ESTIMATING THE NUMBER OF COMPONENTS OF A SPATIAL–EM ALGORITHM: AN R PACKAGE

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A thesis submitted to the faculty of The University of Mississippi in partial fulfillment of the requirement of the Sally Mcdonell Barksdale Honors College.

Oxford
May 2015

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ABSTRACT

The Expectation Maximization algorithm also known as the EM algorithm is an algorithm used to solve the maximum likelihood parameter estimation problem. This problem arises when some of the data involved are missing or incomplete, hence it becomes difficult to know the parameters of the underlying distribution. The EM algorithm mainly comprises of two steps; the E–Step, and the M–Step. In the E–Step, estimated parameter values are used as true values to calculate the maximum likelihood estimate, and in the M–Step, the maximum likelihood calculated is used to estimate the parameters. The E–Step and M–Step iterate through until a specified convergence is met. Applications of the EM algorithm include density estimation in unsupervised clustering, estimating class–conditional densities in supervised learning settings, and for outlier detection purposes. The Spatial – EM algorithm is a novel approach that utilizes median – based location and rank – based scatter estimators to replace the sample mean and sample covariance matrix in the M – Step of an EM algorithm. This helps to enhance the stability and robustness of the Spatial – EM algorithm for finite mixture models. The algorithm is especially robust to outliers. In this research, we use the trimmed Bayesian Information Criterion (BIC) to determine the optimal value of the number of components in the distribution. The algorithm is implemented as an R package, and tested on different datasets.

ACKNOWLEDGEMENTS

I would like to express my sincere appreciation to my advisors Dr. Yixin Chen, Dr. Xin Dang, and Dr. Dawn Wilkins. I have been fortunate to have their support during my undergraduate studies. I am very thankful to them for their guidance and advice throughout this thesis. I would also like to express my appreciation to the Sally McDonnell Barksdale College and the Department of Computer and Information Science for offering me the opportunity to research.

Finally, I would like to thank my family for their continuous love and support.

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CHAPTER 1

INTRODUCTION

1.1 Clustering

Clustering is the most common form of unsupervised learning. Unsupervised learning means that there is no authority that has given the true labels of the data. Clustering can be defined as a process of assigning a set of data into its clusters using the distribution and makeup of the data. The major goal of many clustering algorithms is to create clusters such that data in the same cluster are similar, and data in different clusters are dissimilar.

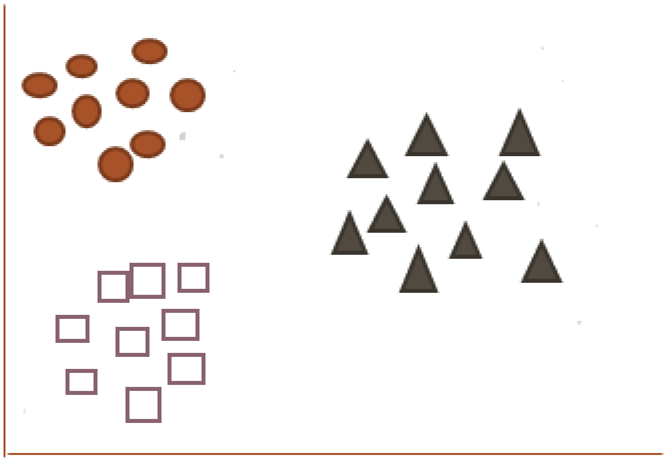


Figure 1.1. Cluster Representation

1.1.1 Clustering Algorithms

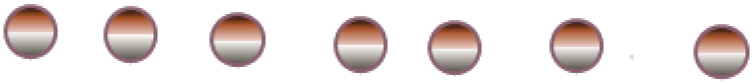
There are mainly two types of clustering algorithms as proposed in [11] namely:

Hard Clustering Algorithms

These algorithms compute a hard assignment i.e. each data is a member of exactly one cluster. An example of a hard clustering algorithm is **K-means**.

Soft Clustering Algorithms

These algorithms compute a soft assignment i.e. each data has a distribution over all the clusters. An example of a soft clustering algorithm is **EM- Algorithm**.



1.1.2 Applications of Clustering

Clustering has many applications in the real–world. Below are a few of the applications of clustering.

1. **Recommender Systems**

   Clustering algorithms are "used to identify groups of consumers who appear to have similar tastes" [14].

2. **Marketing**

   Cluster analysis can be used to identify groups of customers having similar behaviors given a large database of customer data containing their buying preferences.

3. **Insurance**

   Cluster analysis can be used in "Identifying groups of motor insurance policy holders with a high average claim cost; identifying frauds" [2].

4. **Crime Analysis**

   Cluster analysis can be used to identify areas where crime rates are likely to occur by identifying hotspots where a similar crime has happened over time. [16].

5. **Educational Data Mining**

   Students with similar properties can be identified using cluster analysis.[16].

6. **Earthquake Studies**

   Cluster analysis can be used to identify dangerous zones by identifying earthquake epicenters. [2].

Some other applications of clustering include voice mining, image processing, and weather report analysis.

1.2 Expectation Maximization Algorithm

The Expectation Maximization algorithm also known as the EM algorithm is used to solve the maximum likelihood parameter estimation problem. This problem arises when some of the data involved are missing or incomplete. Hence, it becomes difficult to know the parameters of the underlying distribution. The EM algorithm mainly comprises of two steps; the E–Step, and the M–Step. In the E–Step also known as the **Expectation Step**, estimated parameter values are used as true values to calculate the maximum likelihood estimate, and in the M–Step also known as the **Maximization Step**, the maximum likelihood calculated is used to estimate the parameters. The E–Step and M–Step iterate through until a specified convergence is met. Applications of the EM algorithm include density estimation in unsupervised clustering, estimating class–conditional densities in supervised learning settings, and for outlier detection purposes.

1.3 Motivation

The EM algorithm has the problem of being sensitive to outliers, and initial values. To overcome this, various algorithms have been implemented to enhance the robustness of the EM algorithm. Some researchers used a weighted maximum likelihood with low weights to outliers, while others proposed updating the component estimates on the M-Step of the algorithm using some form of robust location and scatter estimates. The Spatial–EM algorithm uses this idea of updating the component estimates on the M–Step of the algorithm using a spatial rank based location and scatter estimate. Spatial refers to the data space and not the geographical space.

1.4 Literature Review

In this section, two papers would be reviewed. These papers explains some of the algorithms developed by researchers to solve the outlier problem of the EM algorithm.

1.4.1 High Breakdown Mixture Discriminant Analysis

Shaheena Bashir, and E.M Carter [3] address the outlier problem of the EM algorithm using a robust S–Estimator in the M–Step of the algorithm. The "parameters estimates obtained are the maximum likelihood estimators of the location vectors and the common covariance matrix which in the presence of outliers, these estimators are non–robust"[3]. The goal of this approach is to replace the M–Step of the algorithm with a robust S–estimator step. The S–estimator estimates a more robust mean and covariance such that there is a high breakdown point. This high breakdown point reduces the sensitivity of the EM algorithm to outliers.

1.4.2 Robust Estimation in the Normal Mixture Model

Fujisawa, and Eguchi [7] approach the outlier problem of the EM algorithm by proposing a β likelihood and a β estimator. This approach was developed because "the maximum likelihood estimator often assigns a certain component to the outlier and causes a single match case. Furthermore, the sensitivity of the maximum likelihood estimator to outlier leads to larger variance, incorrect mixing proportions, and makes statistical inference such as clustering and outlier detection uncertain" [7]. When $\beta = 0$, this is the usual log- likelihood.

In Chapter 2, we propose a new robust algorithm to solve the outlier problem of the EM algorithm. The algorithm proposed is known as the Spatial–EM algorithm.

CHAPTER 2

THE SPATIAL–EM ALGORITHM

2.1 Solution Approach

As stated in [17], a random vector χ is said to follow a K–component mixture distribution if it is characterized by the density function

$$f(x|\theta) = \sum_{j=1}^{K} \tau_j f_j(x|\theta_j)$$

where $f_j(x|\theta_j)$ is the conditional probability density function of x belonging to the j^{th} component which is defined by the parameter θ_j, $\tau_1, ..., \tau_K$ are the mixing proportions with all $\tau_j > 0$ and $\sum_{j=1}^{K} \tau_j = 1$, and $\theta = \{\theta_1, ..., \theta_K, \tau_1, ..., \tau_K\}$ is the set of parameters.

For mixture elliptical distributions, $f(x|\theta_j)$ can be written as

$$f_j(x|\mu_j, \Sigma_j) = |\Sigma_j|^{-\frac{1}{2}} h_j\{(x - \mu_j)^T \Sigma_j^{-1}((x - \mu_j)\},$$

for some $\mu_j \in \mathbb{R}^d$, a positive definite symmetric d × d matrix Σ_j, and a nonnegative function h_j independent to μ_j and Σ_j. μ_j is the symmetric center of the j^{th} component, and Σ_j is proportional to the covariance matrix when it exists. The most widely used mixture elliptical distribution is the mixture of gaussian distributions in which

$$h_j(t) = (2\pi)^{-\frac{d}{2}} e^{-\frac{t}{2}}.$$

Hence, when d=1, and K=1, the conditional probability density function reduces to the standard equation of a normal distribution given by

$$f = \frac{1}{\sigma\sqrt{2\pi}} e^{-\frac{(x-\mu)^2}{2\sigma^2}}$$

In the EM algorithm, the observed sample $\chi = \{x_1, ..., x_n\}$ is viewed as incomplete. The complete data is expressed as $Z = \{x_i, y_i\}_{i=1}^{n}$, where $y_i = (y_{1i}, ..., y_{Ki})^T$ is an unobserved indicator vector with $y_{ji} = 1$ if x_i comes from component j, zero otherwise. Thus,

E–Step: Given χ and the current estimate $\theta^{(t)}$, since Y_{ji} is either 1 or 0, $Pr(Y_{ji} = 1|\theta^{(t)}, x_i)$ is denoted as $T_{ji}^{(t)}$. By the Bayes rule,

$$T_{ji}^{(t)} = \frac{\tau_j^{(t)} f_j(x|\theta_j^{(t)})}{\sum_{i=1}^{K} \tau_j^{(t)} f_j(x|\theta_j^{(t)})}$$

$T_{ji}^{(t)}$'s are the soft labels at the t^{th} iteration.

M–Step:

$$w_{ji}^{(t)} = \frac{T_{ji}^{(t)}}{\sum_{i=1}^{n} T_{ji}^{(t)}}$$

Given a multivariate data χ which is an n x d matrix; where n is the input size, and d is the number of dimensions, we compute a weighted spatial median, and a weighted modified rank covariance matrix. The weighted spatial median is computed from the weighted rank of the matrix. The weighted rank for $x_k \in \chi$ is computed as

$$R_j^{(t)}(x_k) = \sum_{i=1}^{n} w_{ji}^{(t)} \frac{x_k - x_i}{\|x_k - x_i\|}$$

where $\|x_k - x_i\|$ is known as the euclidean norm of the vector $x_k - x_i$.

The weighted spatial median is then computed as

$$\mu_j^{(t+1)} = \arg\min_{x_k} \left\| \sum_{i=1}^{n} w_{ji}^{(t)} \frac{x_k - x_i}{\|x_k - x_i\|} \right\|$$

$\mu_j^{(t+1)}$ is the weighted spatial median for the next iteration.

The weighted modified rank covariance matrix (MRCM) can be computed also from the weighted rank using the formula

$$\Sigma_j^{(t+1)} = \sum_{i=1}^{n} w_{ji}^{(t)} (R_j^{(t)}(x_i))(R_j^{(t)}(x_i))^T$$

The mixture proportion τ for the jth component in the next iteration can be computed using the formula

$$\tau_j^{(t+1)} = \frac{1}{n} \sum_{i=1}^{n} T_{ji}^{(t)}$$

Initial values are assigned such that $\mu_j^{(0)}$ is computed using the K– means, where K is determined from the number of classes in the dataset, and $\Sigma_j^{(0)} = \boldsymbol{I}_{\text{dxd}}$, where **I** is the identity matrix. Spatial–EM iterates until convergence.

