

Exam Review

Rebecca C. Steorts, Duke University

STA 325

Announcements

Exam 2: Released Monday, November 18th. Due Monday November 25th.

Exam 3: Released Monday, December 2. Due Friday December 6.

Questions for the Class

- ▶ Would you like the exam released earlier to have more time to work on it and to ask questions to me on Monday, Wednesday, and Friday (as well as the teaching assistants)?
- ▶ What would be the most helpful?
- ▶ What else can we provide to provide support?
- ▶ I will also post some optional lecture slides in case you wish to learn about some other machine learning methods in case you finish the materials early.

What is clustering?

Clustering is an unsupervised method that divides up data into groups (clusters), so that points in any one group are more similar to each other than to points outside the group.

When might we want to use clustering?

One practical application of clustering is recommender systems, where one clusters users with similar viewing patterns on Netflix/Hulu, etc.

What are other applications we have seen in class or you have encountered?

Machine Learning Algorithms for Clustering

- ▶ Mixture Models and the EM Algorithm
- ▶ k-means
- ▶ hierarchical clustering
- ▶ how to choose the number of clusters

Agenda

- ▶ In this review, I will focus on mixture models
- ▶ Review Exponential Mixture Models
- ▶ Review Derivation of Estimates
- ▶ How to Code These Models Up

Mixture models can be viewed as probabilistic clustering

- ▶ Mixture models put similar data points into “clusters”.
- ▶ This is appealing as we can potentially compare different probabilistic clustering methods by how well they predict (under cross-validation).
- ▶ This contrasts other methods such as k-means and hierarchical clustering as they produce clusters (and not predictions), so it's difficult to test if they are correct/incorrect.

Resources

One resource that is a tutorial on mixture models is the following:
<https://arxiv.org/pdf/1901.06708>

The derivations are adapted from the authors' materials.

Mixture Model

Assume that we have a mixture of K exponential distributions.

Following the notation in the article, assume that

$$g_k(x, \lambda_k) = \lambda_k e^{-\lambda_k x}, x > 0$$

From equation (1) in the article, it follows that

$$f(x, \lambda_1, \dots, \lambda_K) = \sum_{k=1}^K \pi_k \lambda_k e^{-\lambda_k x},$$

which is a K -component exponential distribution with rate parameter λ_k and mixing proportions (or weights) π_k .

EM Algorithm

Because the likelihood and log-likelihood is complex for mixture models, we often utilize an algorithm called the expectation-maximization (EM) algorithm to estimate any unknown parameter values.

Properties of the EM Algorithm

1. It's quite general (see the tutorial), so we can apply it to any type of mixture model.
2. It converges to a local minimum but not a global one.
3. It can get stuck depending on the starting value, so this is something to watch out for in practice.
4. We typically monitor convergence of the algorithm using the log-likelihood.

Derivation of the E-Step

From equation (38) in the tutorial, we can update γ_{ik} as follows:

$$\gamma_{ik} = \frac{\pi_k \lambda_k e^{-\lambda_k x_i}}{\sum_{j=1}^K \pi_j \lambda_j e^{-\lambda_j x_i}}$$

What does this step do in words?

Derivation of the M-Step

Using section 3 of the tutorial, we can work with a function $Q()$ that takes advantage of the latent components/variables.

$$Q(\lambda_1, \dots, \lambda_K) = \sum_{i=1}^n \sum_{k=1}^K \gamma_{ik} \log[\pi_k g_k(x_i, \lambda_k)] \quad (1)$$

$$= \sum_{i=1}^n \sum_{k=1}^K \gamma_{ik} \log[\pi_k \lambda_k e^{-\lambda_k x_i}] \quad (2)$$

$$= \sum_{i=1}^n \sum_{k=1}^K \gamma_{ik} [\log \pi_k + \log \lambda_k - \lambda_k x_i] \quad (3)$$

Note that the following constraint must be satisfied $\sum_{k=1}^K \pi_k = 1$.

Derivation of the M-Step

The Lagrangian¹ becomes

$$\mathcal{L}(\lambda, \pi, \alpha) = \sum_{i=1}^n \sum_{k=1}^K [\gamma_{ik} \log \pi_k + \gamma_{ik} \log \lambda_k - \gamma_{ik} \lambda_k x_i] - \alpha \left(\sum_{k=1}^K \pi_k - 1 \right). \quad (4)$$

This implies that

$$\frac{\partial \mathcal{L}}{\partial \lambda_k} = \sum_{i=1}^n \left[\frac{\gamma_{ik}}{\lambda_k} - \gamma_{ik} x_i \right] = 0 \implies \quad (5)$$

$$\frac{\sum_{i=1}^n \gamma_{ik}}{\lambda_k} = \sum_{i=1}^n \gamma_{ik} x_i \implies \quad (6)$$

$$\lambda_k = \frac{\sum_{i=1}^n \gamma_{ik}}{\sum_{i=1}^n \gamma_{ik} x_i} \quad (7)$$

¹This is a constrained optimization problem.

