DD2434 Machine Learning, Advanced Course

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December 30, 2019

Contents

1 Knowing the rules

Question 2.1.1: *It is mandatory to read the above text. Have you read it?*

Yes, I have read it.

Question 2.1.2: *List all your collaborations concerning the problem formulations in this assignment.*

1. Adrian Campoy
2. Doumitru Nimara
3. Gustavo Teodoro Beck
4. Lucas Gongora
5. Flavia García

Question 2.1.3: *Have you discussed solutions with anybody?*

No, I have not discussed my solutions.

2 Dependencies in a Directed Graphical Model

Question 2.2.4: *In the graphical model of Figure 1, is $\mu_k \perp \tau_k$ (not conditioned by anything)?*

Yes.

Question 2.2.5: *In the graphical model of Figure 1, is $\mu_k \perp \tau_k | X, ..., X^N$?*

No.

Question 2.2.6: *In the graphical model of Figure 2, is $\mu \perp \beta'$ (not conditioned by anything)?*

Yes.

Question 2.2.7 *In the graphical model of Figure 2, is $\mu \perp \beta' | X, ..., X^N$?*

No.

Question 2.2.8 *In the graphical model of Figure 2, is $X^n \perp S^n$ (not conditioned by anything)?*

No.

Question 2.2.9 *In the graphical model of Figure 2, is* $X^n \perp S^n | \mu_k, \tau_k$

No.

3 Likelihood of a tree GM

Question 2.3.10

Question 2.3.11

4 Simple VI

Question 2.4.12

The code can be found in appendix A.

Question 2.4.13

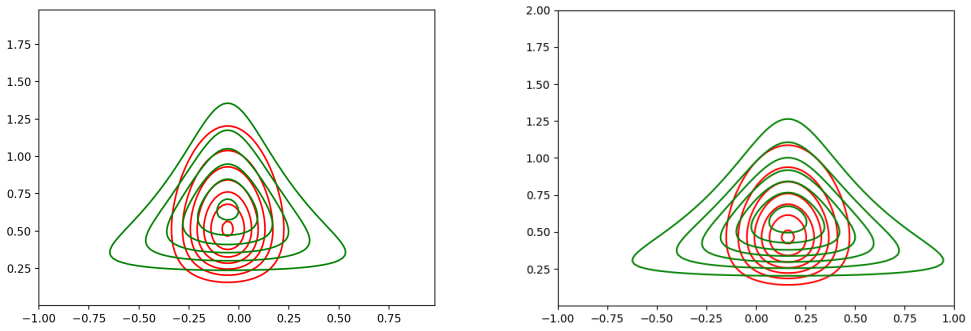
The exact posterior is defined by:

$$p(\mu|\tau) = \mathcal{N}(\mu|\mu_0, (\lambda_0\tau)^{-1})$$
$$p(\tau) = Gam(\tau|a_0, b_0)$$

The joint of these distributions provides the exact posterior.

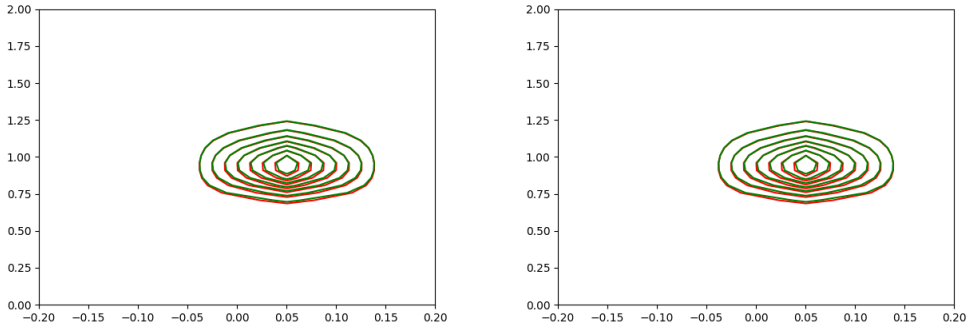
Question 2.4.14

Once the code has been implemented, several tests have been performed, observing the following results:



(a) Estimation 10 samples - 10 iterations (b) Estimation 10 samples - 100 iterations

Figure 1: Approximations with 10 samples



(a) Estimation 100 samples - 10 iterations (b) Estimation 100 samples - 100 iterations

Figure 2: Approximations with 100 samples

The figures above express the different approximations performed by means of the *variational inference* algorithm for different combinations of the number of used samples and the number of iterations of the algorithm. The green shape is the original one and the red one is the one obtained from the approximation, and the horizontal axis represents the values of μ, while the vertical one represents the values of τ.

As it can be seen, in the first two plots the forms obtained are quite similar, even though the number of iterations is 10 times higher in the second one. In the last two, it has been necessary to enlarge the part of the image in which the shapes are drawn. These two show a much smaller area, providing a greater specification of the possible values μ and τ can take.

As a conclusion, it can be said that the number of used samples has a much greater relevance in the procedure, and that the algorithm converges really fast, since the results obtained when only varying the number of iterations are extremely similar.

5 Mixture of trees with observable variables

Question 2.5.15

See appendix B.

Question 2.5.16

Applying the EM algorithm to the provided data, the following results have been obtained:

- The obtained trees for a configuration with 10 nodes, 20 observations and 4 clusters have been the followings:

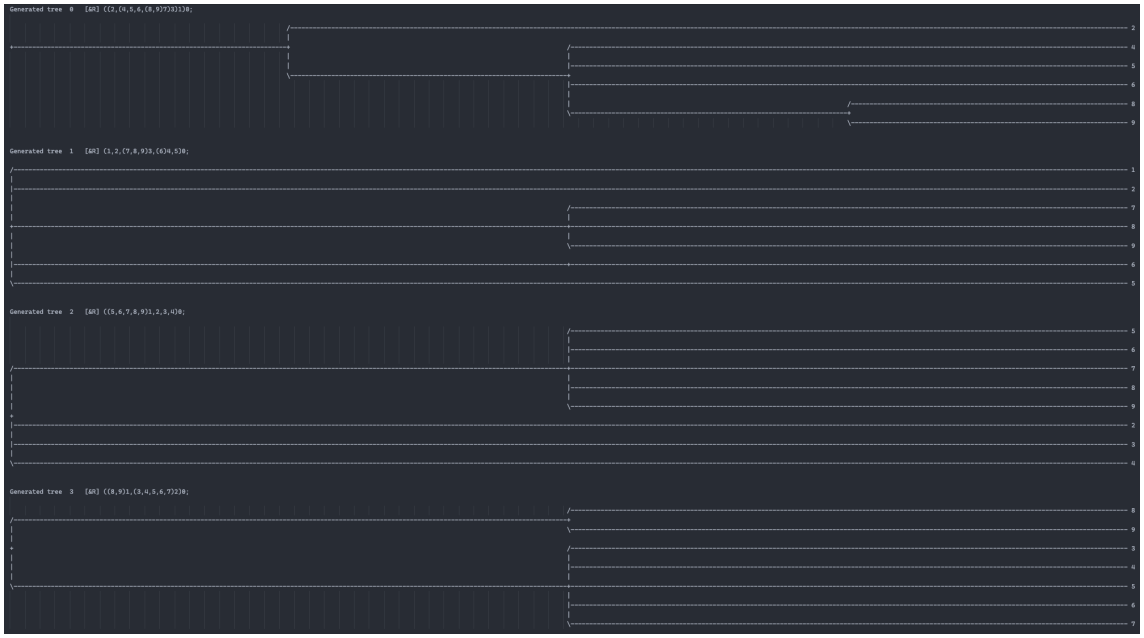


Figure 3: Inferred trees 10 - 20 - 4

- Applying Robinson-Foulds metric, it has been possible to compare the generated trees to the original ones, obtaining the following result:

```
Distances of trees:

Original tree 0 compared to generated tree 0
        Robinson-Foulds distance: 8
Original tree 0 compared to generated tree 1
        Robinson-Foulds distance: 6
Original tree 0 compared to generated tree 2
        Robinson-Foulds distance: 5
Original tree 0 compared to generated tree 3
        Robinson-Foulds distance: 7
Original tree 1 compared to generated tree 0
        Robinson-Foulds distance: 9
Original tree 1 compared to generated tree 1
        Robinson-Foulds distance: 7
Original tree 1 compared to generated tree 2
        Robinson-Foulds distance: 6
Original tree 1 compared to generated tree 3
        Robinson-Foulds distance: 6
Original tree 2 compared to generated tree 0
        Robinson-Foulds distance: 9
Original tree 2 compared to generated tree 1
        Robinson-Foulds distance: 7
Original tree 2 compared to generated tree 2
        Robinson-Foulds distance: 8
Original tree 2 compared to generated tree 3
        Robinson-Foulds distance: 8
Original tree 3 compared to generated tree 0
        Robinson-Foulds distance: 7
Original tree 3 compared to generated tree 1
        Robinson-Foulds distance: 7
Original tree 3 compared to generated tree 2
        Robinson-Foulds distance: 2
Original tree 3 compared to generated tree 3
        Robinson-Foulds distance: 6
```

Figure 4: Distances 10 - 20 - 4

- Finally, the last step taken was comparing likelihood and log-likelihood of the original mixture and the generated one:

