

ASEN 6519 Project Final Project

Using Variational Gaussian Mixture Models for Autonomous Task Segmentation

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Application and Context

Overview

This project will implement and extend prior work on robot trajectory segmentation. A robot trajectory consists of a sequence of robot state data, captured over a given time period, that encodes the progression of movements / actions taken by the robot. State data usually consists of low-level features such as robot joint configuration, end effector position, object position, and object-object relative data etc,. This project will also incorporate high-level features such as behavioral constraints that capture abstract concepts, such as keeping a certain object upright for a determined segment of the task. These trajectories are often used as sample data in robotic learning techniques such as Learning from Demonstration (LfD).

A robot trajectory might constitute a number of sub-tasks that have goal and stylistic behaviors distinct from other sub-task in other parts of the trajectory. Unless explicitly segmented and outline by a human operator, there is no clear obvious indicators that differentiate one sub-task sequence from another sub-task sequence withing the same trajectory. Thus, the goal of autonomous trajectory segmentation is to generate a candidate segmentation sequence for which each segment ideally captures the dynamics (style) and goals (pertinent objects, target locations, constraints etc,.) of some sub-task. For example, the standard pick-and-place task ubiquitously used throughout robotic research might consist of three sub-tasks:

1. **Pick:** The goal of this sub-task is to pick up a target object. Most sub-sequences of a trajectory will consist of data that signifies the end-effector moving towards the target object.
2. **Carry:** This sub-task can be vague, but often consists of the aspect of the pick-and-place task where the robot carries an object over to a the target area for placement.
3. **Place:** The goal of this sub-task is to place. The state data sequence will generally consist of moving towards the target location and releasing the object.

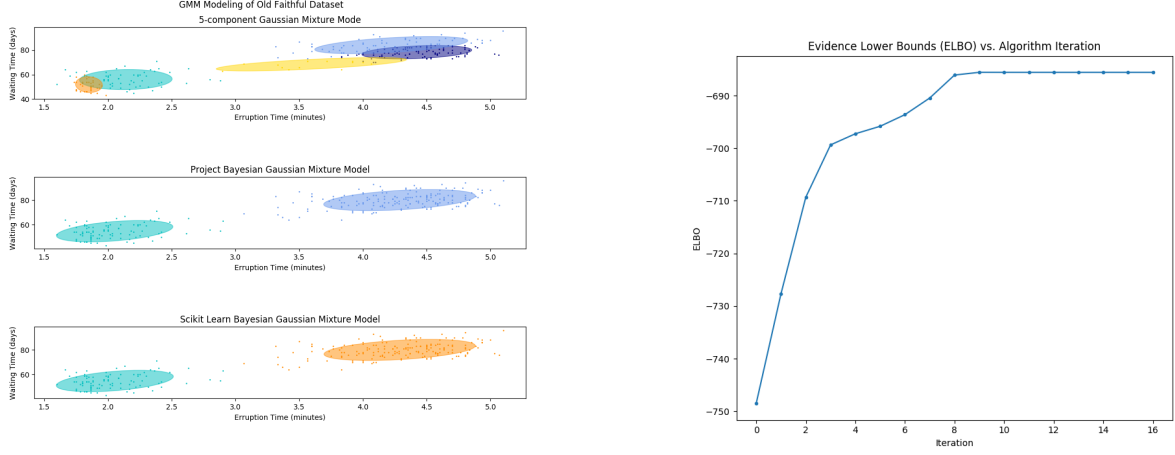
GMM Components as Segments

Many autonomous segmentation techniques make use of Gaussian Mixture Models. Ghahramani et. al. [1] showed how Gaussian Mixture models are a form of linear regression that linearize around the mixture means. In the spirit of this idea, Lee et. al. [2] fit GMM directly to the robot trajectory data where each data point $x_t \in X$, where X is a a sequence of state vectors x_i , is assigned to the best fitting component. Thus each $x_i \in X$ is assigned to a cluster of points representing a segment. Each component is, in a sense, a regression around the data for that specific segment. To capture more of the model dynamics, [3] utilizes the stacked vector of $\begin{bmatrix} x_t \\ x_{t+1} \end{bmatrix}$ and fits a GMM on this newly generated sequence of data. The GMM in this case can be thought of as a switched linear dynamical system in which each component's μ and Σ represent the dynamics for all data most associated with that given component. In either case, these works utilized the clustering of points to their corresponding mixture component to generate a segmentation of the entire trajectory.