2.2 Algorithm

Algorithm 1: Spatial–EM Algorithm

```
1. {Initialization} $\mu_j^{(0)}, \Sigma_j^{(0)} = \mathbb{I}_{d\times d}, \tau_j^{(0)} = 1/K$ for $\forall j, t = 0$
2. Do until $\tau_j^{(t)}$'s converge for all $j$
3.     For $j = 1$ to K
E–Step:
4.         Calculate $T_{ji}^{(t)}$
M–Step:
5.         Update $\tau_j^{(t+1)}$
```

```
        Define $w_{ji}^{(t)}$
        Find $\mu_j^{(t+1)}$
        Find $(\Sigma_j^{(t+1)})^{-1}$ and $|\tilde{\Sigma}_j^{(t+1)}|$ by Algorithm 3
    End
    t=t+1
End
```

Algorithm 2: Compute the weighted spatial median $\mu_j^{(t+1)}$

```
Input $\{x_i\}_{i=1}^n, \{w_{ji}^{(t)}\}_{i=1}^n$
For $l = 1$ to $n$
    $R_j^{(t)}(x_l) = \Sigma_{i=1}^n w_{ji}^{(t)} \boldsymbol{s}(x_l - x_i)$
End
$\mu_j^{(t+1)} = \arg\min_{x_l} \|R_j^{(t)}(x_l)\|$
Output $\{R_j^{(t)}(x_l)\}_{l=1}^n$, $\mu_j^{(t+1)}$
```

Algorithm 3: Compute the inverse of weighted MRCM $\tilde{\Sigma}_j^{(t+1)}$

```
Input $\{R_j^{(t)}(x_i), T_{ji}^{(t)}, w_{ji}^{(t)}\}_{i=1}^n, \mu_j^{(t+1)}, \tau_j^{(t+1)}$
$\Sigma_{R,j}^{(t+1)} = \Sigma_{i=1}^n w_{ji}^{(t)}(R_j^{(t)}(x_i))(R_j^{(t)}(x_i))^T$
Find eigenvectors $U_j = [u_{j,1}, ..., u_{j,d}]$ of $\Sigma_{R,j}^{(t+1)}$
For $m = 1$ to $d$
    $a_m = \{T_{ji}^{(t)} \mu_{j,m}^T (x_i - \mu_j^{(t+1)})\}_{i=1}^n$
    Delete the $\lceil (1 - \tau_j^{(t+1)}) \rceil$ smalles values of $a_m$ denoted as $\{T_{ji_k}^{(t)} \mu_{j,m}^T (x_{i_k} - \mu_j^{(t+1)})\}_{i_k}$
    $\hat{\lambda}_{jm}$=MAD $(\{T_{ji_k}^{(t)} \mu_{j,m}^T (x_{i_k} - \mu_j^{(t+1)})\}_{i_k})$
End
```

9. $\hat{\wedge}_j = \text{diag}\ (\hat{\lambda}^2_{j1}, ..., \hat{\lambda}^2_{jd})$

10. Inverse MRCM $(\tilde{\Sigma}_j^{(t+1)})^{-1} = U_j \hat{\wedge}_j^{-1} U_j^T$

11. Output $(\tilde{\Sigma}_j^{(t+1)})^{-1}$, $\prod_{m=1}^{d}, \hat{\lambda}_{jm}^{-1}$

2.3 Convergence

The Spatial–EM algorithm terminates when the likelihood of successive iterations changes with very small probability (0.0001) compared to the likelihood of the previous iteration, or when the number of iterations reaches a prespecified parameter maxiter. The maxiter is 100 for the Spatial–EM algorithm.

CHAPTER 3

EVALUATION OF THE SPATIAL–EM ALGORITHM

3.1 Comparison with other EM Algorithms

To test the effectiveness of the Spatial EM algorithm, the results computed from the EM algorithm are compared with two other known EM algorithms, the Regular EM algorithm, and the Kotz EM algorithm.

3.1.1 Regular EM

The Regular EM algorithm uses the sample mean and sample covariance to compute the M–Step of the algorithm.

Algorithm: Regular–EM Algorithm

```
1. {Initialization} $\mu_j^{(0)}, \Sigma_j^{(0)} = \mathbb{I}_{d\times d}, \tau_j^{(0)} = 1/K$ for $\forall j, t = 0$
2. Do until $\tau_j^{(t)}$'s converge for all $j$
3.     For $j = 1$ to K
E–Step:
4.         Calculate $T_{ji}^{(t)}$
M–Step:
5.         Update $\tau_j^{(t+1)}$ using the same formula as in the Spatial–EM algorithm
6.         Find $\mu_j^{(t+1)}$ using the formula
               $\mu_j^{(t+1)} = \frac{\sum_{i=1}^n T_{ji}^{(t)} x_i}{\sum_{i=1}^n T_{ji}^{(t)}}$
```

```
7.          Find $\Sigma_j^{(t+1)}$ using the formula
                $\Sigma_j^{(t+1)} = \frac{\sum_{i=1}^{n} T_{ji}^{(t)}(x-\mu_j^{(t+1)})(x-\mu_j^{(t+1)})^T}{\sum_{i=1}^{n} T_{ji}^{(t)}}$
8.      End
9.      t=t+1
10. End
```

3.1.2 Kotz EM

The Kotz EM algorithm uses a Kotz type distribution. A Kotz type distribution is a special type of mixture elliptical distribution studied by Kotz [10] and Fang et.al [6]. The conditional density of a Kotz type distribution is given as

$$f_j(x|\mu_j,\Sigma_j) = |\Sigma_j|^{-\frac{1}{2}} h_j\{(x-\mu_j)^T\Sigma_j^{-1}((x-\mu_j)\},$$

where h_j is given as

$$h_j(t) = \frac{\Gamma(d/2)}{(2\pi)^{d/2}\Gamma(d)} e^{-\sqrt{t}}$$

3.2 Evaluation Metrics

3.2.1 Normalized Mutual Information

The normalized mutual information is the normalized form of the mutual information measure. The Mutual information is an information theory concept which was first introduced by [15]. It measures the mutual dependence between two random variables, i.e., how much information is shared between two random variables. The mutual information is symmetric and always nonnegative. If the two variables are independent, then the mutual information is zero. The normalized mutual information introduces an uncertainty coefficient, **entropy** that determines the degree of association between two variables. This measure is calculated using mutual information and entropy. Let $\boldsymbol{I}$ be mutual information, and $\boldsymbol{H}$ be entropy. Let X and Y be two random variables, then the normalized mutual information between the variables is given by,

$$NMI(X;Y) = \frac{2I(X;Y)}{H(X) + H(Y)}$$

The mutual information is calculated by

$$I(X;Y) = \sum_{y \in Y} \sum_{x \in X} p(x,y) log\left(\frac{p(x,y)}{p(x)p(y)}\right)$$

where $p(x,y)$ is the joint distribution between the two variables, $p(x)$ is the marginal distribution of X, and $p(y)$ is the marginal distribution of Y.

3.2.2 Purity

To compute purity, “each cluster is assigned to the class which is most frequent in the cluster, and then the accuracy of this assignment is measured by counting the number of correctly assigned documents and dividing by N” [11]. The purity can also be used to get the true component that corresponds to the predicted component of a distribution. This is done generally by getting the component with the maximum frequency in the predicted labels given the ground truth. The purity of the distribution is generally calculated as

$$purity(\Omega, \mathbb{C}) = \frac{1}{N} \sum_{k} max_j |\omega_k \cap c_k|$$

$\Omega = \{\omega_1, ..., \omega_k\}$ is the set of components in the distribution and $\mathbb{C} = \{c_1, ..., c_k\}$ are the set of predicted labels belonging to a component in the distribution.

“Bad clusterings have purity values close to 0, a perfect clustering has a purity of 1”[11]. However, purity can be a biased measure when the number of clusters is large. That is, “High purity is easy to achieve when the number of clusters is large in particular, purity is 1 if each document gets its own cluster. Thus, we cannot use purity to trade off the quality of the clustering against the number of clusters" [11].

3.2.3 Rand Index and F–Measure

To calculate the Rand Index and F–Measure, four important concepts need to be explained.

- **True Positive**: The true positive (TP) assigns similar data to the same cluster.
- **False Positive**: The false positive (FP) assigns dissimilar data to the same cluster.
- **True Negative**: The true negative (TN) assigns dissimilar data to different clusters.
- **False Negative**: The false negative (FN) assigns similar data to the different clusters

Below is a figure to show these four concepts

	Same Cluster	Different Cluster
Same Class	TP	FN
Different Class	FP	TN

Table 3.1. Confusion Matrix

Rand Index [13] measures the percentage of the data that are correctly classified, which is the accuracy.

$$RI = \frac{TP + TN}{TP + FP + TN + FN}$$

The Rand Index is not an efficient measure to evaluate a clustering method because "the rand index gives equal weights to false positives and false negatives. This is a problem because sometimes putting similar data in separate clusters is sometimes worse than putting dissimilar data in the same cluster"[11]. To overcome this bias, the F–measure is used.

To understand the **F–measure**, two important concepts need to be understood.

Precision

Precision is the fraction of pairs put in the same cluster. it is calculated as

$$\frac{TP}{TP + FP}$$

Recall

Recall is the fraction of actual pairs that were correctly identified.

$$\frac{TP}{TP + FN}$$

F–measure computes the effectiveness of the algorithm using the precision (P) and recall (R).

$$F_\beta = \frac{(\beta^2 + 1)PR}{\beta^2 P + R}$$

when $\beta = 1$, this is the balanced form of the F–measure. It is the harmonic mean of the precision and recall.

$$F_1 = \frac{2PR}{P + R}$$

Setting β to a higher value can overcome the bias produced by the rand index.

CHAPTER 4

TESTING

4.1 UCI Winsconsin Breast Cancer Dataset

This is the Breast Cancer Wisconsin (Diagnostic) data set in the UCI Machine Learning Repository. This data set is available from *http://archive.ics.uci.edu/ml/datasets*. In this dataset, there are 569 observations from 357 patients with benign tumors and 212 patients with malignant tumors. The dataset is classified using two features : *mean texture* and *extreme area*. Clustering analysis is performed using the Spatial–EM, the Regular–EM, and the Kotz–EM, and the dataset is represented as a **two–component** mixture model. The components of this distribution are malignant and benign.

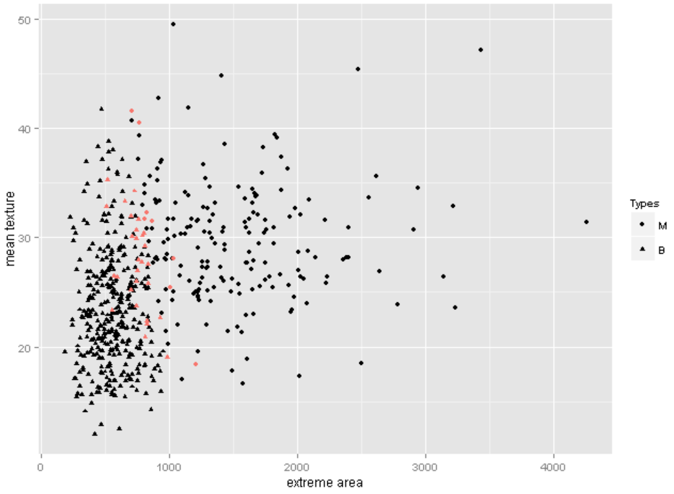


Figure 4.1. Breast Cancer Data (Spatial–EM)

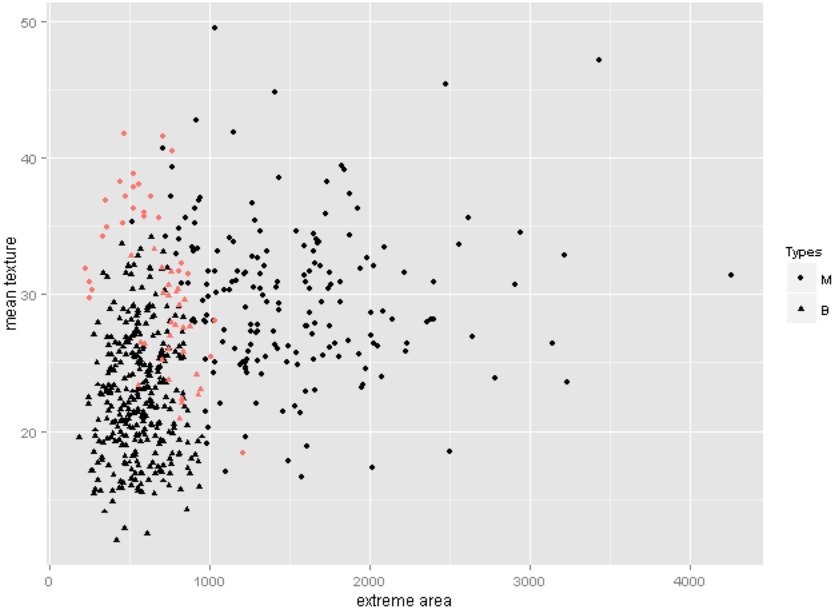


Figure 4.2. Breast Cancer Data (Regular–EM)

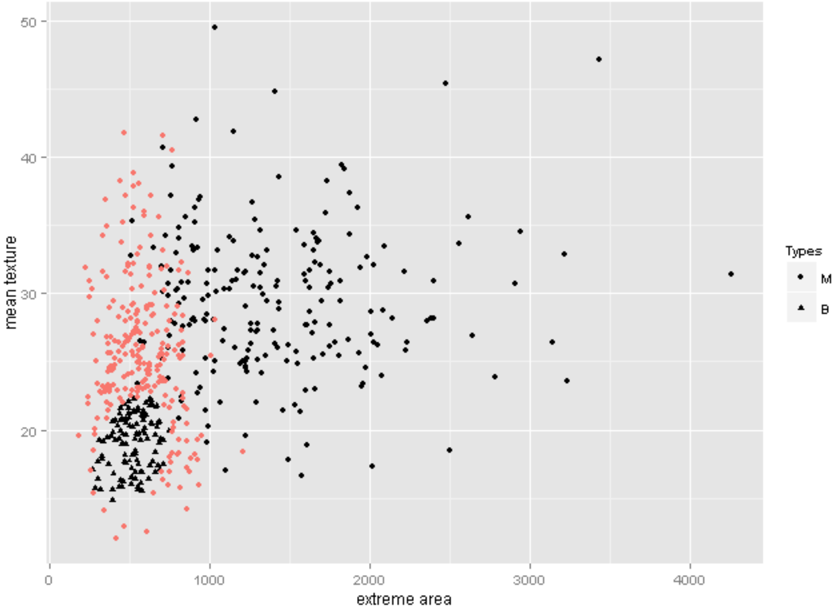


Figure 4.3. Breast Cancer Data (Kotz–EM)