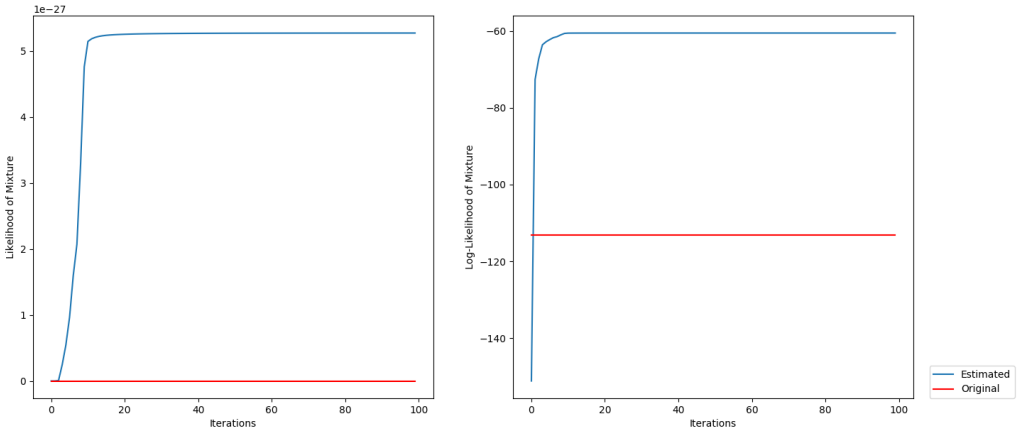


Figure 5: Likelihood and log-likelihood 10 - 20 - 4

Question 2.5.17

The same procedure used in the previous question have been employed with different configurations, obtaining the following results:

- For the case of 20 nodes, 20 observations and 4 clusters:
  - Robinson-Foulds metric:

```
Distances of trees:

Original tree 0 compared to generated tree 0
        Robinson-Foulds distance: 15
Original tree 0 compared to generated tree 1
        Robinson-Foulds distance: 14
Original tree 0 compared to generated tree 2
        Robinson-Foulds distance: 12
Original tree 0 compared to generated tree 3
        Robinson-Foulds distance: 13
Original tree 1 compared to generated tree 0
        Robinson-Foulds distance: 13
Original tree 1 compared to generated tree 1
        Robinson-Foulds distance: 16
Original tree 1 compared to generated tree 2
        Robinson-Foulds distance: 14
Original tree 1 compared to generated tree 3
        Robinson-Foulds distance: 15
Original tree 2 compared to generated tree 0
        Robinson-Foulds distance: 17
Original tree 2 compared to generated tree 1
        Robinson-Foulds distance: 16
Original tree 2 compared to generated tree 2
        Robinson-Foulds distance: 16
Original tree 2 compared to generated tree 3
        Robinson-Foulds distance: 19
Original tree 3 compared to generated tree 0
        Robinson-Foulds distance: 18
Original tree 3 compared to generated tree 1
        Robinson-Foulds distance: 13
Original tree 3 compared to generated tree 2
        Robinson-Foulds distance: 13
Original tree 3 compared to generated tree 3
        Robinson-Foulds distance: 16
```

Figure 6: Distances 20 - 20 - 4

  - Likelihood and log-likelihood comparison:

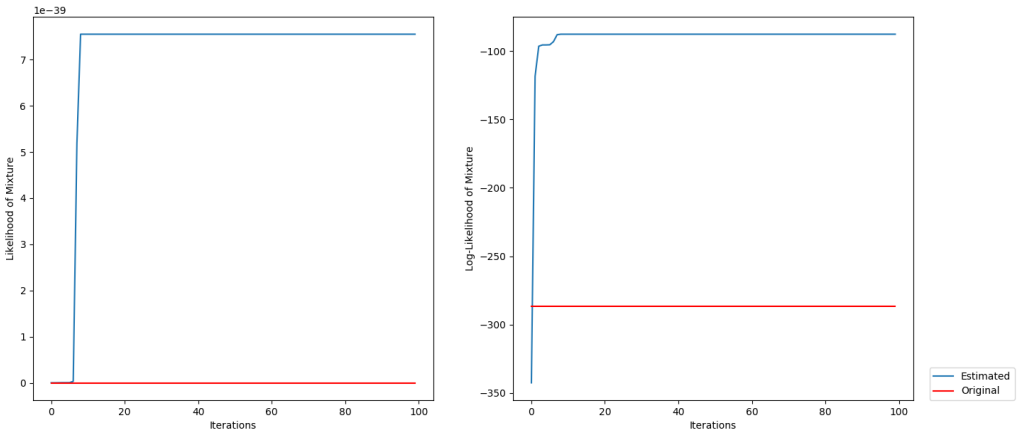


Figure 7: Likelihood and log-likelihood 20 - 20 - 4

- For the case of 10 nodes, 50 observations and 4 clusters:
  - Robinson-Foulds metric:

```
Distances of trees:

Original tree 0 compared to generated tree 0
        Robinson-Foulds distance: 5
Original tree 0 compared to generated tree 1
        Robinson-Foulds distance: 6
Original tree 0 compared to generated tree 2
        Robinson-Foulds distance: 6
Original tree 0 compared to generated tree 3
        Robinson-Foulds distance: 5
Original tree 1 compared to generated tree 0
        Robinson-Foulds distance: 6
Original tree 1 compared to generated tree 1
        Robinson-Foulds distance: 9
Original tree 1 compared to generated tree 2
        Robinson-Foulds distance: 5
Original tree 1 compared to generated tree 3
        Robinson-Foulds distance: 6
Original tree 2 compared to generated tree 0
        Robinson-Foulds distance: 10
Original tree 2 compared to generated tree 1
        Robinson-Foulds distance: 9
Original tree 2 compared to generated tree 2
        Robinson-Foulds distance: 7
Original tree 2 compared to generated tree 3
        Robinson-Foulds distance: 8
Original tree 3 compared to generated tree 0
        Robinson-Foulds distance: 6
Original tree 3 compared to generated tree 1
        Robinson-Foulds distance: 7
Original tree 3 compared to generated tree 2
        Robinson-Foulds distance: 7
Original tree 3 compared to generated tree 3
        Robinson-Foulds distance: 6
```

Figure 8: Distances 10 - 50 - 4

  - Likelihood and log-likelihood comparison:

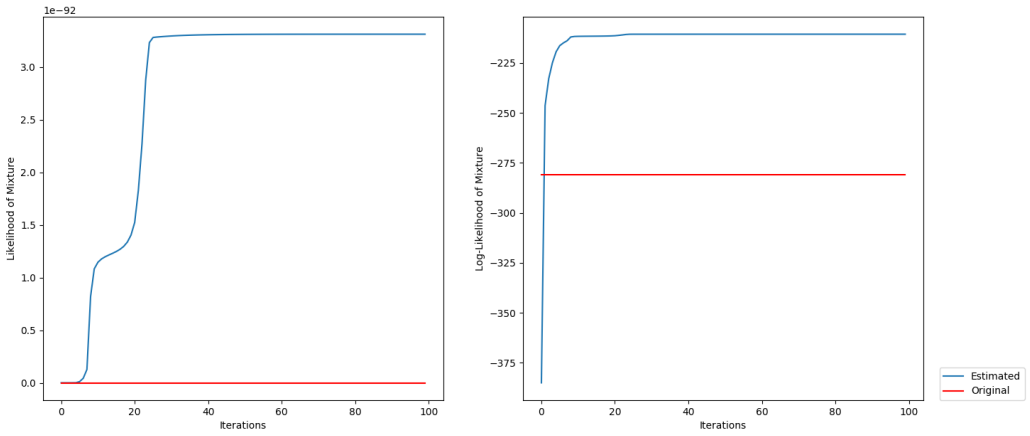


Figure 9: Likelihood and log-likelihood 10 - 50 - 4

- For the case of 10 nodes, 20 observations and 4 clusters, applying mixtures of 3 trees:
  - Robinson-Foulds metric:

```
Distances of trees:

Original tree 0 compared to generated tree 0
        Robinson-Foulds distance: 5
Original tree 0 compared to generated tree 1
        Robinson-Foulds distance: 8
Original tree 0 compared to generated tree 2
        Robinson-Foulds distance: 9
Original tree 1 compared to generated tree 0
        Robinson-Foulds distance: 6
Original tree 1 compared to generated tree 1
        Robinson-Foulds distance: 5
Original tree 1 compared to generated tree 2
        Robinson-Foulds distance: 6
Original tree 2 compared to generated tree 0
        Robinson-Foulds distance: 8
Original tree 2 compared to generated tree 1
        Robinson-Foulds distance: 9
Original tree 2 compared to generated tree 2
        Robinson-Foulds distance: 8
```

Figure 10: Distances 10 - 20 - 4 - mixtures of 3 trees

  - Likelihood and log-likelihood comparison:

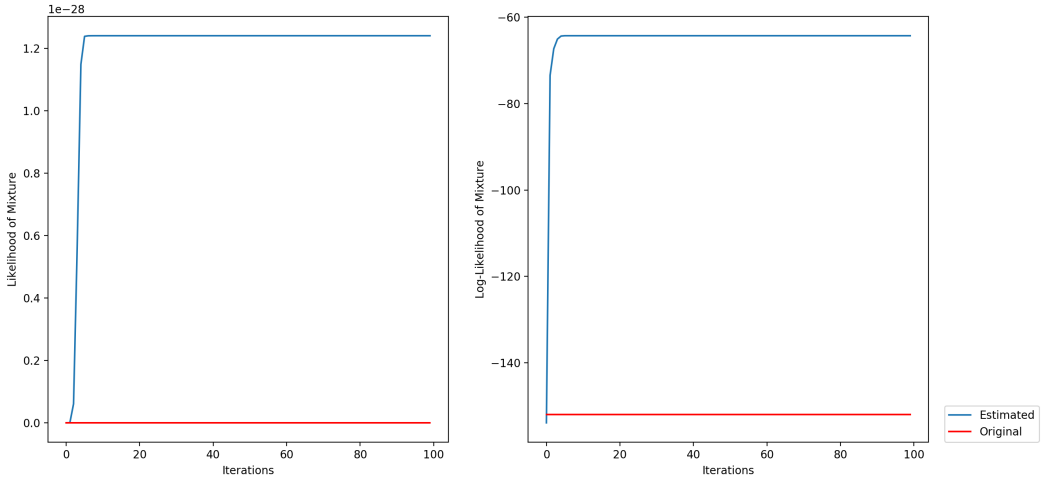


Figure 11: Likelihood and log-likelihood 10 - 20 - 4 - mixtures of 3 trees

As can be seen, the modification of the configuration produces quite different results. When the number of nodes was increased from 10 to 20, the distances between generated trees and the original ones practically doubled those of the previous case. A similar case happens with likelihood and log-likelihood after a proper number of iterations. Given that the number of nodes is much bigger, mixtures are less probable.