Derivation of the M-Step

There are two approaches we can use to find π_k .

1. Using the tutorial, pg. 7 and equation (41), it follows that

$$\pi_k = \frac{\sum_{i=1}^n \gamma_{ik}}{\sum_{i=1}^n \sum_{j=1}^K \gamma_{ij}} = \frac{1}{n} \sum_{i=1}^n \gamma_{ik},$$

where $\sum_{i=1}^n \sum_{j=1}^K \gamma_{ij} = n$.

2. You can also derive the estimate using the Lagrangian.

Derivation of the M-Step

$$\mathcal{L}(\lambda, \pi, \alpha) = \sum_{i=1}^n \sum_{k=1}^K [\gamma_{ik} \log \pi_k + \gamma_{ik} \log \lambda_k - \gamma_{ik} \lambda_k x_i] - \alpha \left(\sum_{k=1}^K \pi_k - 1 \right).$$

$$\frac{\partial \mathcal{L}}{\partial \pi_k} = \frac{\sum_{i=1}^n \gamma_{ik}}{\pi_k} - \alpha = 0 \implies \quad (8)$$

$$\pi_k = \frac{1}{\alpha} \sum_{i=1}^n \gamma_{ik} \implies \quad (9)$$

$$\sum_{k=1}^K \pi_k = \frac{1}{\alpha} \sum_{k=1}^K \sum_{i=1}^n \gamma_{ik} \implies \quad (10)$$

$$1 = \frac{1}{\alpha} \sum_{k=1}^K \sum_{i=1}^n \gamma_{ik} \implies \quad (11)$$

$$\alpha = \sum_{k=1}^K \sum_{i=1}^n \gamma_{ik} = n \quad (12)$$

Derivation of the M-Step

Putting this together, we find that

$$\pi_k = \frac{\sum_{i=1}^n \gamma_{ik}}{\sum_{i=1}^n \sum_{j=1}^K \gamma_{ij}} = \frac{1}{n} \sum_{i=1}^n \gamma_{ik}.$$

Monitor the expected log-likelihood

Again, recall that

$$Q(\lambda_1, \dots, \lambda_K) = \sum_{i=1}^n \sum_{k=1}^K \gamma_{ik} [\log \pi_k + \log \lambda_k - \lambda_k x_i]$$

Formally, this is the expected log-likelihood, which can be used as an approximation to monitor convergence of the EM algorithm.

We cannot calculate the log-likelihood in closed form, so this is why we monitor changes to the expected log-likelihood.

Monitor the expected log-likelihood

Specifically for an iteration $t + 1$ and t we can monitor

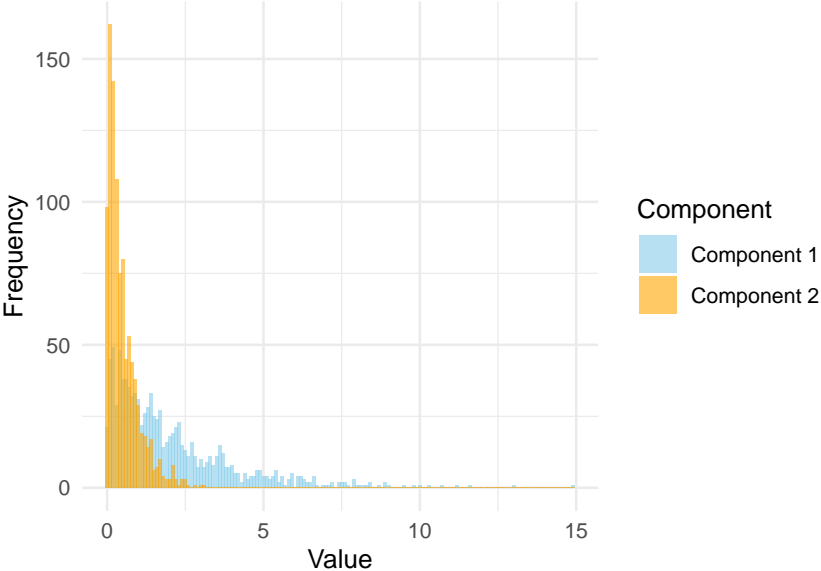
$$\Delta Q^{(t+1)} = |\Delta Q^{(t+1)} - \Delta Q^{(t)}| < \epsilon$$

We often plot the expected log-likelihood versus the number iterations.

Simulation Study

Simulate a two-component exponential mixture model with 2,000 data points. Let the true rates be 0.5 and 2.0. Let the mixing proportions be 0.5 and 0.5.

