mid \boldsymbol{\mu}_k, \boldsymbol{\tau}_k^{-1} I\right) Po\left(\lambda_k\right)}$$

3. Now, we do the Maximization step in which we recompute the parameters using their distributions:

$$\boldsymbol{\mu}_k^* = \frac{1}{N_k} \sum_{n=1}^N r_{nk} \boldsymbol{x}_n$$

$$\boldsymbol{\tau}_k^* = \frac{1}{N_k} \sum_{n=1}^N r_{nk} \left( \boldsymbol{x}_n - \boldsymbol{\mu}_k^* \right) \left( x_n - \boldsymbol{\mu}_k^* \right)^T$$

$$\boldsymbol{\pi}_k^* = \frac{N_k}{N}$$

$$\lambda_k^* = \frac{1}{N_k} \sum_{n=1}^N r_{nk} s_n$$

where 
$$N_k = \sum_{n=1}^N r_{nk}$$

4. Lastly, we evaluate the log-likelihood with the new parameters (\*). If the new log-likelihood has not changed by more than a user defined threshold, we stop. If it has changed more than the threshold, we go to 2.

#### Question 2.4.13

# Implement your EM algorithm

See code in Appendix 4: Expectation-Maximization Code.

#### Question 2.4.14

Apply it to the data provided, give an account of the success, and provide visualizations for a couple of examples. Repeat it for a few different choices of K.

1. Using 3 components: In this section it is shown how the EM algorithm progresses through its first steps to the final result. It can be seen in 13 how the the clusters are initialized to (0.3640, 6.7395) in the case of the red cluster, (0.7429, 7.4138) for the green and (5.7401, 3.7467) for the blue cluster. This is a very bad model of the data, however, it is just the inizialitation. After one iteration, in figure 14 we can see how the cluster means and rates make much more sense and describe the 3 clear groups in the 2-d data. In the next iteration (see figure 15) the model gets even better and the rates make much more sense. Finally, convergence its achieved in the 9th iteration of figure 16. All in all, the model obtained is very good and would generalize well.