The case of increasing the number of observations from 20 to 50 has also affected the final result. Distances between trees do not vary that much; nonetheless, likelihood and log-likelihood are even smaller than in the previous case. Since the sequence of observations is much bigger, it is less probable.

Finally, the configuration was modified by changing the number of trees which compose the mixture from 4 to 3. This has triggered almost no changes in the probabilities shown by the generated trees unlike in the original ones. As the configuration was made for 4 clusters, applying mixtures of 3 has worsened the likelihood of the original trees, being even lower than the one sampled from the original mixture when 4 clusters were used.

6 Super epicentra – EM

Question 2.6.18

The following graphical model and data are given:

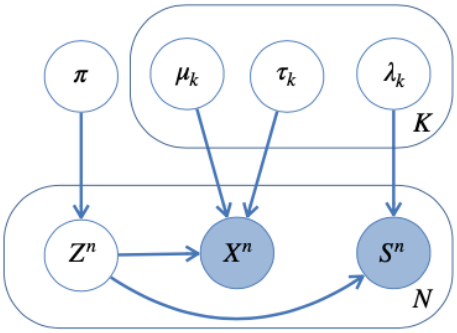


Figure 12: The K super epicentra model with priors

- Each super epicentra is modeled by a 2-dimensional Gaussian determining the location and a Poisson determining the strength.
- The entire model is a mixture of K components.
- The variable Z^n is a class variable that follows a categorical distribution π.
- X^n is modeled by a Gaussian distribution sampled from $\mu_k = (\mu_{k,1}, \mu_{k,2})$ and $\tau_k = (\tau_{k,1}, \tau_{k,2})$.
- S^n is modeled by a Poisson distribution sampled from λ_k.

As Z^n is not observed, the EM algorithm can be applied to find the maximum likelihood solution for the model. To do so, the following expression can be applied:

$$\log(p(X, S|\theta)) = \log\left\{\sum_Z p(X, S, Z|\theta)\right\}$$

Summing over all values of Z, it is possible to get the probability of X and S happening. Nevertheless, Z is not an observed variable, so it is necessary to employ the expected value $\mathbb{E}_Z[\log(p(X, S, Z|\theta))]$ to perform this calculation. Employing the initial equation, the following is obtained:

$$\begin{aligned} p(X, S, Z|\theta) &= p(X|S, Z, \theta)\, p(S|Z, \theta)\, p(Z|\theta) = \\ &= p(X|S, Z, M, T)\, p(S|Z, \Lambda)\, p(Z|\Pi) \end{aligned}$$

According to the provided data, this expression can be rewritten using $p(Z = 1|\Pi)$, since Z

follows a categorical distribution, and when $Z = 0$, all multiplied by it will be equal to 0.

$$Z \sim Cat(\pi_k) = \prod_{n=1}^{N}\prod_{k=1}^{K} \pi_k^{Z_{n,k}}$$
$$p(S|Z=1,\Lambda) = \prod_{n=1}^{N}\prod_{k=1}^{K} Poisson(S_n|\lambda_k)^{Z_{n,k}}$$
$$p(X|Z=1,M,T) = \prod_{n=1}^{N}\prod_{k=1}^{K} \mathcal{N}(X_n|\boldsymbol{\mu}_k,(\boldsymbol{\tau}_k)^{-1}I)^{Z_{n,k}}$$

Using the obtained results, it is possible to get the following:

$$\begin{aligned}\log(p(X,S,Z|\theta)) &= \log(p(X|S,Z,M,T)\,p(S|Z,\Lambda)\,p(Z|\Pi)) \\ &= \log\left(\prod_{n=1}^{N}\prod_{k=1}^{K}(\mathcal{N}(X_n|\boldsymbol{\mu}_k,(\boldsymbol{\tau}_k)^{-1}I)\;Poisson(S_n|\lambda_k)\;\pi_k)^{Z_{n,k}}\right) = \\ &= \sum_{n=1}^{N}\sum_{k=1}^{K} Z_{n,k}\left(\log(\mathcal{N}(X_n|\boldsymbol{\mu}_k,(\boldsymbol{\tau}_k)^{-1}I)) + \log(Poisson(S_n|\lambda_k)) + \log(\pi_k)\right)\end{aligned}$$

Applying this to the expected value, the following is gotten:

$$\begin{aligned}\mathbb{E}_Z[\log(p(X,S,Z|\theta))] &= \mathbb{E}_Z\left[\sum_{n=1}^{N}\sum_{k=1}^{K} Z_{n,k}\left(\log(\mathcal{N}(X_n|\boldsymbol{\mu}_k,(\boldsymbol{\tau}_k)^{-1}I)) + \log(Poisson(S_n|\lambda_k)) + \log(\pi_k)\right)\right] = \\ &= \sum_{n=1}^{N}\sum_{k=1}^{K} \mathbb{E}_Z[Z_{n,k}]\left(\log(\mathcal{N}(X_n|\boldsymbol{\mu}_k,(\boldsymbol{\tau}_k)^{-1}I)) + \log(Poisson(S_n|\lambda_k)) + \log(\pi_k)\right)\end{aligned}$$

Keeping expanding each term, they can be transformed into:

$$\begin{aligned}\log(\mathcal{N}(X_n|\boldsymbol{\mu}_k,(\boldsymbol{\tau}_k)^{-1}I)) &= \log\left(\frac{1}{\sqrt{(2\pi)^K|\boldsymbol{\tau}_k^{-1}|}}\exp\left[\frac{1}{2}(X_n-\boldsymbol{\mu}_k)^T(\boldsymbol{\tau}_k^{-1}I)^{-1}(X_n-\boldsymbol{\mu}_k)\right]\right) = \\ &= -\frac{1}{2}(K(\log(2\pi)) + \log(|\boldsymbol{\tau}_k^{-1}|)) + \left[\frac{1}{2}(X_n-\boldsymbol{\mu}_k)^T(\boldsymbol{\tau}_k^{-1}I)^{-1}(X_n-\boldsymbol{\mu}_k)\right] \\ \log(Poisson(S_n|\lambda_k)) &= \log\left(\frac{\lambda_k^{S_n}e^{-\lambda_k}}{S_n!}\right) = S_n\log(\lambda_k) - \lambda_k - \log(S_n!)\end{aligned}$$

From here, it is possible to obtain (Expectation step):

$$\gamma(Z_{n,k}) = \frac{\mathcal{N}(X_n|\boldsymbol{\mu}_k,(\boldsymbol{\tau}_k)^{-1}I)\;Poisson(S_n|\lambda_k)\;\pi_k}{\sum_{k=1}^{K}\mathcal{N}(X_n|\boldsymbol{\mu}_k,(\boldsymbol{\tau}_k)^{-1}I)\;Poisson(S_n|\lambda_k)\pi_k}$$

And applying this function $\gamma(Z_{n,k})$, the new parameters can be estimated (Maximization step):

$$\boldsymbol{\mu}_k^{new} = \frac{1}{N_k} \sum_{n=1}^{N} \gamma(Z_{n,k}) X_n$$

$$\boldsymbol{\tau}_k^{new} = \frac{1}{N_k} \sum_{n=1}^{N} \gamma(Z_{n,k})(X_n - \boldsymbol{\mu}_k)^T (X_n - \boldsymbol{\mu}_k)$$

$$\pi_k^{new} = \frac{N_k}{N}$$

$$\lambda_k^{new} = \frac{1}{N_k} \sum_{n=1}^{N} \gamma(Z_{n,k}) S_n$$

Knowing that:

$$N_k = \sum_{n=1}^{N} \gamma(Z_{n,k})$$

This procedure is repeated iteratively until either the estimated parameters or the log-likelihood converges.

Question 2.6.19

See appendix C.