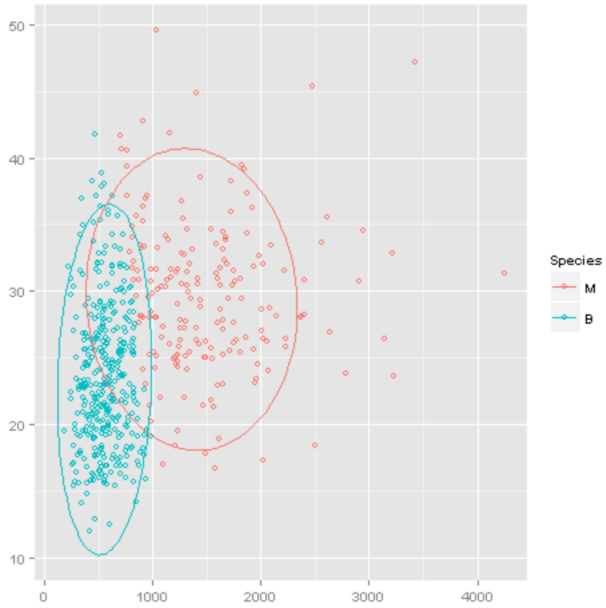


Figure 4.4. Spatial–EM Cluster Plot

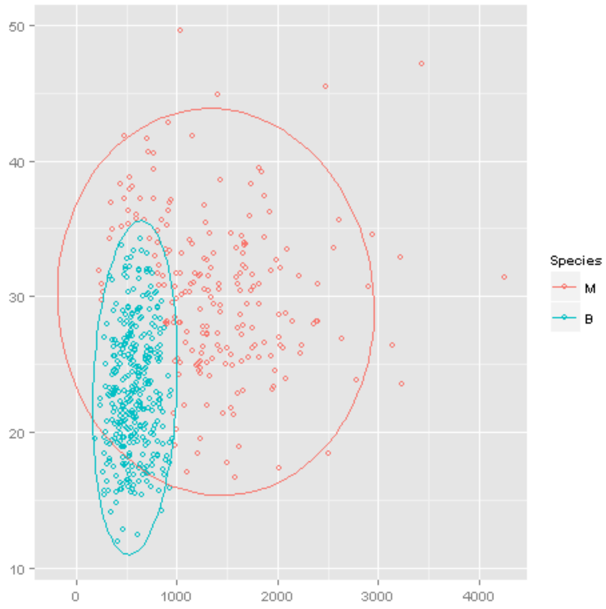


Figure 4.5. Regular–EM Cluster Plot

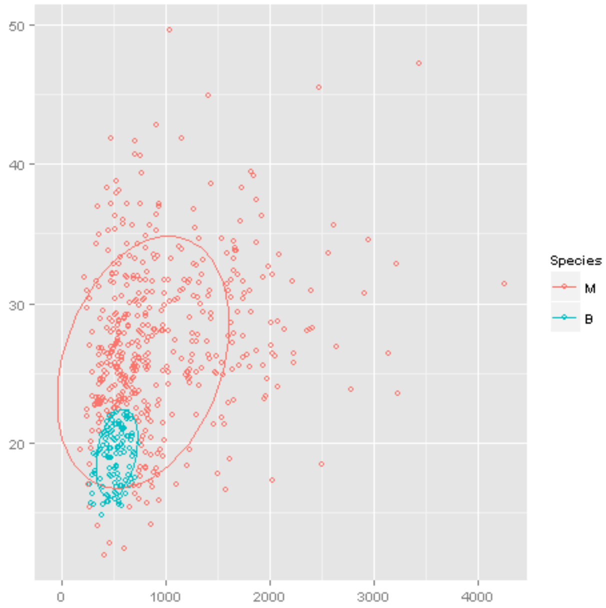


Figure 4.6. Kotz–EM Cluster Plot

4.1.1 Discussion of Results

Figure 4.1, 4.2, and 4.3 show scatter plots of the projection of the UCI Wisconsin diagnostic breast cancer dataset using the two features. ∘ represents benign, and △ represents malignant. The symbols in red represents data that are misclassified. In the health care practice, it is important to be able to correctly classify a patient as having a malignant tumor or a benign tumor. A malignant patient should get more attention, and misclassification can prove fatal especially when a patient with a malignant tumor is classified as benign. From the scatter plots, we can see that the Kotz–EM has a lot of misclassified data compared to the Regular–EM and the Spatial–EM. The results for the classification of this dataset using the three EM algorithms are shown in Table 4.1. From these results, we can see that the Kotz–EM has the lowest Normalized Mutual Information score, and though it has a low False Negative rate, it has a high False Positive rate. Hence, the Kotz–EM is not a good classifier for the breast cancer dataset. On the other hand, the Spatial–EM has a smaller false positive and false negative rate than the Regular–EM. The FPR of

0.0224 of Spatial–EM is around 13 that of Regular–EM. “Medical screening tests that maintain a similar level of FNR but much smaller FPR can save time, money and clinic resource on the follow- up diagnostic procedures and more importantly, relieve unnecessary worries of those false positive diagnostic patients.” [17].

Figure 4.4, 4.5, and 4.6 show cluster plots which represent the 95% probability density contours of each component. This cluster plot provides a visual representation of the data in their clusters or components. The overlap between clusters shows that there are some data whose clusters are really difficult to ascertain.

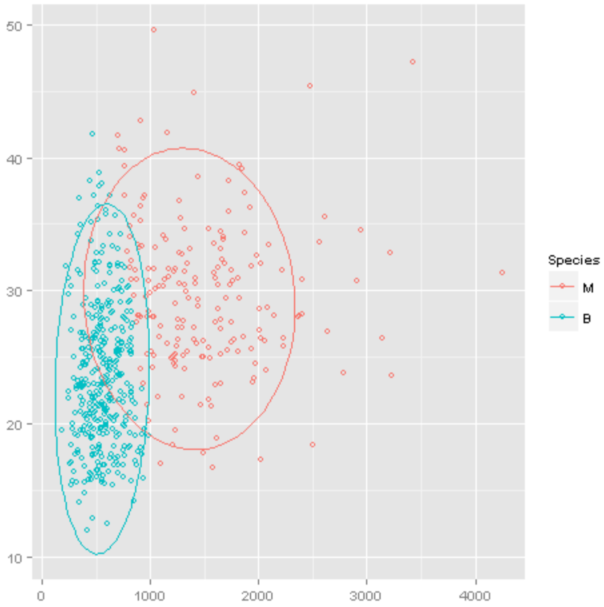


Figure 4.7. Spatial–EM Cluster Plot

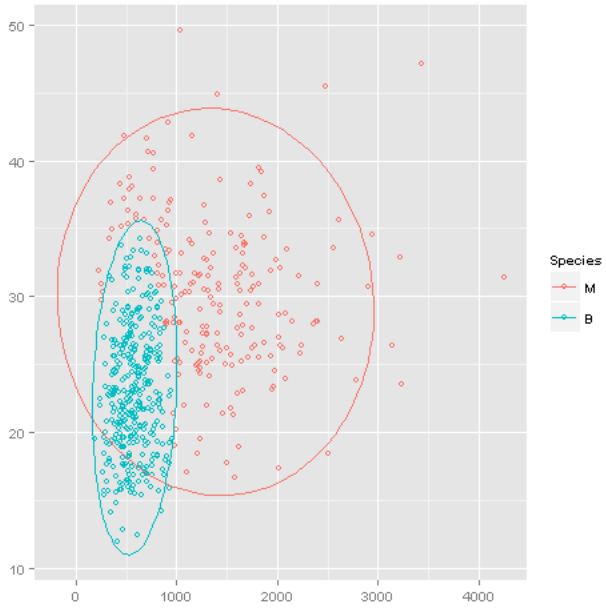


Figure 4.8. Regular–EM Cluster Plot

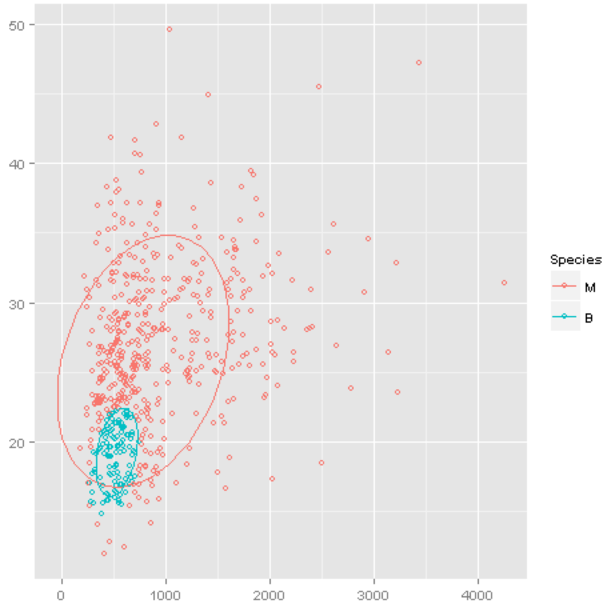


Figure 4.9. Kotz–EM Cluster Plot

	Regular–EM	Spatial–EM	Kotz–EM
FPR	0.07563025	0.02240896	0.32493
FNR	0.13679245	0.13207547	0.00000
NMI	0.51811101	0.6564773	0.1888646

Table 4.1. Classification Results

4.2 Fish Dataset

The Fish dataset is from the Tulane University Museum of Natural History (TUMNH), and contains 2-dimensional landmarks of different views of fishes from the *Catostomidae* family of fishes.

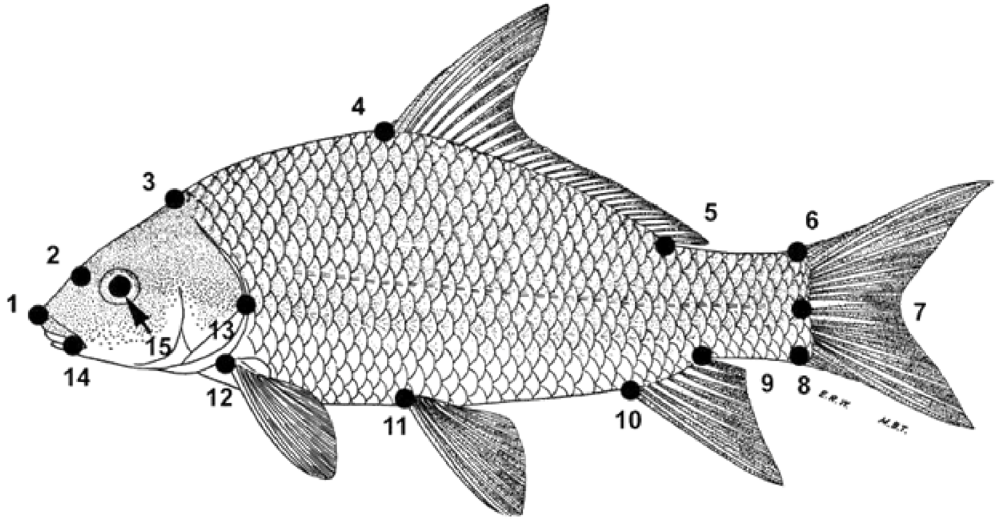
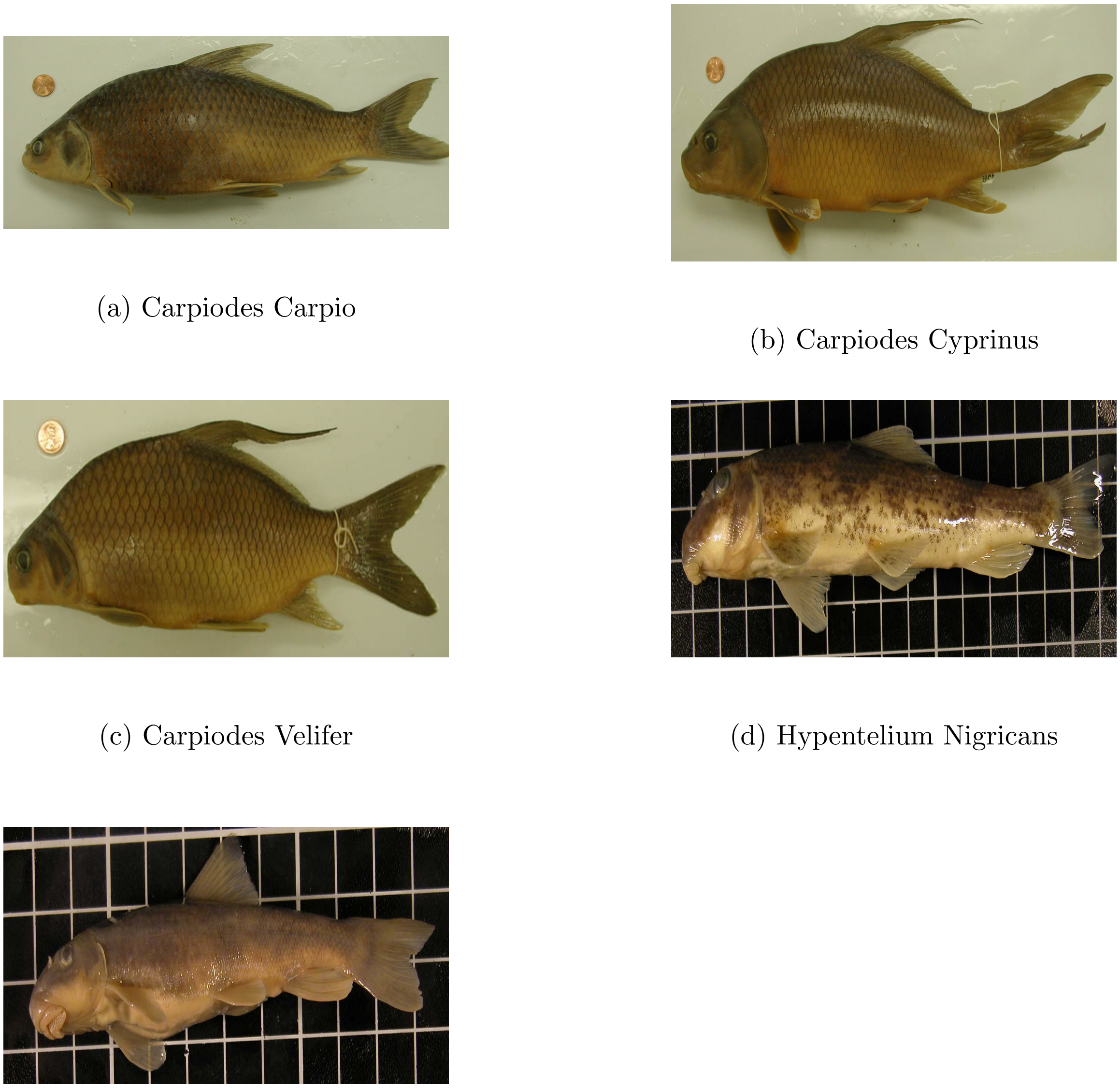


Figure 4.10. Fish Landmarks

There are 10 different species in the Catostomidae family. These species include *Carpiodes Carpio*,*Carpiodes Cyprinus*,*Catostomus Commersoni*,*Carpiodes Velifer*,*Erimyzon Tenuis*,*Hypentelium Nigricans*,*Ictiobus Bubalus*,*Minytrema Melanops*,*Moxostoma Poecilurum*, and *Pantosteus Discobolus*.