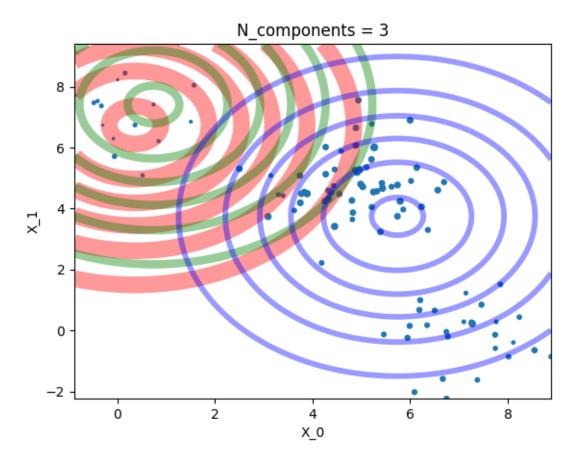


Figure 13: Initialization of EM algorithm

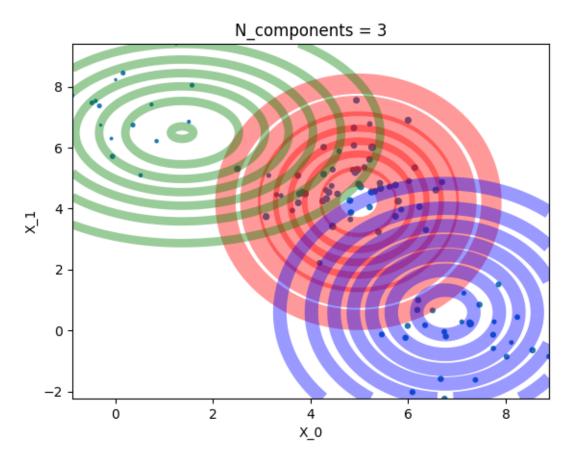


Figure 14: First iteration of EM algorithm

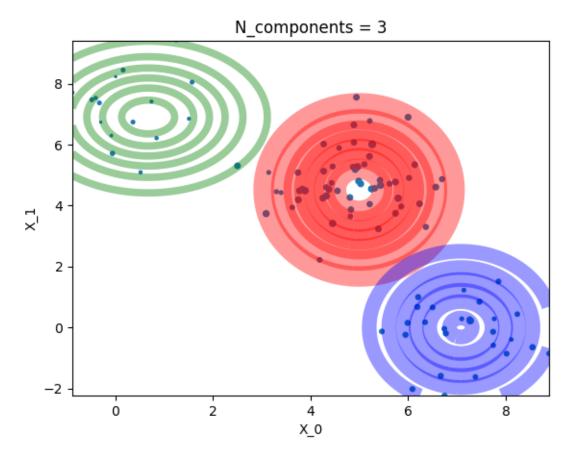


Figure 15: Second iteration of EM algorithm

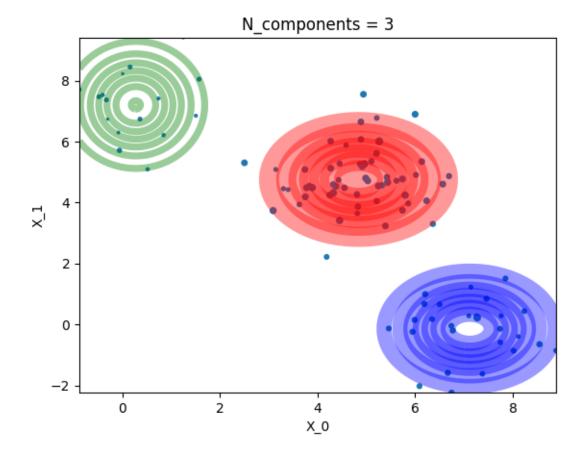


Figure 16: 9th iteration of EM algorithm - Convergence achieved

2. Using < 3 components: In this case we show in figure 17 how a bad election of clusters can lead to bad models. Even though convergence was achieved for a threshold value of 1e-300 the model lacks 1 more cluster to represent the data. This is a clear example of a model which generalizes too much, i.e, a high bias but a very low variance model.

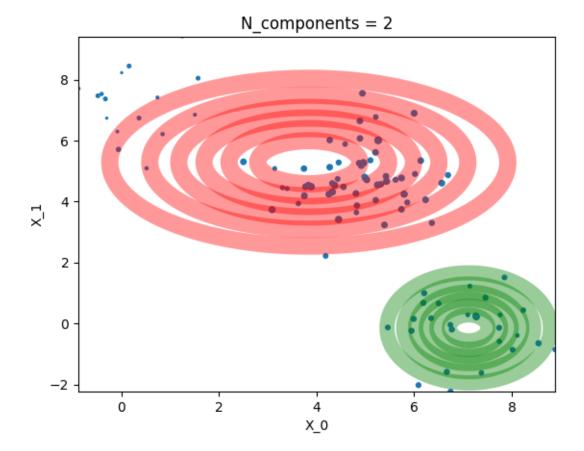


Figure 17: Bad Model - Convergence achieved

3. Using > 3 components: In the case of 18 we show the exact opposite of the previous point. The model overfits the data and tries to create too many clusters which are too specialized. Some of the Poisson rates lead to very complex relationships. This is a clear example of a low bias but high variance model.