Question 2.6.20

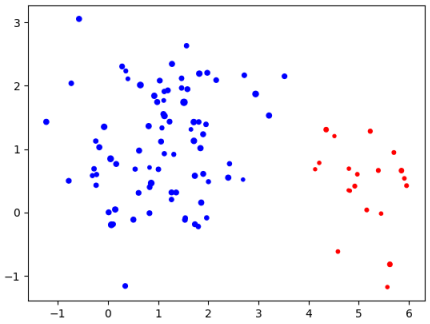
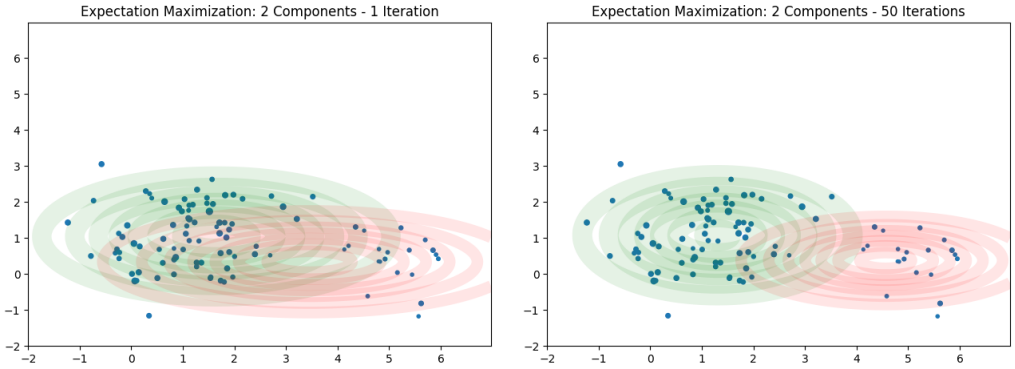


Figure 13: Provided data with 2 components



(a) EM for 2 components with 1 iteration (b) EM for 2 components with 50 iterations

Figure 14: EM algorithm for provided data with 2 components

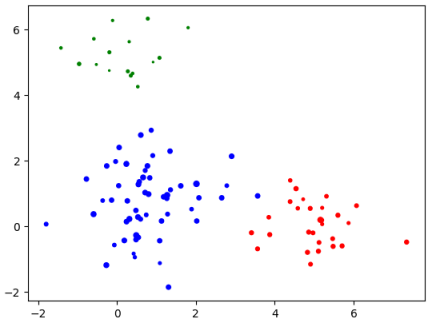
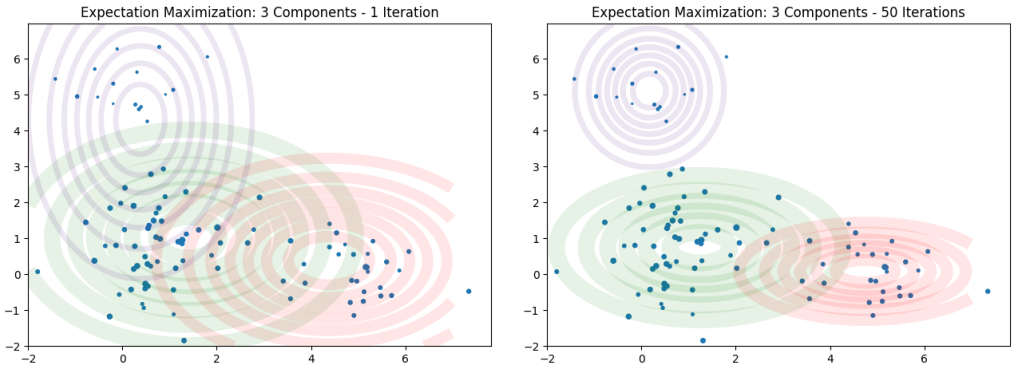


Figure 15: Provided data with 3 components



(a) EM for 3 components with 1 iteration (b) EM for 3 components with 50 iterations

Figure 16: EM algorithm for provided data with 3 components

7 Super epicentra – VI

Question 2.7.21

The following graphical model and data are given:

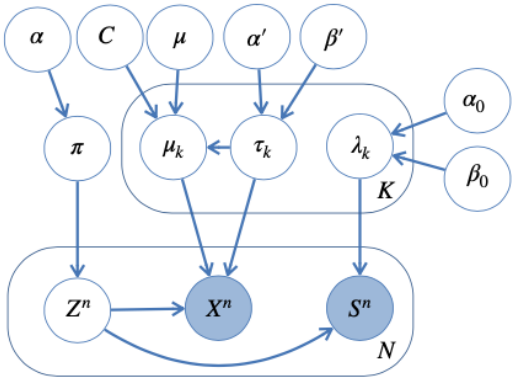


Figure 17: The K super epicentra model with priors

- π has a Dir(α) prior.
- $\tau_{k,i}$ has a Ga(α',β') prior.
- $\mu_{k,i}$ has a $\mathcal{N}(\mu, (C\tau_{k,i})^{-1})$ prior.
- λ_k has a Ga(α_0,β_0) prior.
- Z^n is modeled by a categorical distribution.
- X^n is modeled by a bi-dimensional normal distribution.
- S^n is modeled by a Poisson distribution.

From here, it can be said that:

$$\pi \to \prod_{k=1}^{K} \pi_k^{\alpha_k - 1}$$

$$\tau_{k,i} \to \frac{(\beta')^{\alpha'}}{\Gamma(\alpha')} \tau_{k,i}^{[\alpha'-1]} e^{[-\beta' \tau_{k,i}]}$$

$$\mu_{k,i} \to \sqrt{\frac{C\tau_{k,i}}{2\pi}} e^{[-\frac{C\tau_{k,i}}{2}(\mu_{k,i}-\mu)^2]}$$

$$\lambda_k \to \frac{(\beta_0)^{\alpha_0}}{\Gamma(\alpha_0)} \lambda_k^{[\alpha_0-1]} e^{[-\beta_0 \lambda_k]}$$

The posterior distribution for this graphical model can be obtained by:

$$p(Z, \theta|X, S) = p(Z, \Pi, T, M, \Lambda|X, S)$$
$$\text{Being } \theta = \pi, \underbrace{\tau_{k,\,i}}_{k}, \underbrace{\mu_{k,\,i}}_{k}, \lambda_k$$

Now, considering variational inference:

$$q(Z, \Pi, T, M, \Lambda) = q(Z)\, q(\Pi, T, M, \Lambda)$$
$$\log(q^*(Z)) = \mathbb{E}_{\Pi,T,M,\Lambda}[\log(\underbrace{p(\Pi, T, M, \Lambda, X, S, Z))}_{\text{Joint distribution}}] + const$$

And now, checking independence by means of the provided graphical model:

$$p(\Pi, T, M, \Lambda, X, S, Z) = \underbrace{p(X|Z, M, T)\, p(S|\Lambda, Z)\, p(Z|\Pi)}_{p(X,S,Z|M,T,\Lambda,\Pi)}\ \underbrace{p(M|T)\, p(T)\, p(\Lambda)\, p(\Pi)}_{p(M,T,\Lambda,\Pi)}$$

Focusing on the first term:

$$p(X, S, Z|M, T, \Lambda, \Pi) = \prod_{n=1}^{N} p(X_n|M, T)\, p(S_n|\Lambda)\ \underbrace{p(Z_n|\Pi)}_{\text{Categorical}} =$$
$$= \prod_{n=1}^{N}\prod_{k=1}^{K} (p(X_n|\boldsymbol{\mu}_k, \boldsymbol{\tau}_k)\, p(S_n|\lambda_k)\, p(Z_{n,k} = 1|\pi_k))^{Z_{n,k}}$$

From here, it can be substituted in the expected value expression derived before:

$$\log(q^*(Z)) = \mathbb{E}_\theta \left[\log \left(\prod_{n=1}^{N}\prod_{k=1}^{K} (p(X_n|\boldsymbol{\mu}_k, \boldsymbol{\tau}_k)\, p(S_n|\lambda_k)\, p(Z_{n,k} = 1|\pi_k))^{Z_{n,k}}\, p(M, T, \Lambda, \Pi) \right) \right] + const$$

The term $p(M, T, \Lambda, \Pi)$ does not depend on Z, so it can be included into the constant. Now, splitting the equation by means of logarithms, it is obtained:

$$\mathbb{E}_\theta \left[\log \left(\prod_{n=1}^{N}\prod_{k=1}^{K} p(X_n|\boldsymbol{\mu}_k, \boldsymbol{\tau}_k)^{Z_{n,k}} \right) + \log \left(\prod_{n=1}^{N}\prod_{k=1}^{K} p(S_n|\lambda_k)^{Z_{n,k}} \right) \right.$$
$$\left. + \log \left(\prod_{n=1}^{N}\prod_{k=1}^{K} p(Z_{n,k} = 1|\pi_k \right)^{Z_{n,k}} \right] + const$$

Now, applying some properties:

$$\mathbb{E}_\theta \left[\sum_{n=1}^{N}\sum_{k=1}^{K} Z_{n,k} (\log(p(X_n|\boldsymbol{\mu_k}, \boldsymbol{\tau}_k)) + \log(p(S_n|\lambda_k)) + \log(p(Z_{n,k} = 1|\pi_k))) \right] + const$$