Probabilistic Graphical Model

The model will be the Variational GMM model a la Bishop [4], built upon an observation set of state vectors but augmented with additional “observations” that consists of a vector of boolean, or one-hot, constraints assignments. The motivation is that during any given robot trajectory demonstration, a user might assign a set of boolean evaluated hard constraints. The constraints might include such high-level concepts such as, “keeping a cup upright” or “the object must be over the target before pouring”. These abstract constraints are evaluated on each $x_i \in X$ of the robot state vector i.e. the set of observations.

A demonstration is defined as a single episode of capturing a sequence of robot state trajectory and constraint assignments. Thus a demonstration represents X . For any set of demonstrations associated with a specific skill or task, this model will be run separately. There will be K parameters associated with S components of the mixture model. K will be determined automatically from the way the variational method



(a) Top: Non-Bayesian GMM 5 component fit. Middle: Project Variational GMM fit where three of five components have been nullified. Bottom: Scikit-Learn Equivalent Variational GMM fit.

(b) Evidence Lower Bounds increases at every iteration, plateauing until it the successive difference is below tolerance.

Figure 2: Old Faithful eruption data set with 3 models and the ELBO increase for the project model.

$$KL(q(Z)||p(z|x)) = E[\log(q(z))] - E[\log(p(z, x))] + \log(p(x))$$

$$\mathcal{L} = E[\log(q(z))] - E[\log(p(z, x))]$$

where the term \mathcal{L} is known as the evidence lower bound (ELBO). By maximizing the ELBO (since $p(x)$ is positive), we minimize the KL divergence.

With respect the variational Gaussian Mixture Model outlined in Figure 1, the chosen variational distribution is a factorized distribution built upon the chosen prior distributions of the model itself [4]:

$$q(Z, \pi, \mu, \Lambda) = q(Z)q(\pi, \mu, \Lambda)$$

and the variational lower bounds is represented by [4]:

$$\mathcal{L} = E[\log(q(X, Z, \pi, \mu, \Lambda))] - E[\log(q(Z, \pi, \mu, \Lambda))]$$

The optimization algorithm, akin the the Expectation Maximization algorithm, for the Variational Gaussian mixture model that optimizes the above is outlined in Algorithm 1.

Variational Iterative (EM) Algorithm

```

/* Initial or prior parameters of prior distributions. */
/* W: Prior Wishart scaling matrix */
/*  $\nu$ : Degrees of freedom on Wishart distribution */
/*  $\alpha$ : Prior Dirichlet parameter */
/*  $\beta$ : Prior scale on precisions for normal distribution */
/* tolerance: Lower bound change tolerance to indicate convergence. */
/* maxIter: Maximum number of iterations allowed. */
Input: W,  $\nu$ ,  $\alpha$ ,  $\beta$ , tolerance, maxIter
/*  $\pi$ : Expected weights */
/* means: Expected means */
/*  $\Lambda$ : Expected precisions. */
/* resp: Responsibilities. */
Output:  $\pi$ , means,  $\Lambda$ , resp
/* Initialize all parameters. Often uses KMeans clustering to generate means and
   covariances for prior distributions. */
initialization();
lowerBoundPrior  $\leftarrow$   $-\infty$ ;
for  $i \leftarrow 2$  to  $n$  do
    /* Variational E-Step: */
    logPi  $\leftarrow$  updateExpectedLogPi(); // Log weights
    logLambda  $\leftarrow$  updateExpectedLogLambda(); // Expected log determinant of precisions
    resp  $\leftarrow$  estimateResponsibilities(); // Calculate component responsibilities.

    /* Variational M-Step: */
     $N_k, x_{bar_k}, S_k \leftarrow$  estimateGaussianStatistics(resp); // Calculates current component
        association, means, and covariances
     $\alpha \leftarrow$  updateDirichletPriorParameter( $N_k$ ); // Updates current dirichlet parameter
     $\nu \leftarrow$  updateWishartPriorParameters( $N_k$ ); // Updates component degrees of freedom.
     $\beta \leftarrow$  updateGaussianPriorParameters( $N_k$ ); // Updates beta precision scaling for each
        component.
     $\pi \leftarrow$  estimateWeights( $N_k$ ); // Updates current weights.
    means  $\leftarrow$  estimateMeans( $N_k, x_{bar_k}$ ); // Updates current means.
     $\Lambda \leftarrow$  calculatePrecisionsCholesky(estimateWishartMatrix( $N_k, x_{bar_k}, S_k$ )); // Updates
        precisions from estimated Wishart matrix

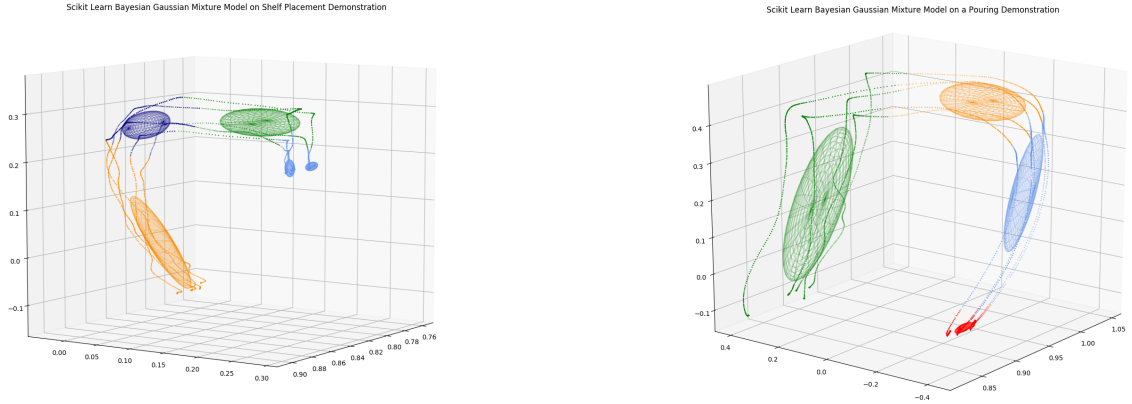
    /* Check for convergence: */
    lowerBoundCurr  $\leftarrow$  calculateELBO(logPi, logLambda, resp,  $\alpha$ ,  $\beta$ , means,  $\Lambda$ ); if
        abs(lowerBoundPrior - lowerBoundCurr)  $\leq$  tolerance then
            break;
        end
end
return  $\pi$ , means,  $\Lambda$ , resp;