(a) Carpiodes Carpio

(b) Carpiodes Cyprinus

(c) Carpiodes Velifer

(d) Hypentelium Nigricans

(b) Pantosteus Discobolus

Figure 4.11. Catostomidae Family

4.2.1 Dorsal View

A classification is performed on the dorsal view of the 10 different species from the catostomidae family of fishes. The number of components K is chosen based on the number of species. Hence, the dataset is modeled as a 10 component finite mixture model. To perform the classification, the features to extract from the species is important.

4.2.1.1 Feature Extraction

Feature extraction was done using pairwise distance. To do this, we normalize the data after removing its mean. Then a pairwise distance is performed and we extract the most discriminative features by selecting the features with the maximum *Inter–Quartile Range*. However, extracting the most discriminative features proved very challenging. This is because some of the species are very similar as can be seen in figure 4.11. To solve this we use the *Recursive Feature Extraction*.

Recursive Feature Extraction "The SVM-RFE algorithm proposed by [8] returns a ranking of the features of a classification problem by training a SVM with a linear kernel and removing the feature with smallest ranking criterion" [1]. The support vector machine recursive feature extraction is applied to the dataset with a parameter C = 5. This parameter determines the trade off between training error and margin.

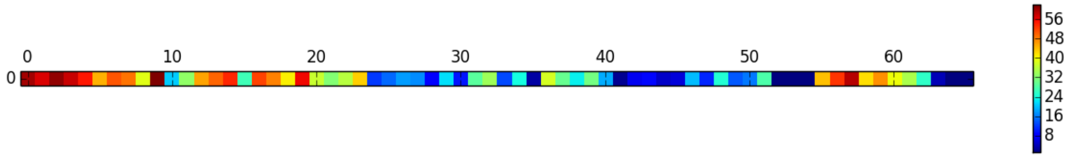


Figure 4.12. Ranking of Features

The number of features chosen is **five**.

4.2.1.2 Results

	Regular–EM	Spatial–EM	Kotz–EM
FPR	0.4341404	0.2128955	0.09950034
FNR	0.154292	0.3448109	0.5754209
RI	0.5944646	0.7736179	0.85187529
F–MEASURE	0.2988977	0.3717261	0.36394386
NMI	0.3730932	0.4737636	0.4899959

Table 4.2. Classification Results using Inter–Quartile Range

	Regular–EM	Spatial–EM	Kotz–EM
FPR	0.1433072	0.2093475	0.07199535
FNR	0.4011179	0.3010627	0.5213911
RI	0.8303404	0.7812778	0.8820692
F–MEASURE	0.4191539	0.3951393	0.4534519
NMI	0.5598887	0.5374111	0.5818194

Table 4.3. Classification Results using Recursive Feature Extraction

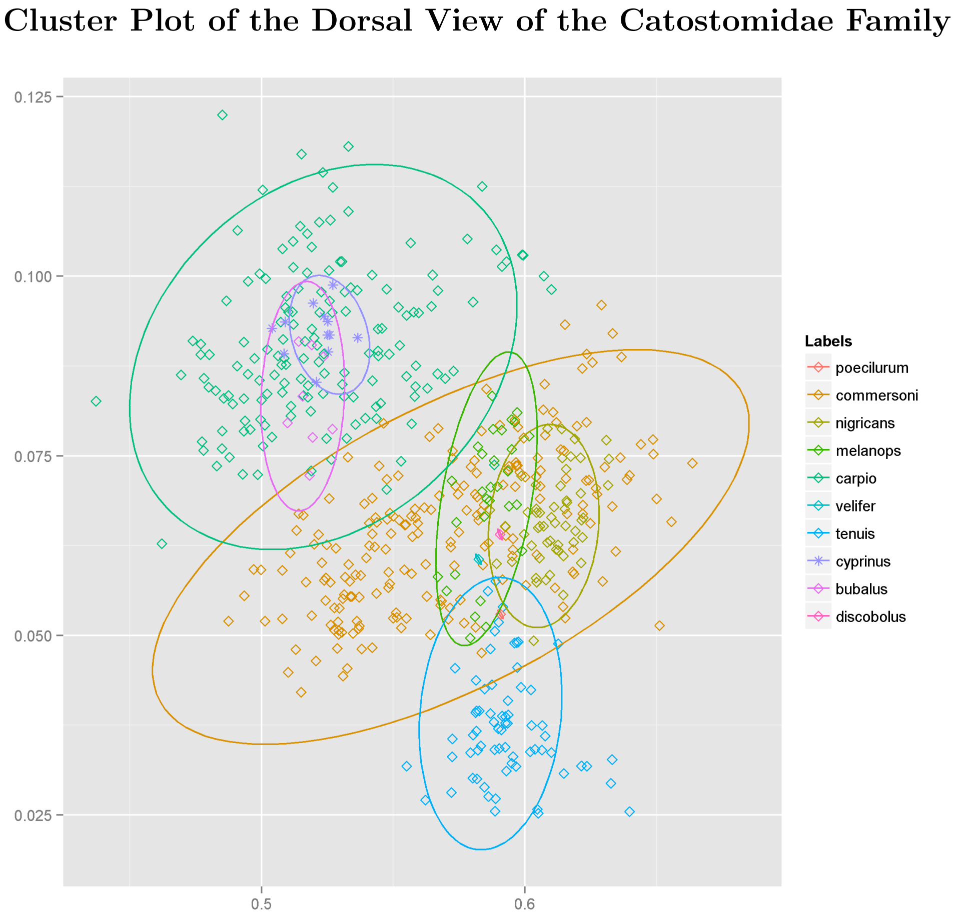


Figure 4.13. Spatial–EM Cluster Plot (Dorsal View)

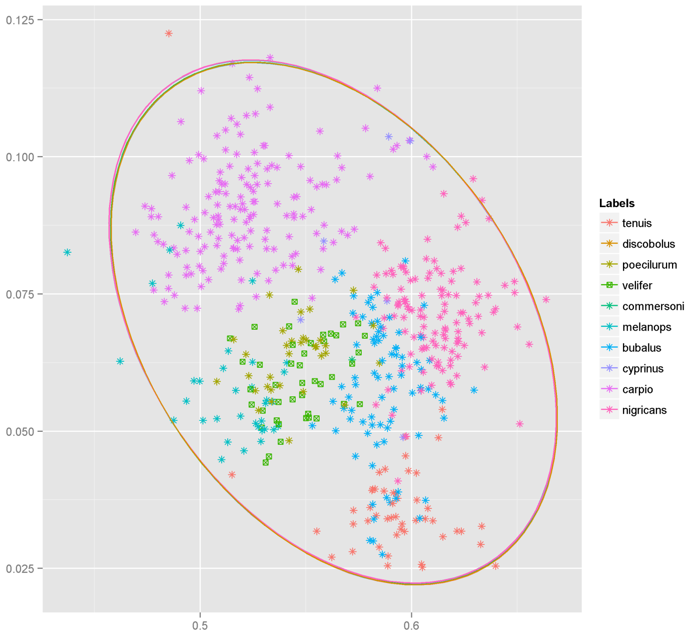


Figure 4.14. Regular–EM Cluster Plot (Dorsal View)

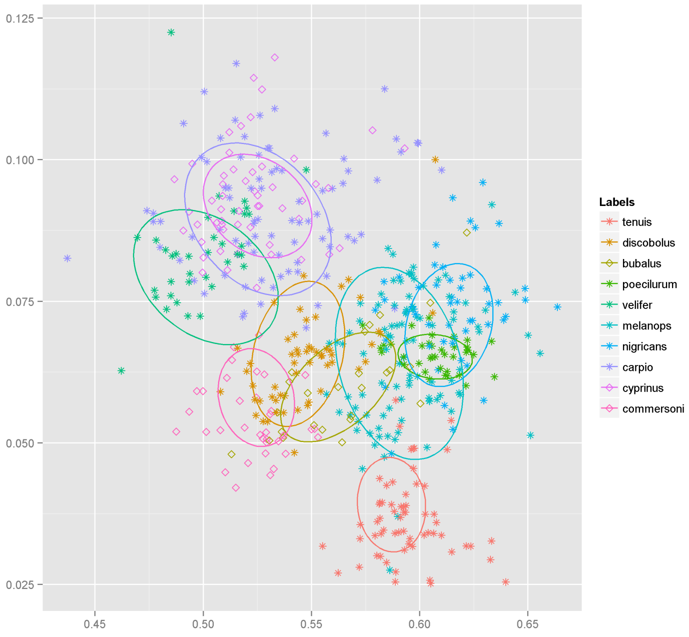


Figure 4.15. Kotz–EM Cluster Plot (Dorsal View)

4.2.2 Lateral View

The same experiment is performed on the lateral view of the 10 different species from the catostomidae family of fishes.

4.2.2.1 Results

	Regular–EM	Spatial–EM	Kotz–EM
FPR	0.2849068	0.2262151	0.08608221
FNR	0.3289567	0.3600071	0.6095339
F–MEASURE	0.329677	0.3610189	0.3691361
NMI	0.4222639	0.4505272	0.4780181

Table 4.4. Classification Results using Recursive Feature Extraction

Cluster Plot of the Lateral View of the Catostomidae Family

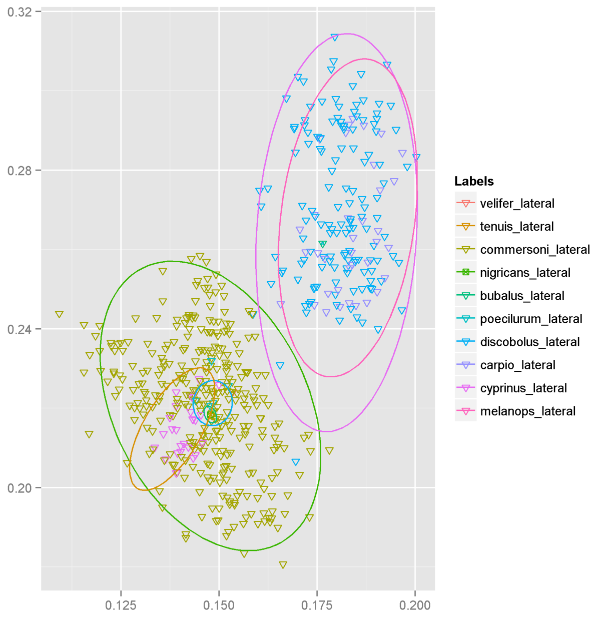


Figure 4.16. Spatial–EM Cluster Plot (Lateral View)

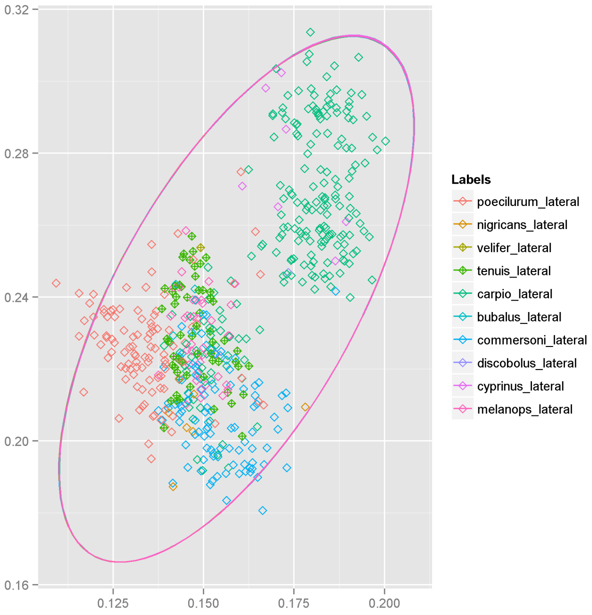


Figure 4.17. Regular–EM Cluster Plot (Lateral View)