Knowing that $X \sim \mathcal{N}(\mu_k|(\tau_k)^{-1})$, $S \sim Poisson(\lambda_k)$ and $Z \sim Cat(\pi_k)$, the expression terms can be transformed into:

$$\log(\mathcal{N}(X_n|\boldsymbol{\mu}_k,(\boldsymbol{\tau}_k)^{-1}I)) = \log\left(\frac{1}{\sqrt{(2\pi)^K|\boldsymbol{\tau}_k^{-1}|}}\exp\left[\frac{1}{2}(X_n-\boldsymbol{\mu}_k)^T(\boldsymbol{\tau}_k^{-1}I)^{-1}(X_n-\boldsymbol{\mu}_k)\right]\right) =$$

$$= -\frac{1}{2}(K(\log(2\pi)) + \log(|\boldsymbol{\tau}_k^{-1}|)) + \frac{1}{2}(X_n-\boldsymbol{\mu}_k)^T(\boldsymbol{\tau}_k^{-1}I)^{-1}(X_n-\boldsymbol{\mu}_k)$$

$$\log(p(S_n|\lambda_k)) = \log\left(\frac{\lambda_k^{S_n}e^{-\lambda_k}}{S_n!}\right) = S_n\log(\lambda_k) - \lambda_k - \log(S_n!)$$

$$\log(p(Z_{n,k}=1|\pi_k)) = \log(\pi_k)$$

Substituting in the expression, it takes the form of:

$$\log(q^*(Z)) = \mathbb{E}_\theta\left[\sum_{n=1}^N\sum_{k=1}^K Z_{n,k}\left(-\frac{1}{2}(K(\log(2\pi)) + \log(|\boldsymbol{\tau}_k^{-1}|)) + \frac{1}{2}(X_n-\boldsymbol{\mu}_k)^T(\boldsymbol{\tau}_k^{-1}I)^{-1}(X_n-\boldsymbol{\mu}_k) + \right.\right.$$

$$\left.\left. + \ S_n\log(\lambda_k) - \lambda_k - \log(S_n!) + \log(\pi_k)\right)\right] + const$$

$$\log(q^*(Z)) = \sum_{n=1}^N\sum_{k=1}^K Z_{n,k}\left(-\frac{1}{2}(K(\log(2\pi)) + \mathbb{E}_\tau[\log(|\boldsymbol{\tau}_k^{-1}|)] + \mathbb{E}_{\mu,\tau}\left[\frac{1}{2}(X_n-\boldsymbol{\mu}_k)^T(\boldsymbol{\tau}_k^{-1}I)^{-1}(X_n-\boldsymbol{\mu}_k)\right] + \right.$$

$$\left. + \ S_n\mathbb{E}_\lambda[\log(\lambda_k)] - \mathbb{E}_\lambda[\lambda_k] - \log(S_n!) + \mathbb{E}_\pi[\log(\pi_k)]\right) + const$$

This equation can be written as a function of ρ, where $\log(\rho)$ will be equivalent to the terms inside the parenthesis:

$$\log(q^*(Z)) = \sum_{n=1}^N\sum_{k=1} Z_{n,k}\log(\rho_{n,k}) + const = \sum_{n=1}^N\sum_{k=1}\log(\rho_{n,k}^{Z_{n,k}}) + const =$$

$$= \log\left(\prod_{n=1}^N\prod_{k=1}^K \rho_{n,k}^{Z_{n,k}}\right) + const$$

$$q^*(Z) = \prod_{n=1}^N\prod_{k=1}^K \rho_{n,k}^{Z_{n,k}} + const \propto \prod_{n=1}^N\prod_{k=1}^K \rho_{n,k}^{Z_{n,k}}$$

Even so, it is necessary to normalize this distribution, since for each value of n, the quantities $Z_{n,k}$ sum to 1 for all values of k, obtaining:

$$q^*(Z) = \prod_{n=1}^N\prod_{k=1}^K r_{n,k}^{Z_{n,k}} \quad \text{where} \quad r_{n,k} = \frac{\rho_{n,k}}{\sum_{k=1}^K \rho_{n,k}}$$

Now, it is necessary to deal with $q^*(M,T,\Lambda,\Pi)$. It is possible to perform a similar derivation than before, just changing the expected value to be over Z instead of being over the parameters:

$$\log(q^*(M,T,\Lambda,\Pi)) = \mathbb{E}_Z[\log(p(\Pi,T,M,\Lambda,X,S,Z))] + const$$

From this expression, as before, it is obtained:

$$p(\Pi, T, M, \Lambda, X, S, Z) = p(X, S, Z|M, T, \Lambda, \Pi)\, p(M, T, \Lambda, \Pi)$$

Nevertheless, in this case, the second term will not be a constant and has to be derived as well:

$$\begin{aligned}\log(q^*(M,T,\Lambda,\Pi)) &= \mathbb{E}_Z\left[\sum_{n=1}^{N}\sum_{k=1}^{K} Z_{n,k}(\log(p(X_n|\boldsymbol{\mu_k},\boldsymbol{\tau}_k)) + \log(p(S_n|\lambda_k)) + \log(p(Z_{n,k}=1|\pi_k)))\right] + \\ &+ \mathbb{E}_Z[\log(p(M,T,\Lambda,\Pi))] + const = \\ &= \mathbb{E}_Z\left[\sum_{n=1}^{N}\sum_{k=1}^{K} Z_{n,k}\left(-\frac{1}{2}(K(\log(2\pi)) + \log(|\boldsymbol{\tau}_k^{-1}|)) + \frac{1}{2}(X_n-\boldsymbol{\mu}_k)^T(\boldsymbol{\tau}_k^{-1}I)^{-1}\right.\right. \\ &\left.\left.(X_n-\boldsymbol{\mu}_k) + S_n\log(\lambda_k) - \lambda_k - \log(S_n!) + \log(\pi_k)\right)\right] + \mathbb{E}_Z[\log(p(M,T,\Lambda,\Pi))] + const\end{aligned}$$

Now, focusing on the second expected value term:

$$\mathbb{E}_Z[\log(p(M,T,\Lambda,\Pi))] = \mathbb{E}_Z[\log(p(M|T)\, p(T)\, p(\Lambda)\, p(\Pi))]$$

As none of these probabilities depends on Z, it is possible to substitute by their correspondent density functions:

$$\begin{aligned}\mathbb{E}_Z[\log(p(M,T,\Lambda,\Pi))] &= \log(p(M|T)\, p(T)\, p(\Lambda)\, p(\Pi))) = \\ &= \sum_{k=1}^{K} -\frac{1}{2}\log(2\pi(C\boldsymbol{\tau}_k)^{-1}) + \frac{(\boldsymbol{\mu}_k-\mu)^2}{2(C\boldsymbol{\tau}_k)^{-1}} + \alpha'\log(\beta') - \log(\Gamma(\alpha')) + \\ &+ (\alpha'-1)\log(\boldsymbol{\tau}_k) - \beta'\boldsymbol{\tau}_k + (\alpha_k-1)\log(\pi_k) + \alpha_0\log(\beta_0) - \log(\Gamma(\alpha_0)) + \\ &+ (\alpha_0-1)\log(\lambda_k) - \beta_0\lambda_k\end{aligned}$$

This is added to the previous equation, obtaining:

$$\begin{aligned}\log(q^*(M,T,\Lambda,\Pi)) &= \sum_{n=1}^{N}\sum_{k=1}^{K}\mathbb{E}_Z[Z_{n,k}]\left(-\frac{1}{2}(K(\log(2\pi)) + \log(|\boldsymbol{\tau}_k^{-1}|)) + \frac{1}{2}(X_n-\boldsymbol{\mu}_k)^T(\boldsymbol{\tau}_k^{-1}I)^{-1}\right. \\ &\left.(X_n-\boldsymbol{\mu}_k) + S_n\log(\lambda_k) - \lambda_k - \log(S_n!) + \log(\pi_k)\right) + \sum_{k=1}^{K} -\frac{1}{2}\log(2\pi(C\boldsymbol{\tau}_k)^{-1}) + \\ &+ \frac{(\boldsymbol{\mu}_k-\mu)^2}{2(C\boldsymbol{\tau}_k)^{-1}} + \alpha'\log(\beta') - \log(\Gamma(\alpha')) + (\alpha'-1)\log(\boldsymbol{\tau}_k) - \beta'\boldsymbol{\tau}_k + (\alpha_k-1)\log(\pi_k) + \\ &+ \alpha_0\log(\beta_0) - \log(\Gamma(\alpha_0)) + (\alpha_0-1)\log(\lambda_k) - \beta_0\lambda_k + const\end{aligned}$$

Which is transformed into the following after removing constants:

$$\log(q^*(M,T,\Lambda,\Pi)) = \sum_{n=1}^{N}\sum_{k=1}^{K}\mathbb{E}_Z[Z_{n,k}]\left(-\frac{1}{2}\log(|\boldsymbol{\tau}_k^{-1}|) + \frac{1}{2}(X_n-\boldsymbol{\mu}_k)^T(\boldsymbol{\tau}_k^{-1}I)^{-1}(X_n-\boldsymbol{\mu}_k) + \right.$$
$$\left. + S_n\log(\lambda_k) - \lambda_k - \log(S_n!) + \log(\pi_k)\right) + \sum_{k=1}^{K} -\frac{1}{2}\log((C\boldsymbol{\tau}_k)^{-1}) + \frac{(\boldsymbol{\mu}_k-\mu)^2}{2(C\boldsymbol{\tau}_k)^{-1}} +$$
$$+ (\alpha'-1)\log(\boldsymbol{\tau}_k) - \beta'\boldsymbol{\tau}_k + (\alpha_0-1)\log(\lambda_k) - \beta_0\lambda_k + (\alpha_k-1)\log(\pi_k) + const$$

And now, applying:

$$q(M,T,\Lambda,\Pi) = q(\Pi)\prod_{k=1}^{K} q(M,T,\Lambda)$$

From the terms of $\log(q^*(M,T,\Lambda,\Pi))$ which depend on Π:

$$\log(q(\Pi)) = \sum_{k=1}^{K}(\alpha_k-1)\log(\pi_k) + \sum_{n=1}^{N}\sum_{k=1}^{K} r_{n,k}\log(\pi_k)$$
$$q(\Pi) = \prod_{k=1}^{K}\pi_k^{(\alpha_k-1)} + \prod_{n=1}^{N}\prod_{k=1}^{K}\pi_k^{r_{n,k}}$$