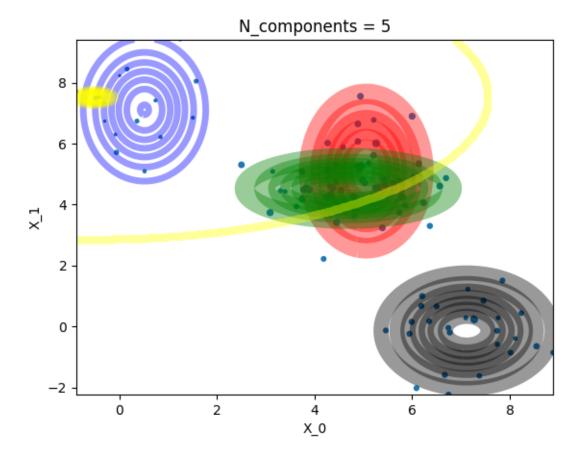


Figure 18: Bad Model - Convergence achieved

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# References

- [1] C. M. Bishop, Pattern recognition and machine learning. Springer, 2016.
- [2] Normal-gamma distribution, May 2021. [Online]. Available: https://en.wikipedia.org/wiki/Normal-gamma\_distribution.

# Appendix 2: Tree Code

""" This file is created as a suggested solution template for question 2.2 in

We encourage you to keep the function templates. However this is not a "must" and you can code however you like. You can write helper functions etc however you want.

If you want, you can use the class structures provided to you (Node and Trifile), and modify them as needed. In addition to the data files given to y test your algorithm with your own simulated data for various cases and and

For those who do not want to use the provided structures, we also saved the format. Let us know if you face any problems.

Also, we are aware that the file names and their extensions are not well-f (i.e example\_tree\_mixture.pkl\_samples.txt). We wanted to keep the template You can change the file names however you want.

For this task, we gave you three different trees ( $q2\_2\_small\_tree$ ,  $q2\_2\_metain Each tree has 5 samples (the inner nodes' values are masked with np.nan). We want you to calculate the likelihoods of each given sample and report is$ 

Note: The alphabet "K" is  $K = \{0, 1, 2, 3, 4\}$ .

Note: A VERY COMMON MISTAKE is to use incorrect order of nodes' values in the table is a list of lists, whose shape is approximately (num\_nodes, For instance, if node "v" has a parent "u", then  $p(v=Zv \mid u=Zu) = v$ 

If you ever doubt your useage of theta, you can double check this  $\sum_{k=1} \hat{k} p(v = k \mid u=Zu) = 1$ 

import numpy as np
from Tree import Tree
from Tree import Node

def calculate\_likelihood(tree\_topology, theta, beta):

This function calculates the likelihood of a sample of leaves.

:param: tree\_topology: A tree topology. Type: numpy array. Dimensions: (nu:param: theta: CPD of the tree. Type: list of numpy arrays. Dimensions (ap:param: beta: A list of node assignments. Type: numpy array. Dimensions: (

Note: Inner nodes are assigned to np.nan. The leaves have value

*" " "* 

```
:return: likelihood: The likelihood of beta. Type: float.
    This is a suggested template. You don't have to use it.
    ,, ,, ,,
    print ("\tCalculating_the_likelihood ...")
    likelihood = 0
   K = len(theta[0])
   num_nodes = tree_topology.size
    s_matrix = np.zeros(shape=(num_nodes, K))
    for node, value in reversed(list(enumerate(beta))):
        if not np. isnan (value): # leaf node
            s_{matrix}[node][int(value)] = 1
        else: # inner node
            children = np.argwhere(tree_topology == node).flatten()
            for k in range(K):
                s_matrix[node][k] = 1
                for child in children:
                    s_{matrix}[node][k] = s_{matrix}[node][k] * 
                        np.dot(s_matrix[child], theta[child][k])
   # End: Example Code Segment
   likelihood = np.dot(theta[0], s_matrix[0])
   return likelihood
def main():
    print("Hello_World!")
    print ("This_file_is_the_solution_template_for_question_2.2.")
   print ("\n1. Load tree data from file and print it \n")
    filenames = ["2_2/data/q2_2.small_tree.pkl"]
                 "2_2/data/q2_2_medium\_tree.pkl", "2_2/data/q2_2_large\_tree.pkl"
    for f in filenames:
        print ('#'*70)
        print ('#'*70)
        t = Tree()
        t.load_tree(f)
       # t. print()
        print("K_of_the_tree:_", t.k, "\talphabet:_", np.arange(t.k))
        print ("\n2._Calculate_likelihood_of_each_FILTERED_sample\n")
       # These filtered samples already available in the tree object.
       \# Alternatively, if you want, you can load them from corresponding tx
        for sample_idx in range(t.num_samples):
            beta = t.filtered_samples[sample_idx]
           \# print("\n\tSample: ", sample\_idx, "\tBeta: ", beta)
```