```

Algorithm 1: Variational EM algorithm.

Project Level Results and Discussion

This project originally sought to emulate the the work of [3] but incorporate the use of conceptual constraints from my own prior work [6]. What the project was able to accomplish is a generation of a a sequence of broad segments using the variational Gaussian Mixture Model which automatically select the number of components. The following outlines the progress made towards each project level:



(a) Mixand ellipsoids overlayed on 5 trajectories of demonstrations of placing an object onto a shelf.

(b) Mixand ellipsoids overlayed on 5 trajectories of demonstrations of a pouring task.

Figure 3: Example of project model fitted onto actual Sawyer trajectory demonstration data two tasks.

Level 1

While implementation woes prevented much progress towards the stated goal of expanding upon the work of [3], the project does successfully reach most of the stated Level 1 goals:

- Implement variational expectation-maximization-like algorithm for the variational model.
- Compare output of implementation to expected results on Old Faithful data set.

The project employs a successful implementation of a Variational Gaussian Mixture Model, mirrors established clustering on the Old Faithful data set (Figure 2a), produces adequate lower bounds increase (Figure 2b), and, lastly, provides reasonable autonomous segmentation of existing demonstration trajectory data from prior work done in [6]. For the lower bound, two approaches were attempted for the lower bound. One used the lower bound equations in chapter 10 of [4], verbatim, but could not successfully integrate with the chosen implementation of using Cholesky decomposed precision matrices in lieu of the standard Wishart scaling matrix. As such, the successful implementation mirrors Scikit-Learn's BayesianGaussianMixture class implementation, and uses the same simplified lower bound / ELBO functions.

Level 2

For level two, the project only managed to reach one goal:

- Use model on robot trajectory demonstration data used in the experiments conducted by Mueller et. al [6].

The variational Gaussian Mixture model provided quite intuitive segmentation based on the mixands (See Figures 3a & 3b). For this project, the model only uses end-effector (X, Y, Z) position and thus the segmentation is inherently confined to variations in trajectories based on the scope of the state data. However, the model successfully segments broad motor movements that outline changes the dynamics of the end-effector movement, as well as segments where the end effector shows little variation in its position. This is usually when the end-effector is doing high-precision movement (pouring or placing the object) but is

localized in a tight X, Y, Z space. This type of dynamics-based segmentation seems to validate the Transition State Clustering approach of [3].

Unfortunately, the planned MIME data set modeling to not come to fruition. The data set only uses robot joint position for the Baxter robot. While the model could be run on this data, running forward kinematics to create easily visualized end-effector data was not possible in the remaining time since updating the project's goals. However, software development kits do exist that could allow this same approach on the Baxter data. This would provide a larger data set to evaluate the segmentation approach.

Level 3

Unfortunately, I did not make any progress towards my level 3 goals. One continued approach to advance this project towards a more substantial research endeavour would be to develop a mechanisms to easily distinguish high variation broad movements from low variation (with respect to euclidean end-effector space) that indicate high precision movements. This would enable a system to autonomously deconstruct a task from a low-level perspective in order to build a more abstracted representation of the task. Additionally, the models do not directly incorporate conceptual constraints. Encoding constraints and generating meaningful segmentation is a next avenue of research. Determining how to encode constraints into the Transition States outlined in [3] will be a challenging extension to explore next.