The same procedure is also applied to $\prod_{k=1}^{K} q(M,T,\Lambda)$:

$$\prod_{k=1}^{K} q(T,M,\Lambda) = \prod_{k=1}^{K} q(M|T)\,q(T)\,q(\Lambda)$$
$$q(M|T)\,q(T) = \prod_{n=1}^{N}\prod_{k=1}^{K}\left(\frac{-1}{\sqrt{\tau_k}} + e^{-\frac{(X_n-\mu_k)^2}{2\tau_k}}\right)^{\mathbb{E}_Z[Z_{n,k}]} + \prod_{k=1}^{K}\frac{-1}{\sqrt{(C\tau_k)^{-1}}}\,e^{\frac{-(\mu_k-\mu)^2}{2(C\tau_k)^{-1}}} + \tau_k^{(\alpha'-1)}\,e^{(-\beta'\tau_k)}$$
$$q(\Lambda) = \prod_{n=1}^{N}\prod_{k=1}^{K}\left(\frac{\lambda_k^{S_n}}{\lambda_k}\right)^{\mathbb{E}_Z[Z_{n,k}]} + \lambda_k^{\alpha_0-1}\,e^{-\beta_0\lambda_k}$$

From this point, with the obtained expressions, it is possible to compute the approximation knowing that:

$$q(Z,\Pi,T,M,\Lambda) = q(Z)\,q(\Pi,T,M,\Lambda)$$

Therefore, the final expression is equal to:

$$q(Z,\Pi,T,M,\Lambda) = \left(\prod_{n=1}^{N}\prod_{k=1}^{K} r_{n,k}^{Z_{n,k}}\right)\left(\prod_{k=1}^{K}\pi_k^{(\alpha_k-1)} + \prod_{n=1}^{N}\prod_{k=1}^{K}\pi_k^{r_{n,k}}\right)\left(\prod_{n=1}^{N}\prod_{k=1}^{K}\left(\frac{-1}{\sqrt{\tau_k}} + e^{-\frac{(X_n-\mu_k)^2}{2\tau_k}}\right)^{\mathbb{E}_Z[Z_{n,k}]} + \right.$$
$$\left. + \prod_{k=1}^{K}\frac{-1}{\sqrt{(C\tau_k)^{-1}}}\,e^{\frac{-(\mu_k-\mu)^2}{2(C\tau_k)^{-1}}} + \tau_k^{(\alpha'-1)}\,e^{(-\beta'\tau_k)}\right)\left(\prod_{n=1}^{N}\prod_{k=1}^{K}\left(\frac{\lambda_k^{S_n}}{\lambda_k}\right)^{\mathbb{E}_Z[Z_{n,k}]} + \lambda_k^{\alpha_0-1}\,e^{-\beta_0\lambda_k}\right)$$

8 Sampling from a tree GM

Question 2.8.22

Question 2.8.23

Question 2.8.24

Question 2.8.25

9 Failing components VI

A Simple VI

```
import numpy as np
import matplotlib.pyplot as plt
import scipy.stats as stats
from tqdm import tqdm

# This function computes the value of tau_N
def compute_tauN(tau_0, mu_0, vector, a_N, b_N):

    result = (tau_0 + len(vector)) * (a_N / b_N)
    return result

# This function computes the values of b_N
def compute_bN(a_0, b_0, vector, mu_0, tau_N):

    term1 = (1 / tau_N) + pow(np.mean(vector),2) + pow(mu_0,2) - 2 * np.mean(vector
    ) * mu_0
    term2 = 0
    for x in vector:
        term2 += pow(x,2) + (1 / tau_N) + pow(np.mean(vector),2) - 2 * np.mean(
    vector) * x
    result = b_0 + 0.5 * tau_0 * term1 + 0.5 * term2

    return result

#This function computes the approximated distribution
def getQ(mu_axis, tau_axis, mu_N, tau_N, a_N, b_N):

    q_mu_tau = np.zeros((len(mu_axis), len(tau_axis)))

    for i in tqdm(range(len(mu_axis))):
        for j in range(len(tau_axis)):
            q_mu = stats.norm(mu_N, 1/(tau_N)).pdf(mu_axis[i])
            q_tau = stats.gamma.pdf(tau_axis[j], a_N, loc=0, scale=(1/b_N))
            q_mu_tau[j][i] = q_mu * q_tau

    return q_mu_tau

#This function computes the original distribution
def getP(mu_axis, tau_axis, mu_N, tau_N, a_N, b_N):

    p_mu_tau = np.zeros((len(mu_axis), len(tau_axis)))

    for i in tqdm(range(len(mu_axis))):
        for j in range(len(tau_axis)):
            if(tau_axis[j] == 0):
```

```
                tau_axis[j] = 0.00001 # Correction for 0 denominator
            p_mu = stats.norm(mu_N, 1/(tau_N * tau_axis[j])).pdf(mu_axis[i])
            p_tau = stats.gamma.pdf(tau_axis[j], a_N, loc=0, scale=(1/b_N))
            p_mu_tau[j][i] = p_mu * p_tau

    return p_mu_tau

if __name__ == "__main__":

    # VARIABLES
    iterations = 10                 # Number of iterations
    n = 10                          # Number of samples
    mu_0 = 0                        # Initial value mu_0
    mu_N = 1                        # Initial value mu_N
    tau_0 = 1                       # Initial value tau_0
    tau_N = 1                       # Initial value mu_N
    a_0 = 0                         # Initial value a_0
    a_N = 1                         # Initial value a_N
    b_0 = 1                         # Initial value b_0
    b_N = 1                         # Initial value b_N
    mu_axis = np.linspace(-1,1,100)  # X axis grid
    tau_axis = np.linspace(0,2,100)  # Y axis grid

    # SAMPLES GENERATION
    vector = np.random.normal(0,1,n)

    mu_N = (tau_0 * mu_0 + np.sum(vector)) / (tau_0 + len(vector))  # mu_N value
    computation (it won't update)
    a_N = a_0 + (len(vector)) / 2                                   # a_N value
    computation (it won't update)

    q_mu_tau = np.zeros((len(mu_axis), len(tau_axis)))
    p_mu_tau = np.zeros((len(mu_axis), len(tau_axis)))

    for i in range(iterations):
        tau_N = compute_tauN(tau_0, mu_0, vector, a_N, b_N)
        b_N = compute_bN(a_0, b_0, vector, mu_N, tau_N)

    p_mu_tau = getP(mu_axis, tau_axis, mu_N, tau_N, a_N, b_N)
    q_mu_tau = getQ(mu_axis, tau_axis, mu_N, tau_N, a_N, b_N)
    #plt.axis([-0.2,0.2, 0, 2])                                     # Uncomment
    this line to modify the grid area
    plt.contour(mu_axis, tau_axis, q_mu_tau, colors='red')
    plt.contour(mu_axis, tau_axis, p_mu_tau, colors='green')
    plt.show()
```