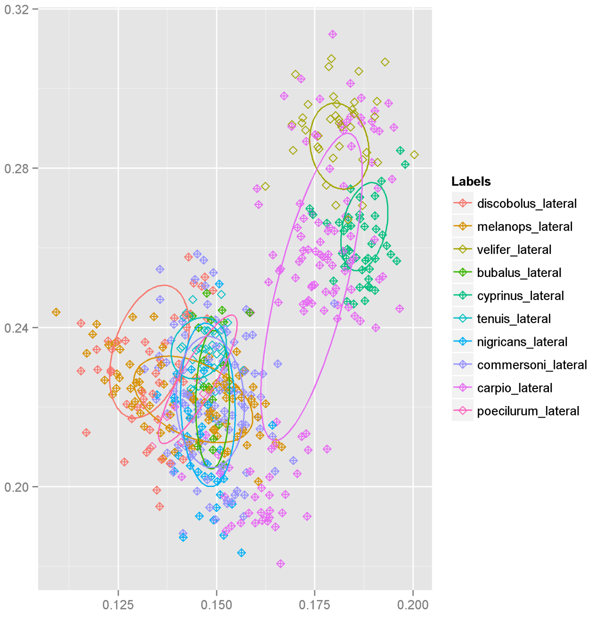


Figure 4.18. Kotz–EM Cluster Plot (Lateral View)

4.2.3 Discussion of Results

To evaluate the algorithm, purity is used to map predicted components given by the algorithm to the true label in the data. A confusion matrix is then computed from the results of using purity and the FPR and FNR are calculated. From the results shown in table 4.2 and table 4.3, we can see that the *recursive feature extraction* improves the effectiveness of the classification than the *inter–quartile range.* The results from tables 4.3 and 4.4 show that the three algorithms are comparable in terms of their classification effect. However, due to the similarity of the species, there is a low F1 score for all three algorithms. Figures 4.10 through 4.15 show the cluster plots of the fish dataset. From these plots, we can see that there is a lot of overlap in the components especially in the cluster plot for the regular–EM algorithm. This overlap emphasizes the similarity between the species in the Catostomidae family and the difficulty in performing cluster analysis on the dataset.

CHAPTER 5

OUTLIER DETECTION

Hawkins [9] defined an outlier as “an observation which deviates so much from the other observations as to arouse suspicions that it was generated by a different mechanism.” “Outlier detection is the process of detecting the data objects that are grossly different or inconsistent with the remaining data” [5]. The goal of this chapter is to show that the Spatial–EM algorithm is robust to outliers. That is, to show that given a group of components of the distribution, the algorithm is able to detect a data in the dataset not belonging to any of the components with little error.

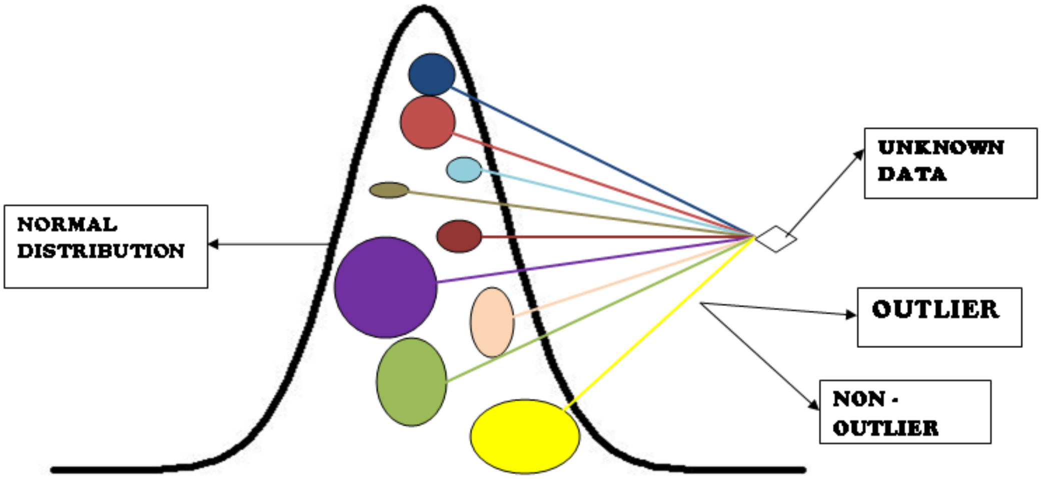


Figure 5.1. Outliers in a Gaussian Distribution

To detect outliers in the Spatial–EM algorithm, two important concepts need to be understood.

5.1 χ^2 Distribution and Mahalanobis Distance

5.1.1 χ^2 Distribution

"The χ^2 distribution results when v independent variables with standard normal distributions are squared and summed" [12]. It is defined by the following probability density function,

$$f(x) = \frac{1}{2^{\frac{d}{2}}\Gamma(\frac{d}{2})} x^{\frac{d}{2}-1} e^{-\frac{d}{2}}$$

where d is the degrees of freedom, Γ is the gamma function.

The cumulative distribution of a χ^2 distribution is given by,

$$F(x) = \frac{\gamma(\frac{d}{2},\frac{x}{2})}{\Gamma(\frac{d}{2})}$$

where γ is the *lower incomplete gamma function*.

5.1.2 Mahalanobis Distance

Introduced by P.C Mahalanobis in 1939. The Mahalanobis distance is a measure of the distance between a point and a distribution. For the Spatial–EM outlier detection problem, the Mahalanobis distance measures the distance between a data object and the components in the underlying gaussian distribution.

Given a d–variate random vector $\boldsymbol{X}$ distributed as $N(\mu, \Sigma)$, the Mahalanobis distance is given as

$$\sqrt{(\boldsymbol{X} - \mu)^T \Sigma^{-1} (\boldsymbol{X} - \mu)}$$

5.2 Outlyingness and Two–type Errors

As stated in [17], Usually, an outlier region is associated with an outlyingness measure. For a finite mixture model, the outlyingness measure is defined as

$$H(x) = \sum_{j=1}^{K} \tau_j G(\xi_j(x))$$

where $\xi_j(x) = (x - \mu_j)^T \Sigma_j^{-1}(x - \mu_j)$ and G is the cumulative distribution function (cdf) of $\chi^2(d)$ distribution."

The Mahalanobis distance is a χ^2 distribution. The corresponding outlier region is defined as

$$\{x \in R^d : H(x) > 1 - \varepsilon\}$$

where ε is a value between 0 and 1.

There are **two types of errors** associated with outlier detection,

Type I error

This is the false positive (alarm) rate. It is the probability that the algorithm identifies a data point as an outlier when the data point is a non-outlier. It is represented as P_{err1}.

$$P_{err1} = \text{ P(identified as outlier| non-outlier)}$$

For a gaussian mixture model, the type I error is ε.

Type II error

This is the false negative rate. It is the probability that the algorithm does not identify a data point as an outlier when the data point is an outlier. It is represented as P_{err2}.

$$P_{err2} = \text{ P(identified as non-outlier| outlier)}$$

These errors are computed to test the performance of the EM algorithms in detecting outliers.

In general, to detect outliers we compute the Mahalanobis distance between an unknown data and each of the components in the distribution. We select the minimum Mahalanobis distance and compare the distance to a χ^2 distribution with a degree of freedom d which is the number of dimensions of the data. If the minimum Mahalanobis distance is a chi–square distribution, then the unknown data belongs to the component that gives the minimum distance, else the unknown data is an outlier.

5.2.1 Testing

The outlier detection method is applied to the dorsal and lateral view of the fish dataset in chapter 4. To accomplish this, a specie is represented as unknown and classification is performed on the remaining nine species. Each data in the unknown specie is tested for outliers.

5.2.1.1 Results

Type I error $= 0.05$

Species	Regular–EM	Spatial–EM	Kotz–EM
Carpiodes Carpio	0.050000000	0.06666667	0.01666667
Carpiodes Cyprinus	0.05263158	0.00000000	0.00000000
Catostomus Commersoni	0.23333333	0.00000000	0.00000000
Carpiodes Velifer	0.12500000	0.15625000	0.03125000
Erimyzon Tenuis	0.01666667	0.00000000	0.00000000
Hypentelium Nigricans	0.06666667	0.18333333	0.00000000
Ictiobus Bubalus	0.02325581	0.00000000	0.00000000
Minetrema Melanops	0.56666667	0.20000000	0.00000000
Moxostoma Poecilurum	0.48333333	0.28333333	0.00000000
Pantosteus Discobolus	0.13333333	0.00000000	0.00000000
Average	**0.1750887**	**0.08895833**	**0.004791667**

Table 5.1. Table showing Type II errors in outlier detection (Dorsal View)

Species	Regular–EM	Spatial–EM	Kotz–EM
Carpiodes Carpio	0.20000000	0.00000000	0.00000000
Carpiodes Cyprinus	0.50000000	0.00000000	0.00000000
Catostomus Commersoni	0.38043478	0.01086957	0.04347826
Carpiodes Velifer	0.03125000	0.00000000	0.00000000
Erimyzon Tenuis	0.00000000	0.00000000	0.00000000
Hypentelium Nigricans	0.03333333	0.00000000	0.00000000
Ictiobus Bubalus	0.00000000	0.00000000	0.00000000
Minetrema Melanops	0.35000000	0.51666667	0.00000000
Moxostoma Poecilurum	0.30000000	0.10000000	0.01666667
Pantosteus Discobolus	0.00000000	0.00000000	0.00000000
Average	**0.17950180**	**0.06275362**	**0.006014493**

Table 5.2. Table showing Type II errors in outlier detection (Lateral View)

5.2.1.2 Discussion of Results

From table 5.1 and 5.2, it can be seen that given an ε value of 0.05 which is a 95% confidence interval, the EM algorithms are able to predict outliers with few errors for some species. The Kotz–EM algorithm in particular does very well for most of the species and has the lowest average Type II error rate, while the Regular–EM has the highest average Type II error rate. In the dorsal view, the Spatial–EM average type II error is about 0.29 that of Regular–EM, and about 9.7 times that of Kotz–EM. Similarly in the lateral view, the Spatial–EM average type II error is about 0.35 that of Regular–EM, and about 10.4 times that of the Kotz–EM. The high Type II error for some of the species in the dataset can be attributed to the similarity between the subspecies in the dataset.

CHAPTER 6

ESTIMATING THE NUMBER OF COMPONENTS

6.1 Bayesian Information Criterion

The Bayesian Information Criterion commonly known as the BIC. "The BIC criterion is well-known in the statistics literature; it has been widely used for model identification in statistical modeling" [4]. In this chapter, a special form of the BIC known as the **trimmed BIC** is used to estimate the number of components in the distribution. The trimmed BIC is computed using the formula,

$$BIC = 2 * (\text{trimmed log likelihood}) - p \log n$$

Where the trimmed log likelihood is a reduction of the values gained by the log likelihood, p is the estimated number of parameters in the model, and n is the sample size.

The trimmed BIC is a "likelihood criterion penalized by the model complexity: the number of parameters in the model" [4]. The BIC criterion is such that the model which maximizes the BIC is chosen. The candidate of the model to be considered is the number of components **K** of the distribution. The parameters of the model are the parameters of the distribution. These parameters are the number of components K, the mixture ratio $\tau = K - 1$, the mean μ whose size is the number of dimensions d, and the covariance Σ whose size is $\frac{d(d+1)}{2}$. Hence the number of parameters p can be estimated as,

$$p = K\left[d + \frac{d(d+1)}{2}\right] + k - 1$$

6.1.1 Log likelihood

The likelihood is a model used for parameter estimation. It can be computed from the conditional density. The likelihood is a measure of the probability that a data belongs to a component given prior knowledge of the data. Hence, it is commonly known as computing the posterior probability. It is assumed that most of the data being observed are independent and identically distributed, hence the likelihood of a dataset can be computed as the product of the likelihood of each data in the dataset. The log likelihood is computed more frequently because the log is a monotonically increasing function, and obtains its maximum value at the same point as the likelihood. The log likelihood of the dataset is the sum of the log likelihood of each data in the dataset. A variation of the log likelihood is the trimmed log likelihood.

6.1.1.1 Trimmed Log Likelihood

The trimmed log likelihood as the name suggests is a reduced version of the values derived from the log likelihood of each of the individual data in the dataset. To trim the log likelihood, we use a threshold value between 0 and 0.5. A threshold value of zero would not trim any of the values, and a threshold of 0.5 would trim off 50% of the values.

To compute the trimmed log likelihood of the dataset, we compute a weighted likelihood for each of the component in the distribution. The weight of a component is greater if the data has a higher possibility of belonging to that component compared to other components. The log likelihood for the data is then computed as the log of the sum of the weighted likelihoods. The trimmed log likelihood is the sum of the highest $(1 - threshold) * 10\%$ of the log likelihood. The formula for the log likelihood is given as

$$\boldsymbol{L}(\theta|x) = \sum_{i=1}^{n} log\Bigg(\sum_{j=1}^{K} \tau_j f(x|\theta_j) \Bigg)$$

where τ_j is the weight for component j, K is the number of components in the distribution, n is the size of the dataset, and $f(x|\theta_j)$ is the conditional density.