Conclusion

I learned a tremendous amount completing this project. I learned how to represent a problem from my research domain as a graphical model. While the model I used was well-established and studied, learning how to apply an existing problem to fit such a model is a tremendous skill to learn. Likewise, I've developed an appreciation for Bayesian approaches to inference and the awesome expressive power they provide over standard expectation maximization approaches.

My advice to those following in my footsteps with regards to Probabilistic Modeling is to not trust the implementations of examples throughout the internet. Only by really deconstructing the algorithms with a deep understanding can one be certain that their own implementation is theoretically correct. This is something I failed to fully accomplish with respect to the evidence lower bound calculation. While I understand and implemented the equations outlined in Bishop's book, my own implementation was different than that used by Scikit-Learn. However, I feel confidence that I am armed with enough knowledge to fully deconstruct the ELBO calculation, and any other probabilistic model.

Thank you for offering such a great course. It was one of my favorites thus far in my graduate career.

Technical Contributors

All technical contributions will be completed by yours truly, Carl Mueller, as I am doing this project by myself.

References

- [1] Zoubin Ghahramani and Michael I Jordan. Supervised learning from incomplete data via an em approach. In *Advances in neural information processing systems*, pages 120–127, 1994.
- [2] Sang Hyoungh Lee, Il Hong Suh, Sylvain Calinon, and Rolf Johansson. Autonomous framework for segmenting robot trajectories of manipulation task. *Autonomous robots*, 38(2):107–141, 2015.
- [3] Sanjay Krishnan, Animesh Garg, Sachin Patil, Colin Lea, Gregory Hager, Pieter Abbeel, and Ken Goldberg. Transition state clustering: Unsupervised surgical trajectory segmentation for robot learning. *The International Journal of Robotics Research*, 36(13-14):1595–1618, 2017.
- [4] Christopher M Bishop. *Pattern recognition and machine learning*. springer, 2006.

- [5] David M Blei, Alp Kucukelbir, and Jon D McAuliffe. Variational inference: A review for statisticians. *Journal of the American Statistical Association*, 112(518):859–877, 2017.
- [6] Carl Mueller, Jeff Venicx, and Bradley Hayes. Robust robot learning from demonstration and skill repair using conceptual constraints. In *2018 IEEE/RSJ International Conference on Intelligent Robots and Systems (IROS)*, pages 6029–6036. IEEE, 2018.

Appendix A: Code

```

1 import numpy as np
2 from scipy import linalg
3 from scipy.special import digamma, logsumexp, gammaln, multigammaln
4 from sklearn.cluster import KMeans
5
6
7 def compute_precisions_cholesky(covariances):
8     # Pulled from sci-kit learn.
9     n_components, n_features, _ = covariances.shape
10    precisions_chol = np.empty((n_components, n_features, n_features))
11    for k, covariance in enumerate(covariances):
12        try:
13            cov_chol = linalg.cholesky(covariance, lower=True)
14        except linalg.LinAlgError:
15            raise ValueError(
16                "Error. Collapsed samples. Try decreasing number of components or ...
17                increasing regularization.")
18        precisions_chol[k] = linalg.solve_triangular(cov_chol,
19                                                    np.eye(n_features),
20                                                    lower=True).T
21
22    return precisions_chol
23
24 def _compute_log_det_cholesky(matrix_chol, n_features):
25     """Compute the log-det of the cholesky decomposition of matrices.
26
27     Parameters
28     -----
29     matrix_chol : array-like
30         Cholesky decompositions of the matrices.
31         'full' : shape of (n_components, n_features, n_features)
32         'tied' : shape of (n_features, n_features)
33         'diag' : shape of (n_components, n_features)
34         'spherical' : shape of (n_components,)
35
36     covariance_type : {'full', 'tied', 'diag', 'spherical'}
37
38     n_features : int
39         Number of features.
40
41     Returns
42     -----
43     log_det_precision_chol : array-like, shape (n_components,)
44         The determinant of the precision matrix for each component.
45     """
46
47     n_components, _, _ = matrix_chol.shape
48     log_det_chol = (np.sum(np.log(
49         matrix_chol.reshape(
50             n_components, -1)[: , :n_features + 1]), 1))
51
52     return log_det_chol
53
54 def _log_dirichlet_norm(dirichlet_concentration):
55     """Compute the log of the Dirichlet distribution normalization term.