Simulation Study



Code

```
exponentialMixture <- function(data, K, max_iter = 1000, tol = 1e-5) {  
  n <- length(data)  
  pi <- rep(1/K, K) # mixing proportions  
  lambda <- runif(K, 0.1, 1) # rate parameters  
  
  log_likelihoods <- numeric(max_iter) # store log-likelihood values  
  
  for (iter in 1:max_iter) { # E-step: numerator of the gammas  
    gamma <- matrix(NA, nrow = n, ncol = K)  
    for (k in 1:K) {  
      gamma[, k] <- pi[k] * dexp(data, rate = lambda[k])  
    }  
    row_sums <- rowSums(gamma) # denominator of the gammas  
    gamma <- gamma / row_sums # normalize probabilities  
  
    pi_old <- pi # M-step: Update mixing proportions and rate parameters  
    lambda_old <- lambda  
  
    pi <- colMeans(gamma) # update mixing proportions  
    for (k in 1:K) {  
      lambda[k] <- sum(gamma[, k]) / sum(gamma[, k] * data) # update rate parameters  
    }  
  
    log_likelihoods[iter] <- sum(log(row_sums)) # calculate log-likelihood  
  
    if (max(abs(pi - pi_old)) < tol && max(abs(lambda - lambda_old)) < tol) {  
      log_likelihoods <- log_likelihoods[1:iter] # trim to the number of iterations  
      cat("Convergence reached at iteration", iter,  
          "with log-likelihood:", log_likelihoods[iter], "\n")  
      break  
    }  
  }  
  return(list(pi = pi, lambda = lambda, log_likelihood = log_likelihoods))  
}
```

Results

```
set.seed(1234)
library(knitr)
# Fit the mixture model
result <- exponentialMixture(data, K = 2)

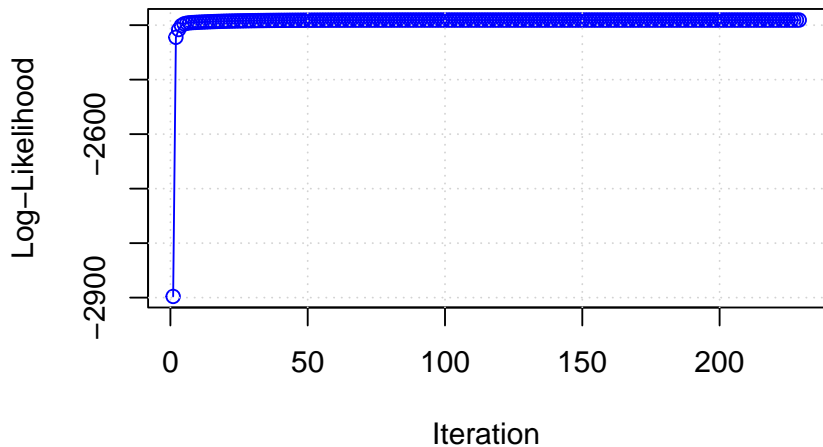
## Convergence reached at iteration 229 with log-likelihood: -2390.612
# Create a data frame to display the results in a table
results_table <- data.frame(
  "Component" = 1:2,
  "Estimated Mixing Proportion" = round(result$pi, 4),
  "Estimated Rate Parameter (lambda)" = round(result$lambda, 4)
)

# move results to a table
kable(results_table, caption = "Estimated Parameters for the Mixture Model", format = "pipe")
```

Table 1: Estimated Parameters for the Mixture Model

Component	Estimated.Mixing.Proportion	Estimated.Rate.Parameter..lambda.
1	0.5135	0.4998
2	0.4865	1.9721

Expected Log-Likelihood Plot



Findings

- ▶ Observe that the parameter estimates are close to the true values.
- ▶ Running this multiple times, should result similar findings and similar estimates each time.
- ▶ Why would the results change even if we re-run things and have a seed?
- ▶ What does the expected log-likelihood plot indicate?

Second Simulation Study

In this part, I am giving you a second simulation study.

Results

The true rate parameters are 0.5 and 1.5. The true mixing proportions are 0.6 and 0.4.

Convergence reached at iteration 720 with log-likelihood: -1383.459

Table 2: Estimated Parameters for the Mixture Model

Component	Estimated.Mixing.Proportion	Estimated.Rate.Parameter..lambda.
1	0.2327	1.9504
2	0.7673	0.5624

Second Simulation Study

Go dig into what you think is going on here!

Next Steps

- ▶ What would you do next for data analysis to investigate this simulation study?
- ▶ How can you utilize this code for the second simulation study?
- ▶ My major recommendation to prepare for the second exam is to go through these review slides and fully understand this material as we have spend a large amount of time on it in and out of class.
- ▶ Exam II will test your knowledge mostly of mixture models to allow you to dig deeply into one problem instead of testing your knowledge at the surface level on many problems.

Exam II

This will look something similar to the exponential exercises that I have released to you, however, most of the code you will have available to make the task easier as this proved to be difficult for students to implement.

Questions?