# Appendix 3: Variational Inference Code

```
import numpy as np
import math
from scipy import stats
import matplotlib.pyplot as plt
import sys
import os
class VI():
    def __init__(self, a0, b0, mu0, lambda0, Etao, threshold):
        self.a0 = a0
        self.b0 = b0
        self.mu0 = mu0
        self.lambda0 = lambda0
        self.Etao = Etao
        self.muN = 0
        self.lambdaN = 0
        self.aN = 0
        self.bN = 0
        self.threshold = threshold
    def fit (self, X):
        print("\tDoing \subset Variational \subseteq Inference \ldots\")
        while True:
             old_Etao = self.Etao
             self.q_mu_update(X)
             self.q_tao_update(X)
             self.Etao = self.aN/self.bN
             if abs(self.Etao - old_Etao) < self.threshold:
                 break
    def q_mu_update(self, X):
        mean, N = np.mean(X), X.shape[0]
        self.muN = ((self.lambda0*self.mu0) + N*mean) / (self.lambda0 + N)
        self.lambdaN = (self.lambda0 + N)*self.Etao
    def q_tao_update(self, X):
        mean, N = np.mean(X), X.shape[0]
        self.aN = self.a0 + N/2
```

```
self.bN = np.dot(X, X) + (N + self.lambda0) * 
            (1/self.lambdaN + math.pow(self.muN, 2))
        self.bN = self.bN - 2*self.muN*(N*mean + self.mu0*self.lambda0)
        self.bN = self.bN + self.lambda0*math.pow(self.mu0, 2)
        self.bN = self.b0 + 0.5*self.bN
    def get_posterior(self, mu_axis, tao_axis):
        mu\_size, tao\_size = len(mu\_axis), len(tao\_axis)
        q = np.zeros(shape=(mu_size, tao_size))
        print('\tCalculating_VI_posterior_approximation...')
        for i in range (mu_size):
            for j in range(tao_size):
                q_tao = stats.gamma.pdf(
                    tao_axis[j], self.aN, loc=0, scale=1/self.bN)
                q_mu = stats.norm.pdf(
                    mu_axis[i], self.muN, np.sqrt(1/self.lambdaN))
                q[j][i] = q_tao*q_mu
        return q
def generate_data(mu, tao, N, mu_axis, tao_axis, lambda0, mu0, a0, b0):
    sigma = np. sqrt (1/tao)
   X = np.random.normal(mu, sigma, N)
    true_posterior = get_true_posterior(
        mu_axis, tao_axis, X, lambda0, mu0, a0, b0)
    return X, true_posterior
def get_true_posterior(mu_axis, tao_axis, X, lambda0, mu0, a0, b0):
    mu_size, tao_size = len(mu_axis), len(tao_axis)
    p = np.zeros(shape=(mu_size, tao_size))
   mean, N = np.mean(X), X.shape[0]
   mu = (N*mean + lambda0*mu0)/(N + lambda0)