```



```

55     Parameters
56     -----
57     dirichlet_concentration : array-like, shape (n_samples,)
58         The parameters values of the Dirichlet distribution.
59
60     Returns
61     -----
62     log_dirichlet_norm : float
63         The log normalization of the Dirichlet distribution.
64     """
65     return (gammaln(np.sum(dirichlet_concentration)) -
66            np.sum(gammaln(dirichlet_concentration)))
67
68
69 def _log_wishart_norm(degrees_of_freedom, log_det_precisions_chol, n_features):
70     """Compute the log of the Wishart distribution normalization term.
71
72     Parameters
73     -----
74     degrees_of_freedom : array-like, shape (n_components,)
75         The number of degrees of freedom on the covariance Wishart
76         distributions.
77
78     log_det_precision_chol : array-like, shape (n_components,)
79         The determinant of the precision matrix for each component.
80
81     n_features : int
82         The number of features.
83
84     Return
85     -----
86     log_wishart_norm : array-like, shape (n_components,)
87         The log normalization of the Wishart distribution.
88     """
89     # To simplify the computation we have removed the np.log(np.pi) term
90     return -(degrees_of_freedom * log_det_precisions_chol +
91            degrees_of_freedom * n_features * .5 * np.log(2.) +
92            np.sum(gammaln(.5 * (degrees_of_freedom -
93                               np.arange(n_features)[:, np.newaxis])), 0))
94
95
96 class VariationalGMM():
97
98     def __init__(self, n_components=3, max_iter=200, tolerance=1e-6, alpha_prior=None, ...
99                 wishart_matrix_prior=None, weights_prior=None, means_prior=None, ...
100                 covariances_prior=None,
101                 regularization=1e-6):
102         self.n_components = n_components # Number of mixture components (K)
103         self.max_iter = max_iter # number of iterations to run iterative update of ...
104         self.varational_inference
105         self.tolerance = tolerance # Log-likelihood tolerance for terminating EM
106         self.alpha_prior = alpha_prior # Dirichlet parameter for prior of weights. (1, K)
107         self.beta_prior = beta_prior # scaling on precisions matrix.
108         self.wishart_matrix_prior = wishart_matrix_prior
109         self.dof = dof # degrees of freedom for Wishart distribution
110         self.covariances_prior = covariances_prior # Initial covariances of mixands.
111         self.weights_prior = weights_prior # Initial weights of mixands
112         self.means_prior = means_prior # Initial means of mixands
113         self.regularization = regularization
114         self.fitted = False
115
116     def _initialize_parameters(self, X):
117         self.n_samples_ = np.shape(X)[0] # number of samples
118         self.n_features_ = np.shape(X)[1] # number of features
119         self.alpha_prior = 1. / self.n_components
120         self.alpha_k = np.full([self.n_components, ], self.alpha_prior) # dirichlet ...
121         parameters

```

```

119     self.means_prior = np.mean(X, axis=0)
120     self.weights = self.weights_prior if self.weights_prior is not None else np.diag(
121         np.random.uniform(0, 1, self.n_components))
122     self.beta_k = np.full(self.n_components, self.beta_prior) # scale of precision ...
123         matrix.
124     self.log_pi = digamma(self.alpha_k) - digamma(np.sum(self.alpha_k))
125     self.log_lambda = np.zeros(self.n_components)
126     self.dof = self.dof if self.dof is not None else self.n_features_
127     self.nu_k = np.full([self.n_components, ], self.dof)
128     self.W_k = np.zeros(
129         [self.n_components, self.n_features_, self.n_features_]) # scaling matrix of ...
130         wishart distribution
131     self.W_lb = np.zeros(
132         [self.n_components, self.n_features_,
133         self.n_features_]) # Collects inverse Wishart scaling matrices for use in ...
134         lowerbound
135     self.W_prior = self.wishart_matrix_prior if self.wishart_matrix_prior is not None ...
136         else np.atleast_2d(
137         np.cov(X.T))
138     self.W_prior.inv = np.linalg.inv(self.W_prior) # Inverse of initial wishart component
139     self._kmeans.initialize(X)
140
141     def _kmeans.initialize(self, X):
142         kmeans = KMeans(n_clusters=self.n_components, n_init=1,
143             random_state=None).fit(
144             X)
145         resp = np.zeros((self.n_samples_, self.n_components))
146         resp[np.arange(self.n_samples_), kmeans.labels_] = 1
147         self.means = kmeans.cluster_centers_.T
148         self._initialize(X, resp)
149
150     def _initialize(self, X, resp):
151         """Initialization of the mixture parameters.
152
153         Parameters
154         -----
155         X : array-like, shape (n_samples, n_features)
156
157         resp : array-like, shape (n_samples, n_components)
158         """
159         N_k, x_bar_k, S_k = self._estimate_gaussian_statistics(X, resp)
160         self._update_dirichlet_prior_parameter(N_k)
161         self._update_wishart_prior_parameters(N_k)
162         self._update_gaussian_prior_parameters(N_k)
163         self._estimate_weights(N_k)
164         self._estimate_means(N_k, x_bar_k)
165         self._estimate_wishart_matrix(N_k, x_bar_k, S_k)
166
167     def e_step(self, X):
168         self._update_expected_log_pi()
169         self._update_expected_log_lambda()
170         # In the variational E step, the ultimate goal is to calculate the responsibilities.
171         return self.estimate_responsibilities(X)
172
173     def m_step(self, X, resp):
174         N_k, x_bar_k, S_k = self._estimate_gaussian_statistics(X, resp)
175         self._update_dirichlet_prior_parameter(N_k)
176         self._update_wishart_prior_parameters(N_k)
177         self._update_gaussian_prior_parameters(N_k)
178         self._estimate_weights(N_k)
179         self._estimate_means(N_k, x_bar_k)
180         self._estimate_wishart_matrix(N_k, x_bar_k, S_k)
181         return N_k, x_bar_k, S_k
182
183     def fit(self, X):
184         self._initialize_parameters(X)
185
186         self.lower_bounds_ = []