6.1.2 Testing

6.1.2.1 Simulation

The BIC is applied to an artificial dataset created from a multivariate normal distribution. The dataset has three components, and contains some outliers. Given the ground truth of three components, we use the BIC and trimmed BIC to estimate the number of components. We expect the trimmed BIC to work better than the BIC because the trimmed BIC is more efficient for data with outliers. Below are the graphs showing the results.

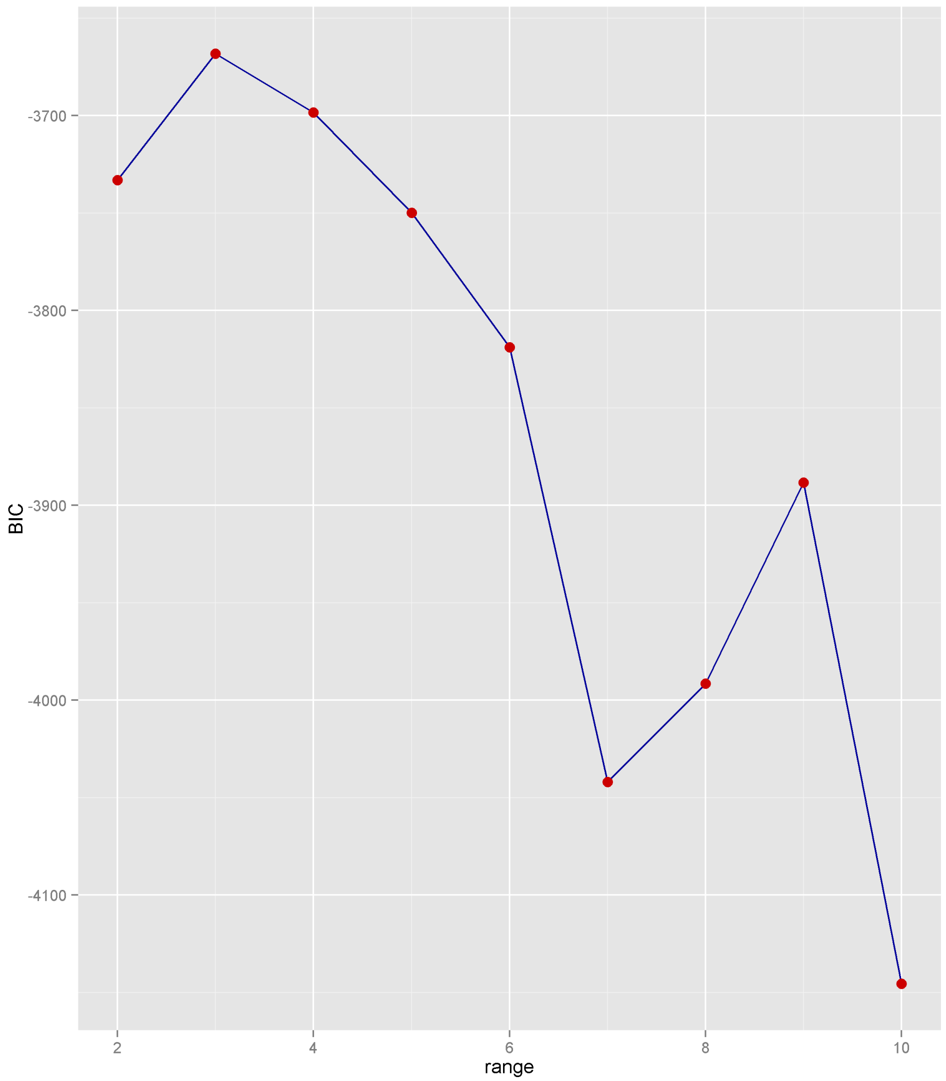


Figure 6.1. BIC using Spatial–EM

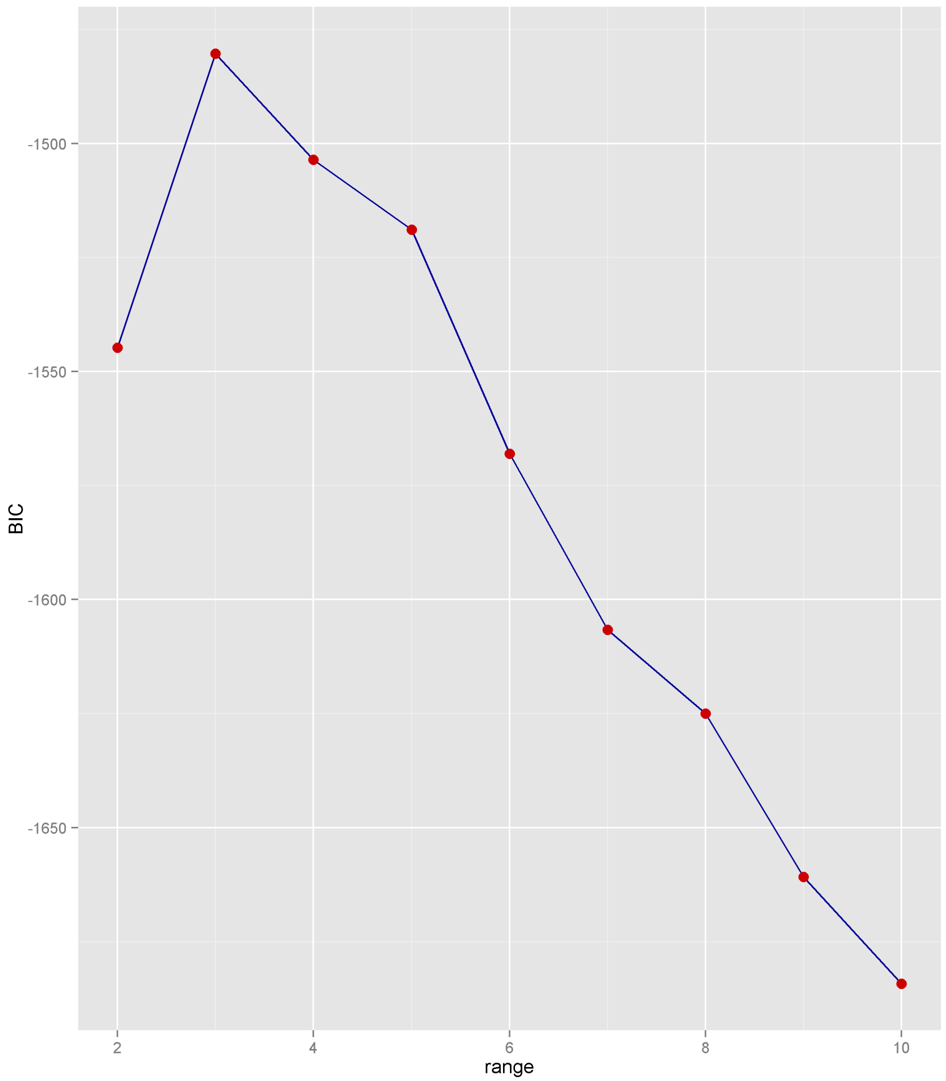


Figure 6.2. Trimmed BIC using Spatial–EM

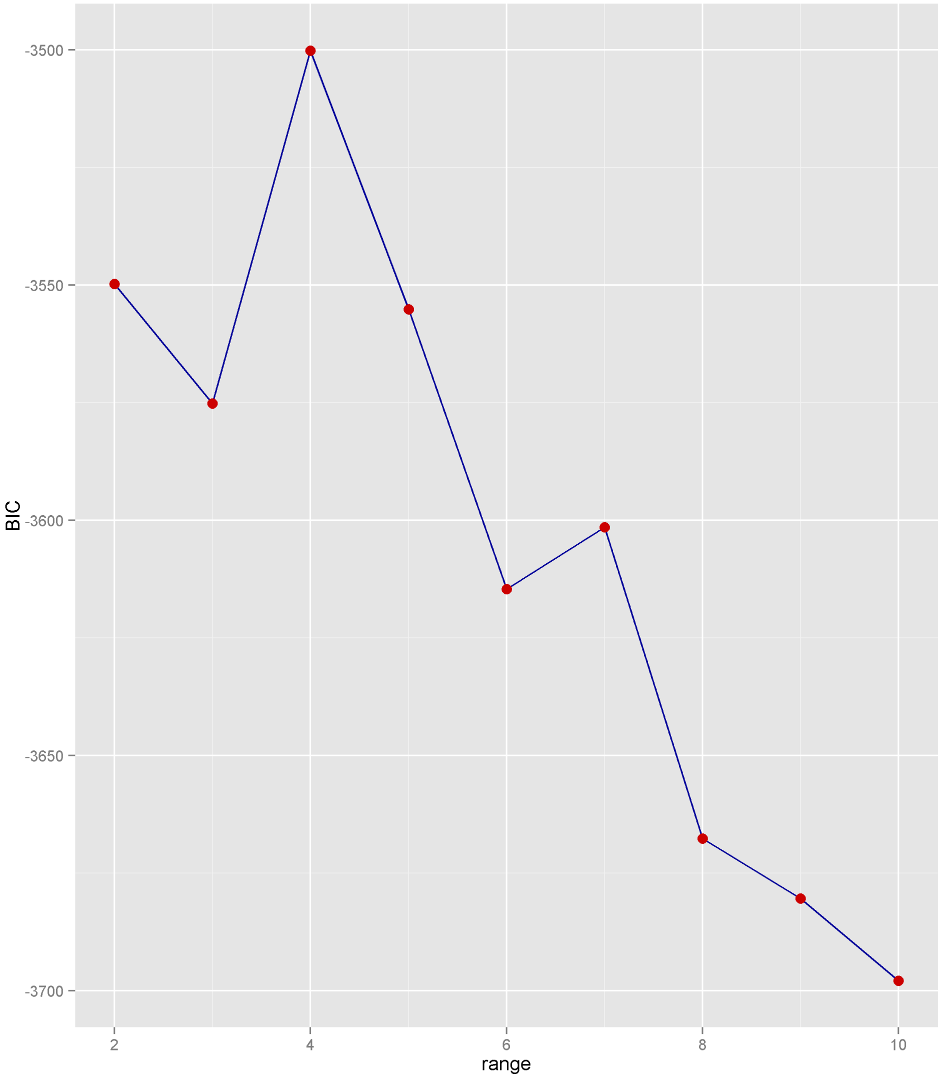


Figure 6.3. BIC using Regular–EM

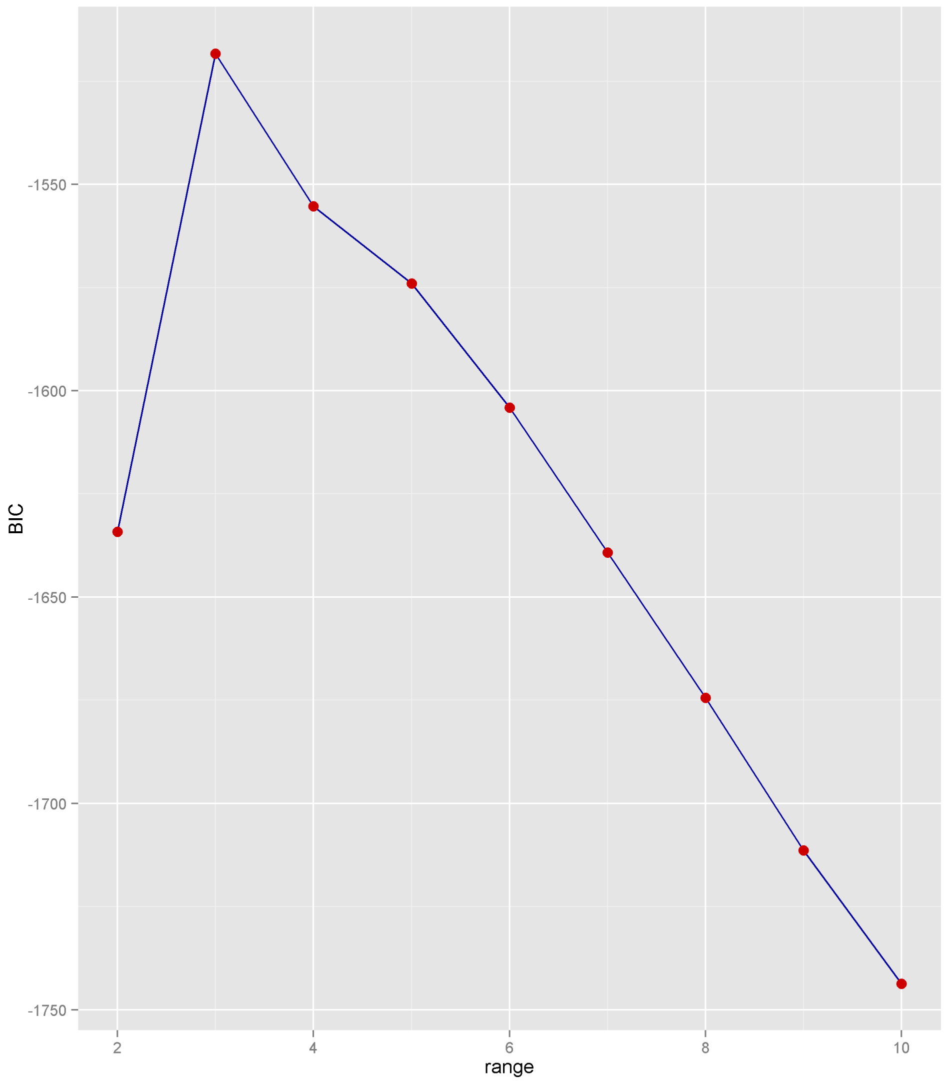


Figure 6.4. Trimmed BIC using Regularl–EM

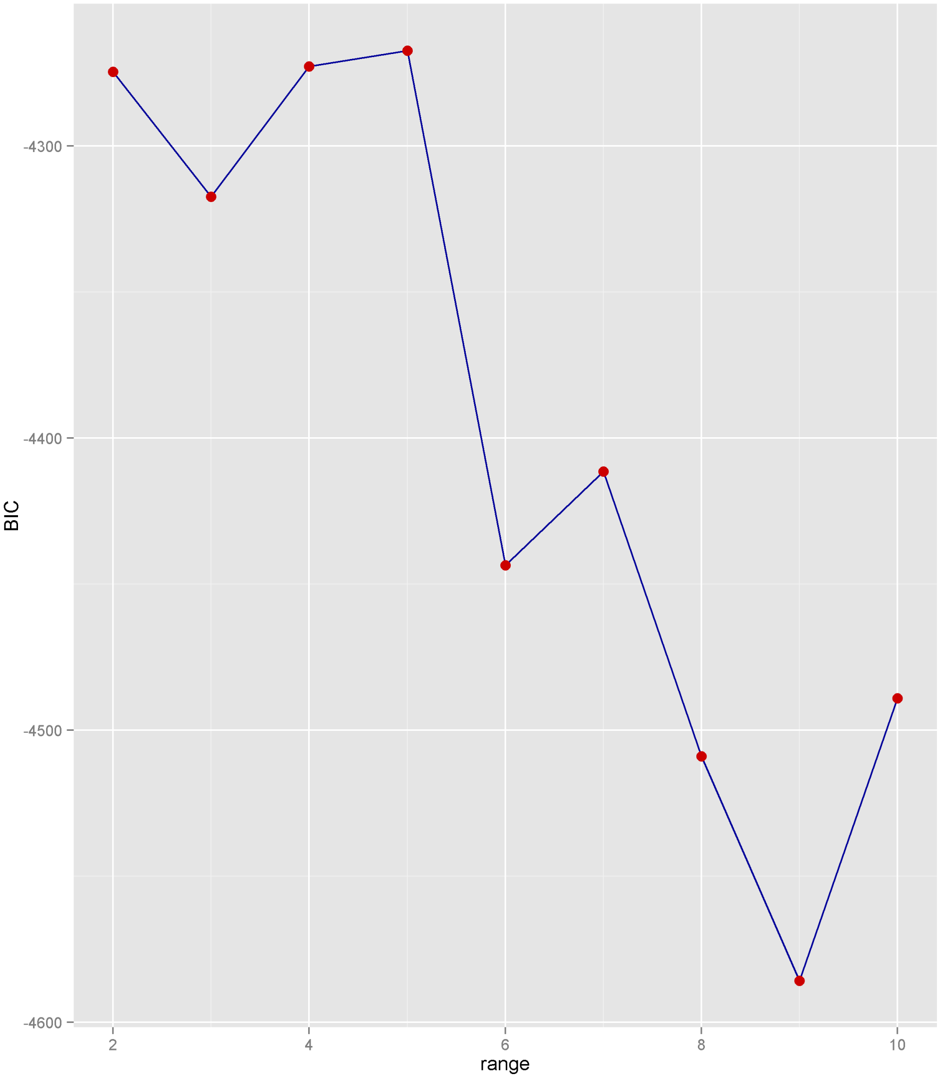


Figure 6.5. BIC using Kotz–EM