    a = a0 + N/2
   b = b0 + 0.5 * (np.dot(X, X) + lambda0*mu0**2 -
                    (N*mean + lambda0*mu0)**2/(N+lambda0))
    print('\tCalculating_true_posterior...')
    for i in range (mu_size):
        for j in range(tao_size):
            tao = (tao_axis[j]*(N+lambda0)) + sys.float_info.epsilon
            sigma = np. sqrt(1/tao)
            p_{tao} = stats.gamma.pdf(tao_axis[j], a, loc=0, scale=1/b)
            p_mu = stats.norm.pdf(mu_axis[i], mu, sigma)
            p[j][i] = p_tao*p_mu
    return p
```

```
def plot_contours (mu_axis, tao_axis, VI_posterior, true_posterior, filename, t
            filename = f'2_3/plots/{filename}'
            plt.figure()
            CS_inferred = plt.contour(mu_axis, tao_axis, VI_posterior, colors='green')
            CS_true = plt.contour(mu_axis, tao_axis, true_posterior, colors='red')
           # Plot density of pdf on the contour line
           \# plt.clabel(CS\_inferred, fmt="%1.2f")
           \# plt.clabel(CS_true, fmt="\%1.2f")
            labels = ["Inferred_Posterior", "True_Posterior"]
            lines = [CS_inferred.collections[0], CS_true.collections[0]]
            plt.legend(lines, labels)
            plt.xlabel("Mu")
            plt.ylabel("Tao")
            plt.title(title)
            plt.savefig(f'{filename}.png')
def main():
           np.random.seed(1)
           # Init parameters
           a0, b0, mu0, lambda0 = 1, 1, 1, 1
           Etao = 1
            threshold = 1e-300
           # Generate data
           mu, tao, N = 0, 1, 1000
           mu_axis = np. linspace(-0.05, 0.15, 100)
            tao_axis = np.linspace(0.9, 1.2, 100)
           X, true_posterior = generate_data(
                       mu, tao, N, mu_axis, tao_axis, lambda0, mu0, a0, b0)
           VI_{model} = VI(a0, b0, mu0, lambda0, Etao, threshold)
            VI_{-model}. fit (X)
            VI_posterior = VI_model.get_posterior(mu_axis, tao_axis)
           \# a0-b0-mu0-lambda0-Etao-thres-mu-tao-N
            filename = f'\{a0\}-\{b0\}-\{mu0\}-\{lambda0\}-\{str(threshold)\}-\{mu\}-\{tao\}-\{N\}'\}
            title = f'[a0=\{a0\}\_b0=\{b0\}\_mu0=\{mu0\}\_lambda0=\{lambda0\}]\_N(\{mu\},\{tao\})\_N=\{N(\{mu\},\{tao\})\_N=\{nu0\}\}\_nu0=\{nu0\}\_nu0=\{nu0\}\_nu0=\{nu0\}\_nu0=\{nu0\}\_nu0=\{nu0\}\_nu0=\{nu0\}\_nu0=\{nu0\}\_nu0=\{nu0\}\_nu0=\{nu0\}\_nu0=\{nu0\}\_nu0=\{nu0\}\_nu0=\{nu0\}\_nu0=\{nu0\}\_nu0=\{nu0\}\_nu0=\{nu0\}\_nu0=\{nu0\}\_nu0=\{nu0\}\_nu0=\{nu0\}\_nu0=\{nu0\}\_nu0=\{nu0\}\_nu0=\{nu0\}\_nu0=\{nu0\}\_nu0=\{nu0\}\_nu0=\{nu0\}\_nu0=\{nu0\}\_nu0=\{nu0\}\_nu0=\{nu0\}\_nu0=\{nu0\}\_nu0=\{nu0\}\_nu0=\{nu0\}\_nu0=\{nu0\}\_nu0=\{nu0\}\_nu0=\{nu0\}\_nu0=\{nu0\}\_nu0=\{nu0\}\_nu0=\{nu0\}\_nu0=\{nu0\}\_nu0=\{nu0\}\_nu0=\{nu0\}\_nu0=\{nu0\}\_nu0=\{nu0\}\_nu0=\{nu0\}\_nu0=\{nu0\}\_nu0=\{nu0\}\_nu0=\{nu0\}\_nu0=\{nu0\}\_nu0=\{nu0\}\_nu0=\{nu0\}\_nu0=\{nu0\}\_nu0=\{nu0\}\_nu0=\{nu0\}\_nu0=\{nu0\}\_nu0=\{nu0\}\_nu0=\{nu0\}\_nu0=\{nu0\}\_nu0=\{nu0\}\_nu0=\{nu0\}\_nu0=\{nu0\}\_nu0=\{nu0\}\_nu0=\{nu0\}\_nu0=\{nu0\}\_nu0=\{nu0\}\_nu0=\{nu0\}\_nu0=\{nu0\}\_nu0=\{nu0\}\_nu0=\{nu0\}\_nu0=\{nu0\}\_nu0=\{nu0\}\_nu0=\{nu0\}\_nu0=\{nu0\}\_nu0=\{nu0\}\_nu0=\{nu0\}\_nu0=\{nu0\}\_nu0=\{nu0\}\_nu0=\{nu0\}\_nu0=\{nu0\}\_nu0=\{nu0\}\_nu0=\{nu0\}\_nu0=\{nu0\}\_nu0=\{nu0\}\_nu0=\{nu0\}\_nu0=\{nu0\}\_nu0=\{nu0\}\_nu0=\{nu0\}\_nu0=\{nu0\}\_nu0=\{nu0\}\_nu0=\{nu0\}\_nu0=\{nu0\}\_nu0=\{nu0\}\_nu0=\{nu0\}\_nu0=\{nu0\}\_nu0=\{nu0\}\_nu0=\{nu0\}\_nu0=\{nu0\}\_nu0=\{nu0\}\_nu0=\{nu0\}\_nu0=\{nu0\}\_nu0=\{nu0\}\_nu0=\{nu0\}\_nu0=\{nu0\}\_nu0=\{nu0\}\_nu0=\{nu0\}\_nu0=\{nu0\}\_nu0=\{nu0\}\_nu0=\{nu0\}\_nu0=\{nu0\}\_nu0=\{nu0\}\_nu0=\{nu0\}\_nu0=\{nu0\}\_nu0=\{nu0\}\_nu0=\{nu0\}\_nu0=\{nu0\}\_nu0=\{nu0\}\_nu0=\{nu0\}\_nu0=\{nu0\}\_nu0=\{nu0\}\_nu0=\{nu0\}\_nu0=\{nu0\}\_nu0=\{nu0\}\_nu0=\{nu0\}\_nu0=\{nu0\}\_nu0=\{nu0\}\_nu0=\{nu0\}\_nu0=\{nu0\}\_nu0=\{nu0\}\_nu0=\{nu0\}\_nu0=\{nu0\}\_nu0=\{nu0\}\_nu0=\{nu0\}\_nu0=\{nu0\}\_nu0=\{nu0\}\_nu0=\{nu0\}\_nu0=\{nu0\}\_nu0=\{nu0\}\_nu0=\{nu0\}\_nu0=\{nu0\}\_nu0=\{nu0\}\_nu0=\{nu0\}\_nu0=\{nu0\}\_nu0=\{nu0\}\_nu0=\{nu0\}\_nu0=\{nu0\}\_nu0=\{nu0\}\_nu0=\{nu0\}\_nu0=\{nu0\}\_nu0=\{nu0\}\_nu0=\{nu0\}\_nu0=\{nu0\}\_nu0=\{nu0\}\_nu0=\{nu0\}\_nu0=\{nu0\}\_nu0=\{nu0\}\_nu0=\{nu0\}\_nu0=\{nu0\}\_nu0=\{nu0\}\_nu0=\{nu0\}\_nu0=\{nu0\}\_nu0=\{nu0\}\_nu0=\{nu0\}\_nu0=\{nu0\}\_nu0=\{nu0\}\_nu0=\{nu0\}\_nu0=\{nu0\}\_nu0=\{nu0\}\_nu0=\{nu0\}\_nu0=\{nu0\}\_nu0=\{nu0\}\_nu0=\{nu0\}\_nu0=\{nu0\}\_nu0=\{nu0\}\_nu0=\{nu0\}\_nu0=\{nu0\}\_nu0=\{nu0\}\_nu0=\{nu0\}\_nu0=\{nu0\}\_nu0=\{nu0\}\_nu0=\{nu0\}\_nu0=\{nu0\}\_nu0=\{nu0\}\_nu0=\{nu0\}\_nu0=\{nu0\}\_nu0=\{nu0\}\_nu0=\{nu0\}\_nu0=\{nu0\}\_nu0=\{nu0\}\_nu0=\{nu0\}\_nu0=\{nu0\}\_nu0=\{nu0\}\_nu0=\{nu0\}\_nu0=\{nu0\}\_nu0=\{nu0\}\_nu0=\{nu0\}\_nu0=\{nu0\}\_nu0=\{nu0\}\_nu0=\{nu0
            plot_contours (mu_axis, tao_axis, VI_posterior,
                                                      true_posterior, filename, title)
if _-name_- = "_-main_-":
           main()
```