```

```

183     prior_lb = -np.inf
184     for n in range(0, self.max_iter):
185         # E-M Step
186         self.log_resp, self.resp = self.e_step(X)
187         N_k, x_bar_k, S_k = self.m_step(X, self.resp)
188         new_lb = self._compute_lower_bound()
189         # new_lb = self._calculate_lower_bound(N_k, x_bar_k, S_k)
190         # new_lb = self.elbo()
191
192         self.lower_bounds.append(new_lb)
193         if abs(new_lb - prior_lb) <= self.tolerance:
194             print("Converged.")
195             break
196         prior_lb = new_lb
197     if abs(new_lb - prior_lb) > self.tolerance:
198         print("Algorithm maximum iterations inadequate to achieve convergence ...
199             according to given tolerance.")
200     self.log_resp, self.resp = self.e_step(X)
201     self.fitted = True
202     return self
203
204 def predict(self, X):
205     if self.fitted is True:
206         return self.get_weighted_log_probability(X).argmax(axis=1)
207     else:
208         raise RuntimeError("Model not fitted.")
209
210 def estimate_responsibilities(self, X):
211     log_rho_nk = self.get_weighted_log_probability(X)
212     Z = logsumexp(log_rho_nk, axis=1)
213     log_resp = log_rho_nk - Z[:, np.newaxis]
214     resp = np.exp(log_resp)
215     return log_resp, resp
216
217 def log_gauss(self, X):
218     # Using scikit learns implementation
219
220     # Get the log determinant of the Cholesky decomposed precisions.
221     log_det_chol = (np.sum(np.log(
222         self.precisions.cholesky.reshape(
223             self.n_components, -1)[:, :self.n_features_ + 1]), 1))
224
225     # Get the log probability of the gaussian
226     log_prob = np.empty((self.n_samples_, self.n_components))
227     for k, (mu, prec_chol) in enumerate(zip(self.means_, self.precisions.cholesky)):
228         y = np.dot(X, prec_chol) - np.dot(mu, prec_chol)
229         log_prob[:, k] = np.sum(np.square(y), axis=1)
230
231     return -.5 * (self.n_features_ * np.log(2 * np.pi) + log_prob) + log_det_chol
232
233 def estimate_log_prob(self, X):
234     # log rho, see Bishop 10.46
235     log_gauss = self.log_gauss(X)
236     return log_gauss + .5 * (self.log_lambda - self.n_features_ / self.beta_k)
237
238 def get_weighted_log_probability(self, X):
239     log_prob = self.estimate_log_prob(X)
240     weighted_log_prob = log_prob + self.log_pi
241     return weighted_log_prob
242
243 def _estimate_gaussian_statistics(self, X, resp):
244     S_k = np.zeros(
245         [self.n_components, self.n_features_, self.n_features_]) # estimated ...
246                             # covariances of the components
247     N_k = np.sum(resp,
248         axis=0) + 1e-10 # from Bishop 10.51, sum or responsibilities for ...
249                             # each component i.e. number of data samples in each component
250     x_bar_k = np.dot(resp.T, X) / N_k[:, np.newaxis] # Bishop 10.52