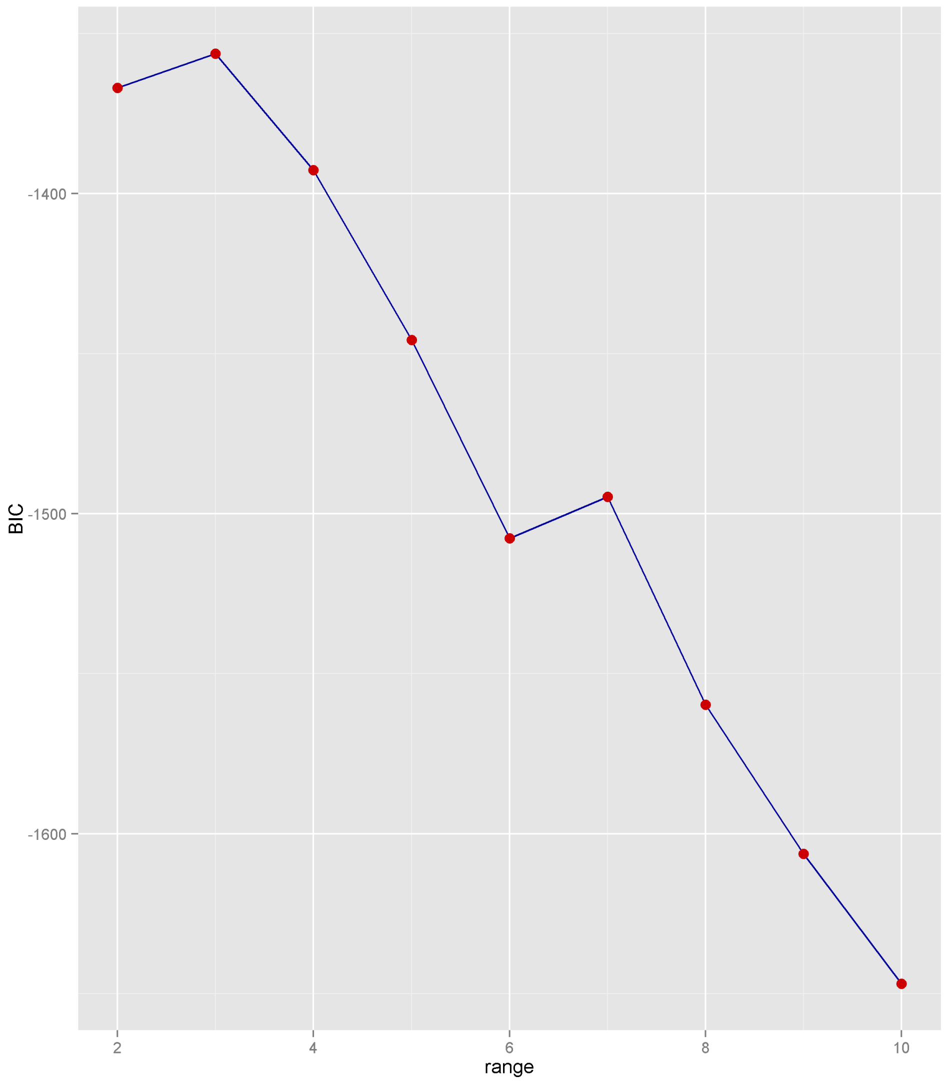


Figure 6.6. Trimmed BIC using Kotz–EM

From the graphs, we can see that for the Spatial–EM, both the BIC and the trimmed BIC estimates 3 components, for the Regular–EM, the BIC estimates 4 while the trimmed BIC estimates 3 components and for the Kotz–EM, the BIC estimates 5 while the trimmed BIC estimates 3 components. Hence, the trimmed BIC is more efficient in estimating the number of components in the distribution of a data containing outliers.

6.1.2.2 Fish Dataset

The BIC is applied to the fish dataset using each of the EM algorithms. To estimate the number of components for the fish dataset, we compute the BIC for $K = 2, ..., 10$ where 10 is the number of species in the data set. The following diagrams show a plot of K against the BIC. The value of K that maximizes the BIC is selected.