B Mixture of trees with observable variables

```
import argparse
import numpy as np
import matplotlib.pyplot as plt
import sys
import networkx as nx
import dendropy
import Kruskal_v1 as kruskal
from Tree import Tree, TreeMixture
from tqdm import tqdm

def save_results(loglikelihood, topology_array, theta_array, filename):
    """ This function saves the log-likelihood vs iteration values,
        the final tree structure and theta array to corresponding numpy arrays. """

    likelihood_filename = filename + "_em_loglikelihood.npy"
    topology_array_filename = filename + "_em_topology.npy"
    theta_array_filename = filename + "_em_theta.npy"
    print("Saving log-likelihood to ", likelihood_filename, ", topology_array to: "
    , topology_array_filename,
          ", theta_array to: ", theta_array_filename, "...")
    np.save(likelihood_filename, loglikelihood)
    np.save(topology_array_filename, topology_array)
    np.save(theta_array_filename, theta_array)

def computeLikelihood(samples, topology, theta):
    result = theta[0][samples[0]]
    for i in range(1, len(topology)):
        result *= theta[i][samples[int(topology[i])]][samples[i]]

    return (result + sys.float_info.epsilon)

def computeLogLikelihood(pi, likelihood):
    result = 0
    for i in range(likelihood.shape[0]):
        aux = 0
        for k in range(likelihood.shape[1]):
            aux += pi[k] * likelihood[i,k]
        result += np.log(aux)

    return result

def computeCondQ(responsibility, samples, node1, node2, value1, value2):
    num = 0
    denom = 0
    for i in range(samples.shape[0]):
```

```
45          if (samples[i,node1] == value1):
46              denom += responsibility[i]
47              if (samples[i,node2] == value2):
48                  num += responsibility[i]
49
50      return (num / (denom + sys.float_info.epsilon))
51
52  def computeQ(responsibility, samples, node, val):
53      num = 0
54      for i in range(samples.shape[0]):
55          if (samples[i,node] == val):
56              num += responsibility[i]
57      denom = np.sum(responsibility) + sys.float_info.epsilon
58
59      return (num / denom)
60
61  def computeQJoint(responsibility, samples, node1, node2, val1, val2):
62      num = 0
63      for i in range(samples.shape[0]):
64          if (samples[i,node1] == val1) and (samples[i,node2] == val2):
65              num += responsibility[i]
66      denom = np.sum(responsibility) + sys.float_info.epsilon
67
68      return (num / denom)
69
70  def computeResponsibility(num_clusters, samples, pi, likelihood):
71      result = np.zeros((samples.shape[0], num_clusters))
72      for i in range(samples.shape[0]):
73          for k in range(num_clusters):
74              result[i,k] = pi[k] * likelihood[i,k]
75          result[i] = (result[i] + sys.float_info.epsilon) / (np.sum(result[i]) +
    num_clusters * sys.float_info.epsilon)
76
77      return result
78
79  def calculateI(responsibility, samples, node1, node2):
80      result = 0
81      for i in range(2):
82          for j in range(2):
83              q_node1 = computeQ(responsibility, samples, node1, i)
84              q_node2 = computeQ(responsibility, samples, node2, j)
85              q_joint = computeQJoint(responsibility, samples, node1, node2, i, j)
86              if (q_joint != 0):
87                  if (q_node1 == 0):
88                      q_node1 = sys.float_info.epsilon
89                  if (q_node2 == 0):
90                      q_node2 = sys.float_info.epsilon
```

```
                if ((q_node1 * q_node2) == 0):
                    result += q_joint * np.log(q_joint / (sys.float_info.min))
                else:
                    result += q_joint * np.log(q_joint / (q_node1 * q_node2))

    return result

def computeTheta(theta_list, responsibility, samples, topology, num_nodes,
    num_clusters):
    result = theta_list
    for k in range(num_clusters):
        for i in range(num_nodes):
            if (i == 0):
                result[k][0,0] = computeQ(responsibility[:,k], samples, 0, 0)
                result[k][0,1] = computeQ(responsibility[:,k], samples, 0, 1)
            else:
                result[k][i,0][0]= computeCondQ(responsibility[:,k], samples, int(
    topology[k][i]), i, 0, 0)
                result[k][i,0][1]= computeCondQ(responsibility[:,k], samples, int(
    topology[k][i]), i, 0, 1)
                result[k][i,1][0]= computeCondQ(responsibility[:,k], samples, int(
    topology[k][i]), i, 1, 0)
                result[k][i,1][1]= computeCondQ(responsibility[:,k], samples, int(
    topology[k][i]), i, 1, 1)

    return result

def computationsEM(iterations, samples, num_clusters, tm, topology_list, theta_list
    ):
    pi = tm.pi
    loglikelihood = np.zeros(iterations)

    for it in range(iterations):
        num_samples = samples.shape[0]
        num_nodes = samples.shape[1]
        likelihood = np.zeros((num_samples, num_clusters)) # Probability of having
    this sample per tree

        # Compute likelihood per sample
        for i in range(num_samples):
            for k in range(num_clusters):
                likelihood[i,k] = computeLikelihood(samples[i,:], topology_list[k],
     theta_list[k])

        # Computation of responsibilities
        responsibility = computeResponsibility(num_clusters, samples, pi,
    likelihood)
```

```
129
130         # Computation of pi'
131         res_sum = np.sum(responsibility, axis=0)
132         total_sum = np.sum(res_sum)
133         pi = np.zeros(len(res_sum))
134         for i in range(len(res_sum)):
135             pi[i] = res_sum[i] / total_sum
136
137         # Get the IQ for using as weights
138         IQ = np.zeros((num_nodes, num_nodes, num_clusters))
139         for k in range(num_clusters):
140             for i in range(len(topology_list[k])):
141                 for j in range(len(topology_list[k])):
142                     if (i != j):
143                         IQ[i,j,k] = calculateI(responsibility[:,k], samples, i, j)
144
145         # Create the graphs
146         graphs = list()
147         for k in range(num_clusters):
148             graphs.append(kruskal.Graph(num_nodes))
149             for i in range(num_nodes):
150                 for j in range(i+1, num_nodes):
151                     graphs[-1].addEdge(i, j, IQ[i,j,k])
152
153         # Get the Maximum Spanning Tree from each graph
154         tree = np.zeros((num_nodes-1, 3, num_clusters))
155         for k in range(num_clusters):
156             result = graphs[k].maximum_spanning_tree()
157             cnt = 0
158             for u_aux, v_aux, weight_aux in result:
159                 tree[cnt,0,k] = u_aux
160                 tree[cnt,1,k] = v_aux
161                 tree[cnt,2,k] = weight_aux
162                 cnt += 1
163
164         # Creation of the tree
165         topology_list = list()
166         for k in range(num_clusters):
167             topology_list.append(np.zeros(num_nodes))
168             topology_list[-1][0] = np.nan
169             max_tree = nx.Graph()
170             for i in range(tree.shape[0]):
171                 max_tree.add_edge(tree[i,0,k], tree[i,1,k])
172             finaltree = list(nx.bfs_edges(max_tree, 0))
173             for i in range(num_nodes - 1):
174                 topology_list[-1][int(finaltree[i][1])] = finaltree[i][0]
175
```

```
176         # Computation of theta'
177         theta_list = computeTheta(theta_list, responsibility, samples,
    topology_list, num_nodes, num_clusters)
178 
179         loglikelihood[it] = computeLogLikelihood(pi, likelihood)
180 
181     return loglikelihood
182 
183 
184 def em_algorithm(seed_val, samples, num_clusters, max_num_iter):
185 
186     # Initialize the needed variables
187     sieving = 100
188     max_log = float("-inf")
189     best_seed = 0
190 
191     # Get the best seed for likelihood
192     for siev in tqdm(range(sieving)):
193         # Set the seed
194         aux_seed = seed_val + siev # Try with all seeds from @param:seed_val to
    @param:seed_val + sieving
195         np.random.seed(aux_seed)
196 
197         # Generate tree mixture
198         tm = TreeMixture(num_clusters=num_clusters, num_nodes=samples.shape[1])
199         tm.simulate_pi(seed_val=aux_seed)
200         tm.simulate_trees(seed_val=aux_seed)
201         topology_list = []
202         theta_list = []
203 
204         for i in range(num_clusters):
205             topology_list.append(tm.clusters[i].get_topology_array())
206             theta_list.append(tm.clusters[i].get_theta_array())
207 
208         # Run 10 iterations according to this mixture
209         loglikelihood = computationsEM(10, samples, num_clusters, tm, topology_list
    , theta_list)
210 
211         aux = loglikelihood[-1]
212         if (aux > max_log):
213             max_log = aux
214             best_seed = aux_seed
215 
216     # -------------------- End of sieving -------------------- #
217 
218     # Variable initialization
219     np.random.seed(best_seed)
```

```
    topology_list = [] # Dimensions: (num_clusters, num_nodes)
    theta_list = [] # Dimensions: (num_clusters, num_nodes, 2)
    tm = TreeMixture(num_clusters = num_clusters, num_nodes = samples.shape[1])
    tm.simulate_pi(seed_val = best_seed)
    tm.simulate_trees(seed_val = best_seed)

    for k in range(num_clusters):
        topology_list.append(tm.clusters[k].get_topology_array())
        theta_list.append(tm.clusters[k].get_theta_array())

    # Beginning of iterations
    pi = tm.pi
    loglikelihood = computationsEM(max_num_iter, samples, num_clusters, tm,
    topology_list, theta_list)

    return loglikelihood, topology_list, theta_list


def main():
    # Code to process command line arguments
    parser = argparse.ArgumentParser(description='EM algorithm for likelihood of a
    tree GM.')
    parser.add_argument('sample_filename', type=str,
                        help='Specify the name of the sample file (i.e data/
    example_samples.txt)')
    parser.add_argument('output_filename', type=str,
                        help='Specify the name of the output file (i.e data/
    example_results.txt)')
    parser.add_argument('num_clusters', type=int, help='Specify the number of
    clusters (i.e 3)')
    parser.add_argument('--seed_val', type=int, default=42, help='Specify the seed
    value for reproducibility (i.e 42)')
    parser.add_argument('--real_values_filename', type=str, default="",
                        help='Specify the name of the real values file (i.e data/
    example_tree_mixture.pkl)')
    # You can add more default parameters if you want.

    print("This file demonstrates the flow of function templates of question 2.5.")

    print("\n0. Load the parameters from command line.\n")

    args = parser.parse_args()
    print("\tArguments are: ", args)

    print("\n1. Load samples from txt file.\n")

    samples = np.loadtxt(args.sample_filename, delimiter="\t", dtype=np.int32)
```

```
260     num_samples, num_nodes = samples.shape
261     print("\tnum_samples: ", num_samples, "\tnum_nodes: ", num_nodes)
262     print("\tSamples: \n", samples)
263 
264     print("\n2. Run EM Algorithm.\n")
265     max_iterations = 100 # Maximum number of iterations for the EM algorithm
266     loglikelihood, topology_array, theta_array = em_algorithm(args.seed_val,
        samples, args.num_clusters, max_iterations)
267 
268     print("\n3. Save, print and plot the results.\n")
269 
270     save_results(loglikelihood, topology_array, theta_array, args.output_filename)
271 
272     for i in range(args.num_clusters):
273         print("\n\tCluster: ", i)
274         print("\tTopology: \t", topology_array[i])
275         print("\tTheta: \t", theta_array[i])
276 
277     print("\n4. Retrieve real results and compare.\n")
278     if args.real_values_filename != "":
279         print("\tComparing the results with real values...")
280 
281         print("\t4.1. Make the Robinson-Foulds distance analysis.\n")
282 
283         tns = dendropy.TaxonNamespace()
284         original_tree = list()
285         original_topology = list()
286 
287         for k in range(args.num_clusters):
288             filename = args.real_values_filename + "_tree_" + str(k) + "_topology.
    npy"
289             original_topology.append(np.load(filename))
290             original_tree.append(Tree())
291             original_tree[-1].load_tree_from_direct_arrays(original_topology[-1])
292             original_tree[-1] = dendropy.Tree.get(data = original_tree[-1].newick,
    schema = "newick", taxon_namespace = tns)
293 
294         generated_tree = list()
295 
296         for k in range(args.num_clusters):
297             generated_tree.append(Tree())
298             generated_tree[-1].load_tree_from_direct_arrays(topology_array[k])
299             generated_tree[-1] = dendropy.Tree.get(data = generated_tree[-1].newick
    , schema = "newick", taxon_namespace = tns)
300             print("Generated tree ", k, " ",generated_tree[-1].as_string("newick"))
301             generated_tree[-1].print_plot()
302 
```

```
303         print("\tDistances of trees:\n")
304         for k in range(args.num_clusters):
305             for i in range(args.num_clusters):
306                 print("\tOriginal tree",k,"compared to generated tree",i)
307                 print("\t\tRobinson-Foulds distance:", dendropy.calculate.
    treecompare.symmetric_difference(original_tree[k], generated_tree[i]))
308 
309 
310         print("\n\t4.2. Make the likelihood comparison.\n")
311 
312         original_theta = list()
313         for k in range(args.num_clusters):
314             filename = args.real_values_filename + "_tree_" + str(k) + "_theta.npy"
315             original_theta.append(np.load(filename, allow_pickle = True))
316 
317         filename = args.real_values_filename + "_pi.npy"
318         original_pi = np.load(filename)
319         original_likelihood = np.zeros((num_samples, args.num_clusters))
320         for i in range(num_samples):
321             for k in range(args.num_clusters):
322                 original_likelihood[i,k] = computeLikelihood(samples[i,:],
    original_topology[k], original_theta[k])
323 
324         original_log_likelihood = computeLogLikelihood(original_pi,
    original_likelihood)
325         original_log_likelihood_array = [original_log_likelihood for i in range(
    max_iterations)]
326 
327         plt.figure(figsize=(16, 7))
328         plt.subplot(121)
329         plt.plot(np.exp(loglikelihood), label='Estimated')
330         plt.plot(np.exp(original_log_likelihood_array), label='Real',color = 'r')
331         plt.ylabel("Likelihood of Mixture")
332         plt.xlabel("Iterations")
333         plt.subplot(122)
334         plt.plot(loglikelihood, label='Estimated')
335         plt.plot(original_log_likelihood_array, label='Original',color = 'r')
336         plt.ylabel("Log-Likelihood of Mixture")
337         plt.xlabel("Iterations")
338         plt.legend(loc=(1.04, 0))
339         plt.show()
340 
341         print("End of execution.\n")
342 
343 if __name__ == "__main__":
344     main()
```