# Appendix 4: Expectation-Maximization Code

```
from scipy.stats import multivariate_normal, poisson
def load_data(X_file, S_file):
    X, S = [], []
    with open(f"2_4/data/{X_file}", 'r') as f:
         for line in f.readlines():
             X. append (line.split (''_'))
         X = np. array(X). astype(float)
    with open(f"2_4/data/\{S_file\}", 'r') as f:
         for line in f.readlines():
             S.append(line.split()[0])
         S = np. array(S). astype(float)
    return X, S
def plot_contours(X, S, mu_k, covar_k, lambda_k):
    N_{\text{points}} = 300
    N_{components} = mu_k.shape[0]
    X0_{\text{-min}}, X0_{\text{-max}} = \text{np.min}(X[:, 0]), \text{np.max}(X[:, 0])
    X1_min, X1_max = np.min(X[:, 1]), np.max(X[:, 1])
    X0_{\text{-axis}} = \text{np.linspace}(X0_{\text{-min}}, X0_{\text{-max}}, N_{\text{-points}})
    X1_axis = np.linspace(X1_min, X1_max, N_points)
    X0, X1 = np. meshgrid (X0_axis, X1_axis)
    plt.figure()
    # plot X points
    plt.scatter(X[:, 0], X[:, 1], s=S)
    # Draw Mixture of Gaussians
    colors = ['red', 'green', 'blue', 'yellow', 'black']
    for k in range (N_components):
         mu = mu_k[k]
         covar = covar_k[k]
         rv = multivariate_normal(mu, covar)
         Z = rv.pdf(np.dstack((X0, X1)))
         plt.contour(X0, X1, Z, colors=colors[k],
                      linewidths=lambda_k[k], alpha=0.4)
    plt.\,xlabel\,("\,X_-0"\,)
    plt.ylabel("X<sub>-</sub>1")
    plt.title(f"N_components==_{N_components}")
    plt.savefig(f"2_4/plots/{N_components}.png")
class GaussianPoissonEM:
    def __init__ (self , N_components , threshold ):
```