```

```

248     for k in range(0, self.n_components):
249         x_cen = X - x_bar_k[k]
250         S_k[k] = np.dot(resp[:, k] * x_cen.T, x_cen) / N_k[k] # Bishop equation 10.53
251         S_k[k].flat[:, self.n_features_ + 1] += self.regularization
252     return N_k, x_bar_k, S_k
253
254 def _update_dirichlet_prior_parameter(self, N_k):
255     self.alpha_k = self.alpha_prior + N_k # from Bishop 10.58
256
257 def _estimate_weights(self, N_k):
258     self.weights = (self.alpha_prior + N_k) / (
259         self.n_components * self.alpha_prior + self.n_samples_) # Bishop 10.69
260     # self.weights = (self.alpha_prior + N_k) # scikit learn doesn't divide by ...
261     # anything...why?
262
263 def _update_wishart_prior_parameters(self, N_k):
264     self.nu_k = self.dof + N_k # from Bishop 10.63 and according to sci-kit learn, it ...
265     # shouldn't have the +1
266
267 def _update_gaussian_prior_parameters(self, N_k):
268     self.beta_k = self.beta_prior + N_k # from Bishop 10.60
269
270 def _estimate_means(self, N_k, x_bar_k):
271     self.means = (self.beta_prior * self.means_prior + N_k[:, np.newaxis] * x_bar_k) / ...
272     self.beta_k[:, np.newaxis] ...
273     # ...
274     # ...
275     from ...
276     Bishop ...
277     10.61
278
279     self.means_ = self.means
280
281 def _estimate_wishart_matrix(self, N_k, x_bar_k, S_k):
282     for k in range(0, self.n_components):
283         mean_diff = x_bar_k[k] - self.means_prior
284         self.W_k[k] = (self.W_prior + N_k[k] * S_k[k] + N_k[k] * self.beta_prior \
285             / self.beta_k[k] * np.outer(mean_diff,
286                 mean_diff)) # from Bishop 10.62
287         self.W_lb[k] = np.linalg.inv(self.W_k[k])
288         self.W_k /= self.nu_k[:, np.newaxis, np.newaxis]
289         self.covariances_ = self.W_k
290         self.precisions_cholesky_ = compute_precisions_cholesky(self.covariances_)
291
292 def _update_expected_log_pi(self):
293     self.log_pi = digamma(self.alpha_k) - digamma(np.sum(self.alpha_k)) # from Bishop ...
294     10.66
295
296 def _update_expected_log_lambda(self):
297     for k in range(0, self.n_components):
298         digamma_sum = 0
299         for i in range(1, self.n_features_ + 1):
300             digamma_sum += digamma((self.nu_k[k] + 1 - i) / 2)
301         self.log_lambda[k] = digamma_sum + self.n_features_ * np.log(2) + ...
302         np.log(np.linalg.det(self.precisions_cholesky_[k])) # from Bishop 10.65
303
304 def logB(self, W, nu):
305     n_col = np.shape(W)[1]
306
307     gamma_sum = 0
308     for i in range(1, n_col + 1):
309         gamma_sum += gammaln(0.5 * (nu + 1 - i))
310     # Compute logB function via Bishop B.79
311     return (-0.5 * nu * np.log(np.linalg.det(W)) - (0.5 * nu * n_col * np.log(2) + ...
312         0.25 * n_col * (n_col - 1) *
313         np.log(np.pi) + gamma_sum))