C Super epicentra – EM

```
import numpy as np
import matplotlib.pyplot as plt
import matplotlib.mlab as mlab
from scipy.stats import multivariate_normal, poisson
import math


def generate_data(n_data, means, covariances, weights, rates):
    n_clusters, n_features = means.shape
    data = np.zeros((n_data, n_features))
    poission_data = np.zeros(n_data)
    colors = np.zeros(n_data, dtype='str')
    for i in range(n_data):
        # pick a cluster id and create data from this cluster
        k = np.random.choice(n_clusters, size=1, p=weights)[0]
        x = np.random.multivariate_normal(means[k], covariances[k])
        data[i] = x
        poission_data[i] = np.random.poisson(rates[k])
        if k == 0:
            colors[i] = 'red'
        elif k == 1:
            colors[i] = 'blue'
        elif k == 2:
            colors[i] = 'green'

    return data, poission_data, colors


# means, covs: means and covariances of Gaussians
# rates: rates of Poissons
# title: title of the plot defining which EM iteration
def plot_contours(X, S, means, covs, title, rates):
    plt.figure()
    plt.scatter(X[:, 0], X[:, 1], s=S)

    delta = 0.025
    k = means.shape[0]
    x = np.arange(-2.0, 7.0, delta)
    y = np.arange(-2.0, 7.0, delta)
    X, Y = np.meshgrid(x, y)
    col = ['green', 'red', 'indigo']
    for i in range(k):
        mean = means[i]
        cov = covs[i]
        positions = np.dstack((X,Y))
```

```
        Z = multivariate_normal(mean, cov)
        plt.contour(X, Y, Z.pdf(positions), colors=col[i], linewidths=rates[i], alpha=0.1)

    plt.title(title)
    plt.tight_layout()


class EM:

    def __init__(self, n_components, n_iter, tol, seed):
        self.n_components = n_components
        self.n_iter = n_iter
        self.tol = tol
        self.seed = seed

    def fit(self, X, S):

        # data's dimensionality
        self.n_row, self.n_col = X.shape

        # initialize parameters
        np.random.seed(self.seed)
        chosen = np.random.choice(self.n_row, self.n_components, replace=False)
        self.means = X[chosen]
        self.weights = np.full(self.n_components, 1 / self.n_components)
        if self.n_components == 3:
            self.rates = (np.mean(S) * np.ones(self.n_components) / np.array([1, 2, 3])[np.newaxis]).flatten()
        elif self.n_components == 2:
            self.rates = (np.mean(S) * np.ones(self.n_components) / np.array([1, 2])[np.newaxis]).flatten()
        shape = self.n_components, self.n_col, self.n_col
        self.covs = np.full(shape, np.cov(X, rowvar=False))
        new_covs = []
        for c in self.covs:
            new_covs = np.append(new_covs, np.diag(np.diag(c))) # making the covariances diagonal (question assumption)
        self.covs = np.array(new_covs).reshape(self.n_components, 2, 2)

        log_likelihood = 0
        self.converged = False

        for i in range(self.n_iter):
            self._do_estep(X, S)
            self._do_mstep(X, S)
            log_likelihood_new = self._compute_log_likelihood(X, S)
```

```
89
90              if (log_likelihood - log_likelihood_new) <= self.tol:
91                  self.converged = True
92                  break
93
94              log_likelihood = log_likelihood_new
95
96          return self
97
98      def _do_estep(self, X, S):
99          num = np.zeros((self.n_row, self.n_components))
100         denom = np.zeros(self.n_row)
101         self.gamma = np.zeros((self.n_row, self.n_components))
102         for i in range(self.n_row):
103             for j in range(self.n_components):
104                 num[i,j] = self.weights[j] * multivariate_normal(self.means[j],
    self.covs[j]).pdf(X[i]) * poisson(self.rates[j]).pmf(S[i])
105         self.gamma = (num.T / num.sum(1)).T
106
107         return self
108
109     def _do_mstep(self, X, S):
110         n_k = self.gamma.sum(0)
111         elems = self.n_row
112         for i in range(self.n_components):
113             for j in range(self.n_col):
114                 self.means[i,j] = sum(self.gamma[:,i] * X[:,j]) / n_k[i]
115                 diff = X[:,j] - self.means[i,j]
116                 self.covs[i,j,j] = sum(self.gamma[:,i] * diff * np.transpose(diff))
     / n_k[i]
117                 self.rates[i] = sum(self.gamma[:,i] * S[:]) / n_k[i]
118             self.weights[i] = n_k[i] / elems
119
120         return self
121
122     def _compute_log_likelihood(self, X, S):
123         log_likelihood = 0
124         for i in range(self.n_components):
125             log_likelihood = sum(self.gamma[:,i] * (self.weights[i] *
    multivariate_normal(self.means[i], self.covs[i]).pdf(X[:]) * poisson(self.
    rates[i]).pmf(S[:])))
126         log_likelihood = np.log(log_likelihood).sum()
127
128         return log_likelihood
129
130 # params for 3 clusters
131 means = np.array([
```

```
    [5, 0],
    [1, 1],
    [0, 5]
])

covariances = np.array([
    [[.5, 0.], [0, .5]],
    [[.92, 0], [0, .91]],
    [[.5, 0.], [0, .5]]
])

weights = [1 / 4, 1 / 2, 1 / 4]

# params for 2 clusters
means_2 = np.array([
    [5, 0],
    [1, 1]
])

covariances_2 = np.array([
    [[.5, 0.], [0, .5]],
    [[.92, 0], [0, .91]]
])

weights_2 = [1 / 4, 3 / 4]

np.random.seed(3)

rates = np.random.uniform(low=.2, high=20, size=3)
print("Poisson rates for 3 components:")
print(rates)

rates_2 = np.random.uniform(low=.2, high=20, size=2)
print("Poisson rates for 2 components:")
print(rates_2)

# generate data
X, S, colors = generate_data(100, means, covariances, weights, rates)
plt.scatter(X[:, 0], X[:, 1], s=S, c=colors) # the Poisson data is shown through
    size of the points: s
plt.show()

X_2, S_2, colors_2 = generate_data(100, means_2, covariances_2, weights_2, rates_2)
plt.scatter(X_2[:, 0], X_2[:, 1], s=S_2, c=colors_2) # the Poisson data is shown
    through size of the points: s
plt.show()

```

```
# Plots of EM results #

em = EM(n_components=3, n_iter=1, tol=1e-4, seed=1)
em.fit(X, S)
# plot: call plot_contours and give it the params updated from EM with 3 components
    (after 1 iteration)
plot_contours(X, S, means=em.means,covs=em.covs, title="Expectation Maximization: 3
    Components - 1 Iteration", rates=em.rates)
plt.show()

em = EM(n_components=3, n_iter=50, tol=1e-4, seed=1)
em.fit(X, S)
# plot: call plot_contours and give it the params updated from EM with 3 components
    (after 50 iterations)
plot_contours(X, S, means=em.means,covs=em.covs, title="Expectation Maximization: 3
    Components - 50 Iterations", rates=em.rates)
plt.show()

em_2 = EM(n_components=2, n_iter=1, tol=1e-4, seed=1)
em_2.fit(X_2, S_2)
# plot: call plot_contours and give it the params updated from EM with 2 components
    (after 1 iteration)
plot_contours(X_2, S_2, means=em_2.means,covs=em_2.covs, title="Expectation
    Maximization: 2 Components - 1 Iteration", rates=em_2.rates)
plt.show()

em_2 = EM(n_components=2, n_iter=50, tol=1e-4, seed=1)
em_2.fit(X_2, S_2)
# plot: call plot_contours and give it the params updated from EM with 2 components
    (after 50 iterations)
plot_contours(X_2, S_2, means=em_2.means,covs=em_2.covs, title="Expectation
    Maximization: 2 Components - 50 Iterations", rates=em_2.rates)
plt.show()
```

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