import matplotlib.pyplot as plt

```
self.N_components = N_components
    self.threshold = threshold
def fit (self, X, S):
    self.init_params(X, S)
    old_log_likelihood = 0
    iter = 0
    print('\tFitting_Expectation_Maximization...')
    while True:
        self.E_step(X, S)
        self.M_step(X, S)
        new_log_likelihood = self.log_likelihood(X, S)
        if abs(old_log_likelihood - new_log_likelihood) < self.threshold:
            break
        old_log_likelihood = new_log_likelihood
        iter = iter + 1
    self.log_likelihood = new_log_likelihood
    print(f'\tIterations=_{{}}{iter}')
def init_params(self, X, S):
    N_{\text{points}}, N_{\text{dim}} = X_{\text{shape}}
    self.pi_k = np.full(self.N_components, 1/self.N_components)
    self.mu_k = X[np.random.choice(
        N_{points}, self.N_{components}, replace=False)
    self.covar_k = np.full(
        (self.N_components, N_dim, N_dim), np.cov(X, rowvar=False))
    self.lambda_k = np.full(self.N_components, np.mean(S))
    self.lambda_k = self.lambda_k / \setminus
        np.array([i for i in range(1, self.N_components+1)])
    # Exercise assumes covariances diagonal so...
    covar_k = []
    for c in self.covar_k:
        covar_k = np.append(covar_k, np.diag(np.diag(c)))
    self.covar_k = np.array(covar_k).reshape(self.N_components, 2, 2)
def get_params(self):
    return self.pi_k, self.mu_k, self.covar_k, self.lambda_k
def E_step(self, X, S):
    N_{points} = X. shape [0]
    r_nk = np.zeros((N_points, self.N_components))
    for n in range (N_points):
        for k in range (self. N_components):
            r_nk[n][k] = self.pi_k[k] *
                 multivariate\_normal(self.mu_k[k], self.covar_k[k]).pdf(X[n])
                 poisson(self.lambda_k[k]).pmf(S[n])
        r_n k [n] = r_n k [n] / r_n k [n] . sum()
```

```
\# Set responsibility, i.e, E[I(Z_n=class_k)]
          self.r_nk = r_nk
     def M_step(self , X, S):
          N_k = self.r_nk.sum(axis=0)
          N_{points}, N_{dim} = X_{shape}
          for k in range (self. N_components):
               self.pi_k[k] = N_k[k]/N_points
               self.lambda_k[k] = np.sum(self.r_nk[:, k] * S[:]) / N_k[k]
               for d in range (N_dim):
                    self.mu_k[k][d] = np.sum(self.r_nk[:, k] * X[:, d])/N_k[k]
                    self.covar_k[k][d][d] = np.sum(self.r_nk[:, k] *
                                                           (X[:, d] - self.mu_k[k][d]) *
                                                           \operatorname{np.transpose}(X[:, d] - \operatorname{self.mu})
     def log_likelihood(self, X, S):
          log_likelihood = np.zeros(self.N_components)
          for k in range (self. N_components):
               \log_{-1} \operatorname{likelihood}[k] = \operatorname{sum}(\operatorname{self.r_nk}[:, k] * (\operatorname{self.pi_k}[k] * \operatorname{multivar})
                    self.mu_k[k], self.covar_k[k]).pdf(X[::]) * poisson(self.lambda)
          \log_{-1} \text{likelihood} = \text{np.sum}(\text{np.log}(\log_{-1} \text{likelihood}))
          return log_likelihood
     def print_params (self):
          for k in range (self. N_components):
               print(f'\tComponent_{k}:')
               pi = self.pi_k[k]
               mu_0, mu_1 = self.mu_k[k][0], self.mu_k[k][1]
               c_{-0}, c_{-1} = self.covar_k[k][0][0], self.covar_k[k][1][1]
               rate = self.lambda_k[k]
               print (
                    f' \setminus t \setminus tpi = [\{pi : .4 f\}] \setminus n \setminus t \setminus tNormal([\{mu_0 : .4 f\}, ..\{mu_1 : .4 f\}], [\{c_0 \}] \cap t \setminus tNormal([\{mu_0 : .4 f\}, ...\{mu_1 : .4 f\}])]
def main():
     np.random.seed(1)
     X_{file}, S_{file} = "X.txt", "S.txt"
    X, S = load_data(X_file, S_file)
     N_{\text{-}}components = [2, 3, 5]
     threshold = 1e-10
     for k in N_components:
          print ('#'*10, f'\t{k}_Components\t', '#'*10)
          EM_model = GaussianPoissonEM(k, threshold)
          EM_model.fit(X, S)
          EM_model.print_params()
          pi_k, mu_k, covar_k, lambda_k = EM_model.get_params()
          plot_contours(X, S, mu_k, covar_k, lambda_k)
```