```

```

305
306 def _calculate_lower_bound(self, N_k, x_bar_k, S_k):
307     # DECREASES
308     log_px = 0
309     log_pml = 0
310     log_pml2 = 0
311     log_qml = 0
312     for k in range(0, self.n_components):
313         # Here we collect all terms that require summations index by the k-th component.
314         diff = x_bar_k[k] - self.means[k]
315         # see Bishop 10.71; we remove (- self.n_features_ * np.log(2 * np.pi)) since ...
316         # it is an additive constant.
317         log_px = log_px + N_k[k] * (
318             self.log_lambda[k] - self.n_features_ / self.beta_k[k] - self.nu_k[k] ...
319             * np.trace(
320                 np.dot(S_k[k], self.W_lb[k])) - self.nu_k[k] * np.dot(
321                 np.dot(diff, self.W_lb[k]), diff) - self.n_features_ * np.log(2 * np.pi)
322
323         # see Bishop 10.74
324         log_pml = log_pml + self.n_features_ * np.log(self.beta_prior / (2 * np.pi)) + ...
325         self.log_lambda[k] - \
326         (self.n_features_ * self.beta_prior) / self.beta_k[k] - ...
327         self.beta_prior * self.nu_k[k] * np.dot(
328         np.dot(np.transpose(self.means[k] - self.means_prior),
329             self.W_lb[k]), self.means[k] - self.means_prior)
330
331         # see Bishop 10.74
332         log_pml2 = log_pml2 + self.nu_k[k] * np.trace(np.dot(self.W_prior_inv, ...
333             self.W_lb[k]))
334
335         # see Bishop 10.77
336         log_qml = log_qml + 0.5 * self.log_lambda[k] + 0.5 * self.n_features_ * np.log(
337             self.beta_k[k] / (2 * np.pi)) \
338             - 0.5 * self.n_features_ - (-self.logB(W=self.W_lb[k], ...
339             nu=self.nu_k[k]) \
340             - 0.5 * (self.nu_k[k] - self.n_features_ ...
341             - 1) * self.log_lambda[
342             k] + 0.5 * self.nu_k[
343             k] * self.n_features_)
344
345         log_px = 0.5 * log_px # see Bishop 10.71
346         log_pml = 0.5 * log_pml + self.n_components * self.logB(W=self.W_prior, ...
347             nu=self.dof) + 0.5 * (
348             self.dof - self.n_features_ - 1) * np.sum(self.log_lambda) - 0.5 * ...
349             log_pml2 # see Bishop 10.74
350         log_pz = np.sum(np.dot(self.resp, self.log_pi)) # see Bishop 10.72
351         log_qz = np.sum(self.resp * self.log_resp) # 10.75
352         log_pp = np.sum((self.alpha_prior - 1) * self.log_pi) + ...
353             gammaln(np.sum(self.n_components * self.alpha_prior)) - \
354             self.n_components * np.sum(gammaln(self.alpha_prior)) # 10.73
355
356         log_qp = np.sum((self.alpha_k - 1) * self.log_pi) + gammaln(np.sum(self.alpha_k)) ...
357             - np.sum(
358             gammaln(self.alpha_k)) # 10.76
359
360         # Sum all parts to compute lower bound\
361         print(log_px + log_pz + log_pp + log_pml - log_qz - log_qp - log_qml)
362         return log_px + log_pz + log_pp + log_pml - log_qz - log_qp - log_qml
363
364 def elbo(self):
365     # ELBO: evidence lower bounds in order to test for convergence.
366     # DECREASES
367     lb = gammaln(np.sum(self.alpha_prior)) - np.sum(gammaln(self.alpha_prior)) \
368         - gammaln(np.sum(self.log_lambda)) + np.sum(gammaln(self.log_pi))
369     lb -= self.n_samples_ * self.n_features_ / 2. * np.log(2. * np.pi)
370     for k in range(0, self.n_components):
371         lb += (- (self.dof * self.n_features_ * np.log(2.) / 2.) \

```

```

362         + ((self.nu.k[k] * self.n.features_ * np.log(2.)) / 2.)
363     lb += - multigammaln(self.dof / 2., self.n.features_) \
364         + multigammaln(self.nu.k[k] / 2., self.n.features_)
365     lb += (self.n.features_ / 2.) * np.log(np.absolute(self.beta_prior)) \
366         - (self.n.features_ / 2.) * np.log(np.absolute(self.beta.k[k]))
367     lb += (self.dof / 2.) * np.log(np.linalg.det(self.W_prior)) \
368         - (self.nu.k[k] / 2.) * np.log(np.linalg.det(self.W.lb[k]))
369     lb -= np.dot(np.log(self.alpha.k[k]).T, self.alpha.k[k])
370     return lb
371
372 def _compute_lower_bound(self):
373     """Estimate the lower bound of the model.
374
375     The lower bound on the likelihood (of the training data with respect to
376     the model) is used to detect the convergence and has to decrease at
377     each iteration.
378
379     Parameters
380     -----
381     X : array-like, shape (n_samples, n_features)
382
383     log_resp : array, shape (n_samples, n_components)
384         Logarithm of the posterior probabilities (or responsibilities) of
385         the point of each sample in X.
386
387     log_prob_norm : float
388         Logarithm of the probability of each sample in X.
389
390     Returns
391     -----
392     lower_bound : float
393     """
394     # Contrary to the original formula, we have done some simplification
395     # and removed all the constant terms.
396     n_features, = self.means_prior.shape
397
398     # We removed `.5 * n_features * np.log(self.degrees_of_freedom)`
399     # because the precision matrix is normalized.
400     log_det_precisions_chol = (_compute_log_det_cholesky(
401         self.precisions_cholesky_, n_features) -
402         .5 * n_features * np.log(self.nu.k))
403
404
405     log_wishart = np.sum(_log_wishart_norm(
406         self.nu.k, log_det_precisions_chol, n_features))
407
408     log_norm_weight = _log_dirichlet_norm(self.alpha.k)
409
410     return (-np.sum(np.exp(self.log_resp) * self.log_resp) -
411            log_wishart - log_norm_weight -
412            0.5 * n_features * np.sum(np.log(self.beta.k)))

```