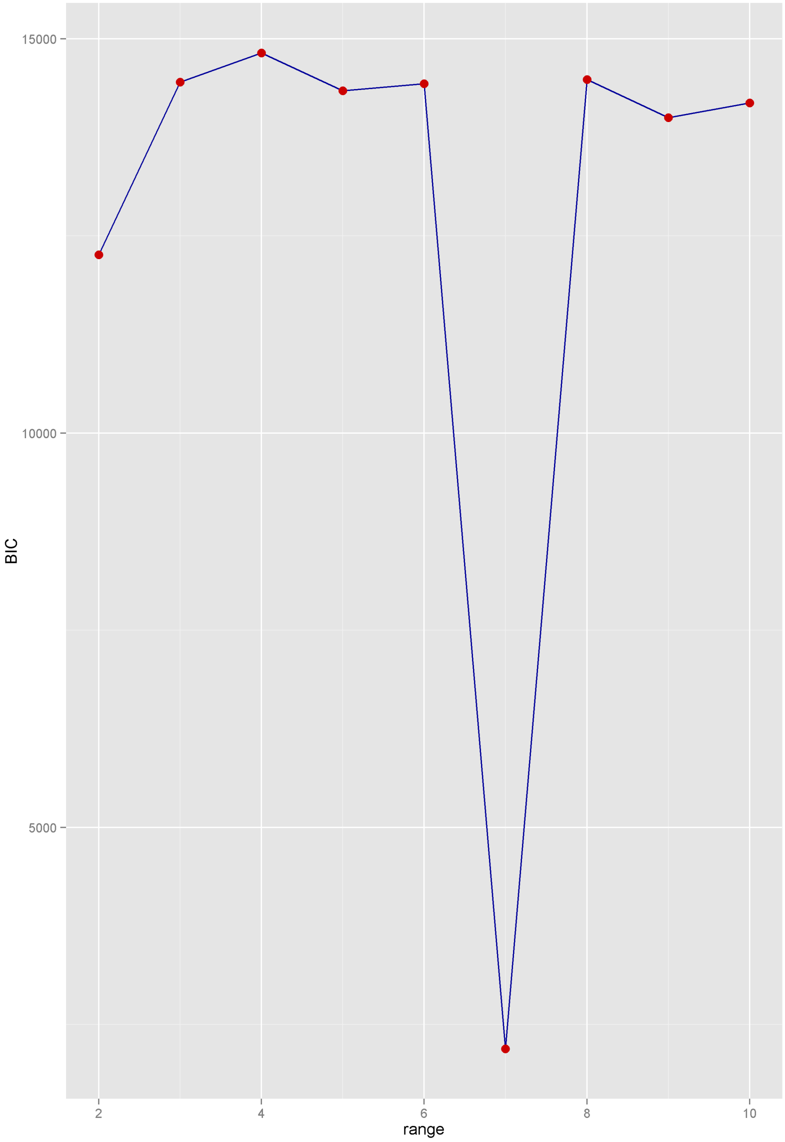


Figure 6.7. BIC plot using the Spatial–EM

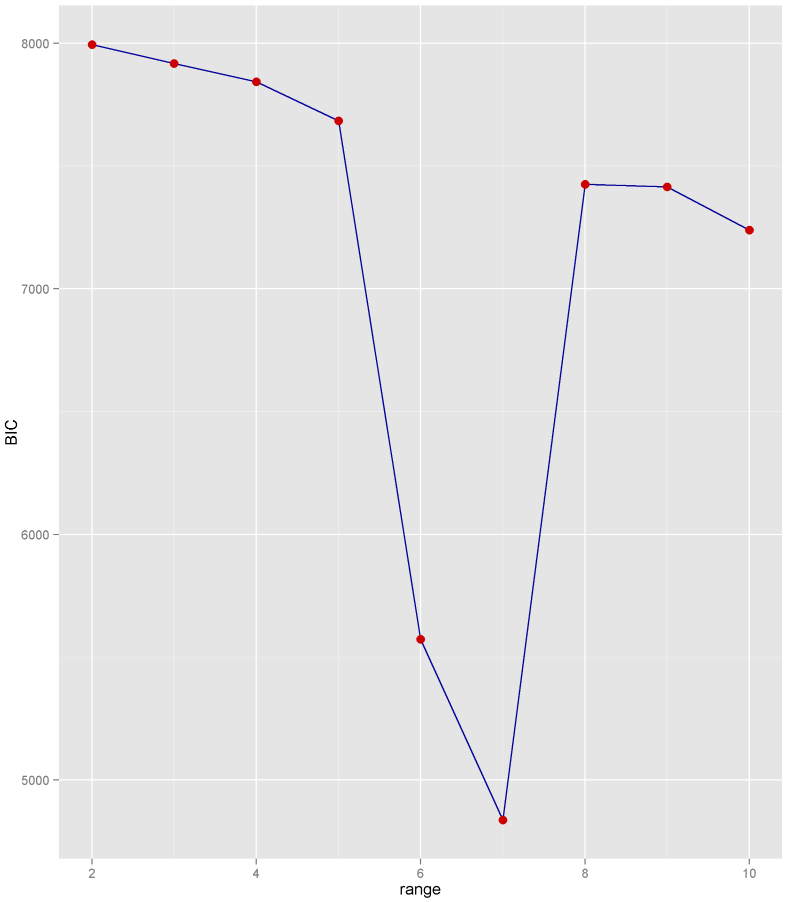


Figure 6.8. Trimmed BIC plot using the Spatial–EM

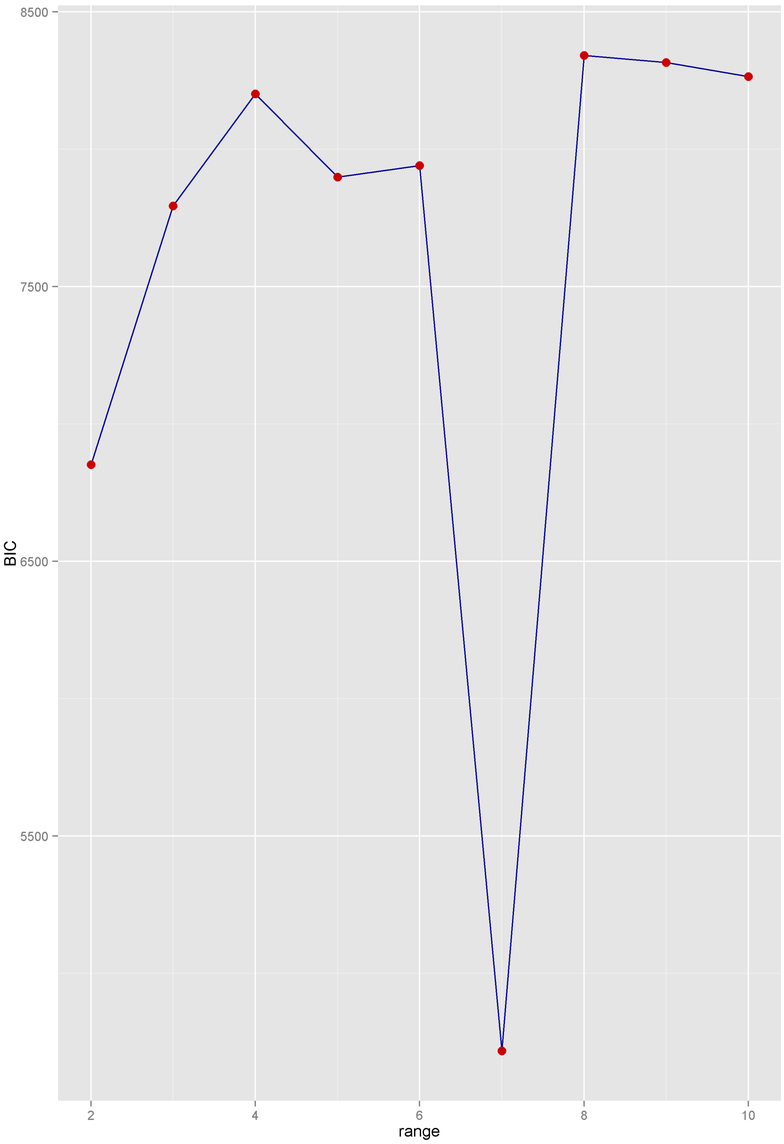


Figure 6.9. BIC plot using the Kotz–EM

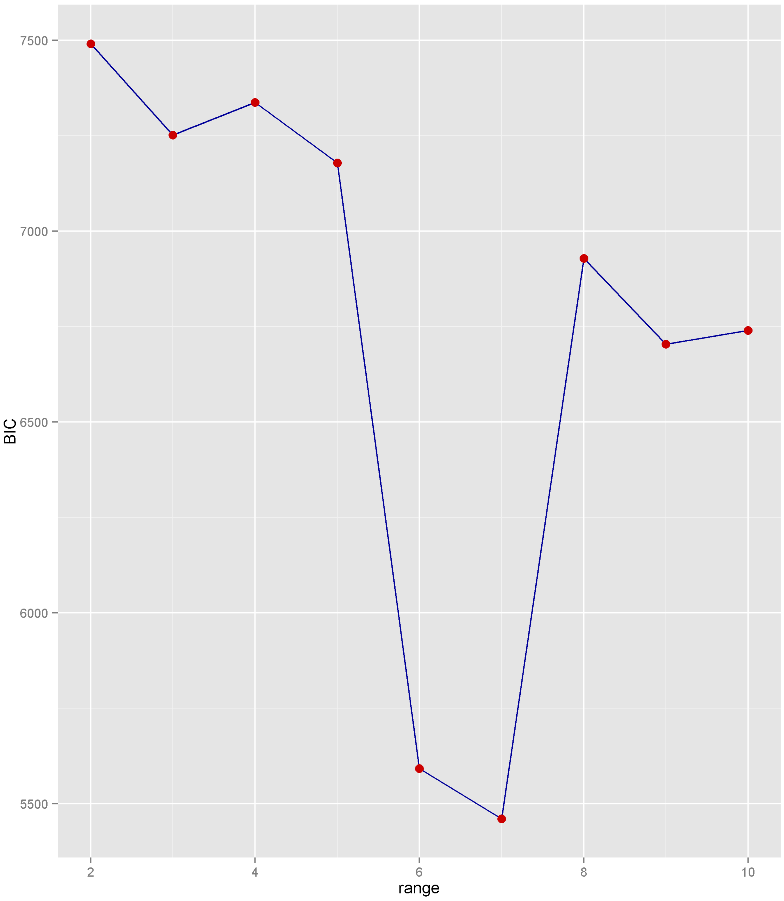


Figure 6.10. Trimmed BIC plot using the Kotz–EM

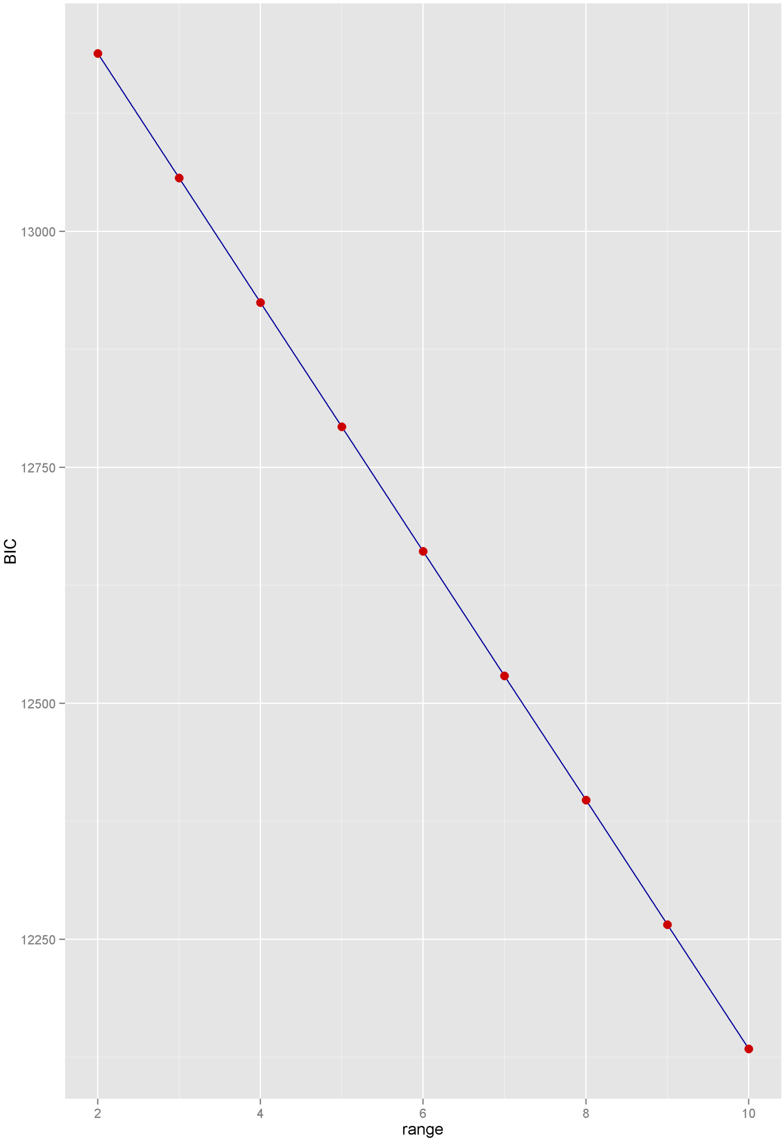


Figure 6.11. BIC plot using the Regular–EM

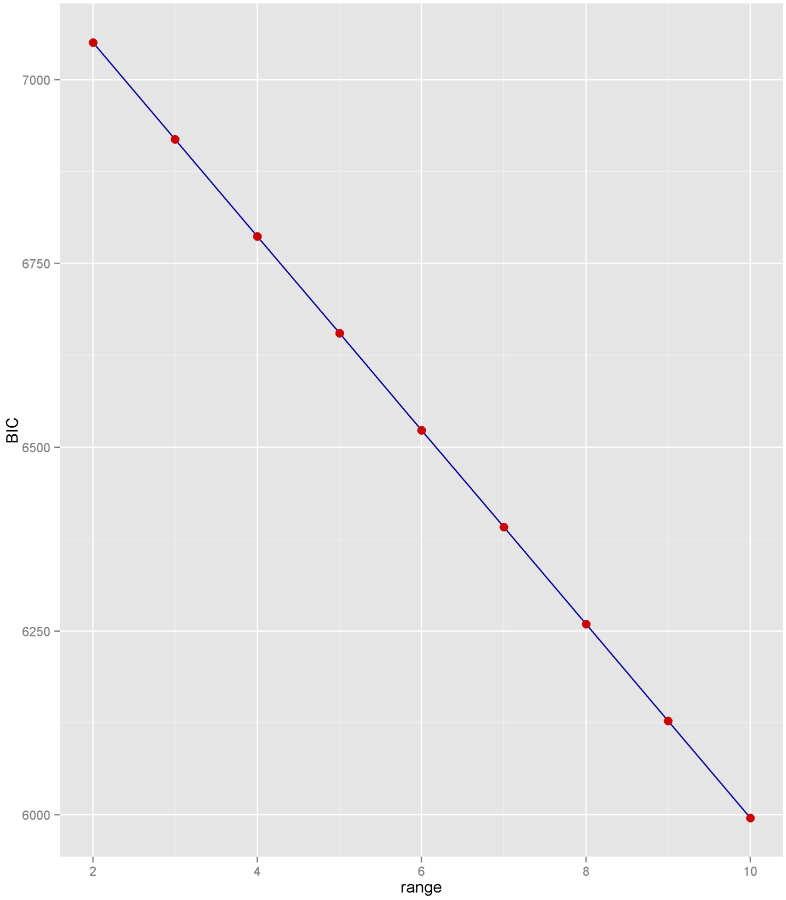


Figure 6.12. Trimmed BIC plot using the Regular–EM

From the above plots, we can observe that the number of components predicted by the Spatial–EM is **4** for BIC and **2** for trimmed BIC, Kotz–EM is **8** for BIC and **2** for trimmed BIC, Regular–EM is **2** for both the BIC and trimmed BIC. For this dataset, the trimmed BIC does not perform more efficiently than the BIC. Hence, to find the optimal number of components, we use *normalized mutual information* to test the efficiency of the classifier based on the number of components estimated by the BIC.

Regular–EM	Spatial–EM	Kotz–EM
0.3893141	0.6086364	0.5291653

Table 6.1. NMI scores for the BIC

From table 6.1, the estimated number of components is the component with the highest average NMI which is **4**.

BIC Cluster Plot of the Dorsal View of the Catostomidae Family

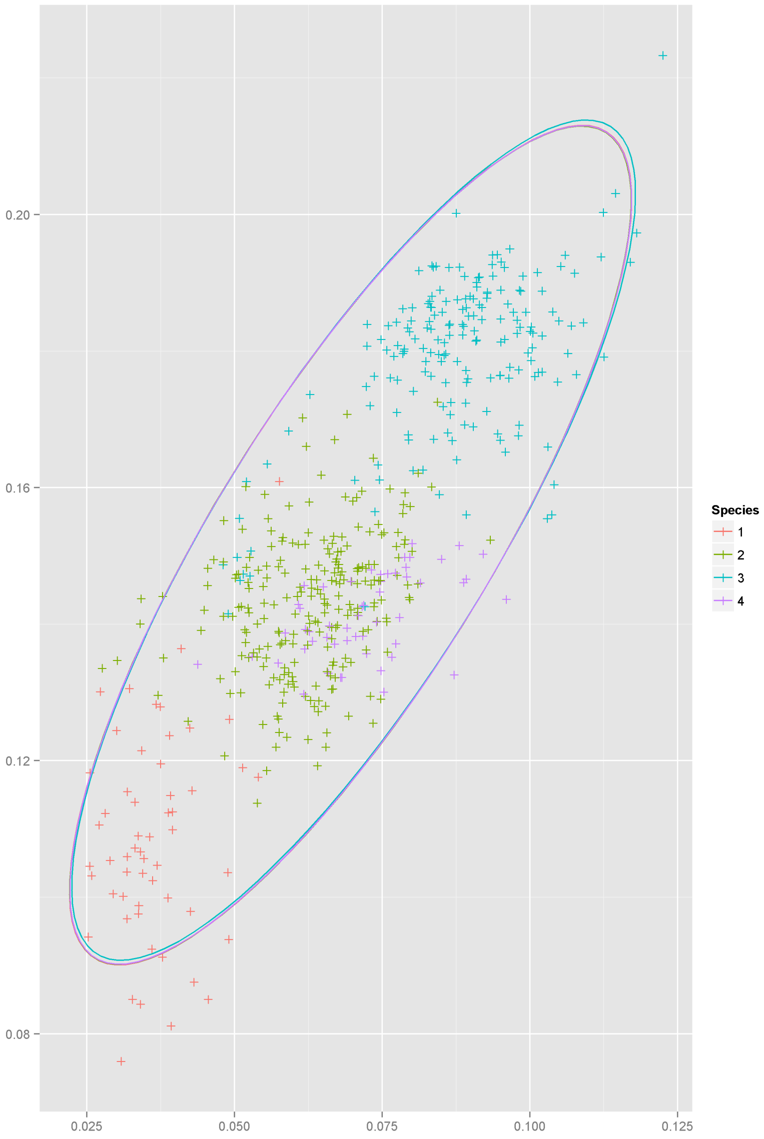


Figure 6.13. Regular–EM BIC Cluster Plot

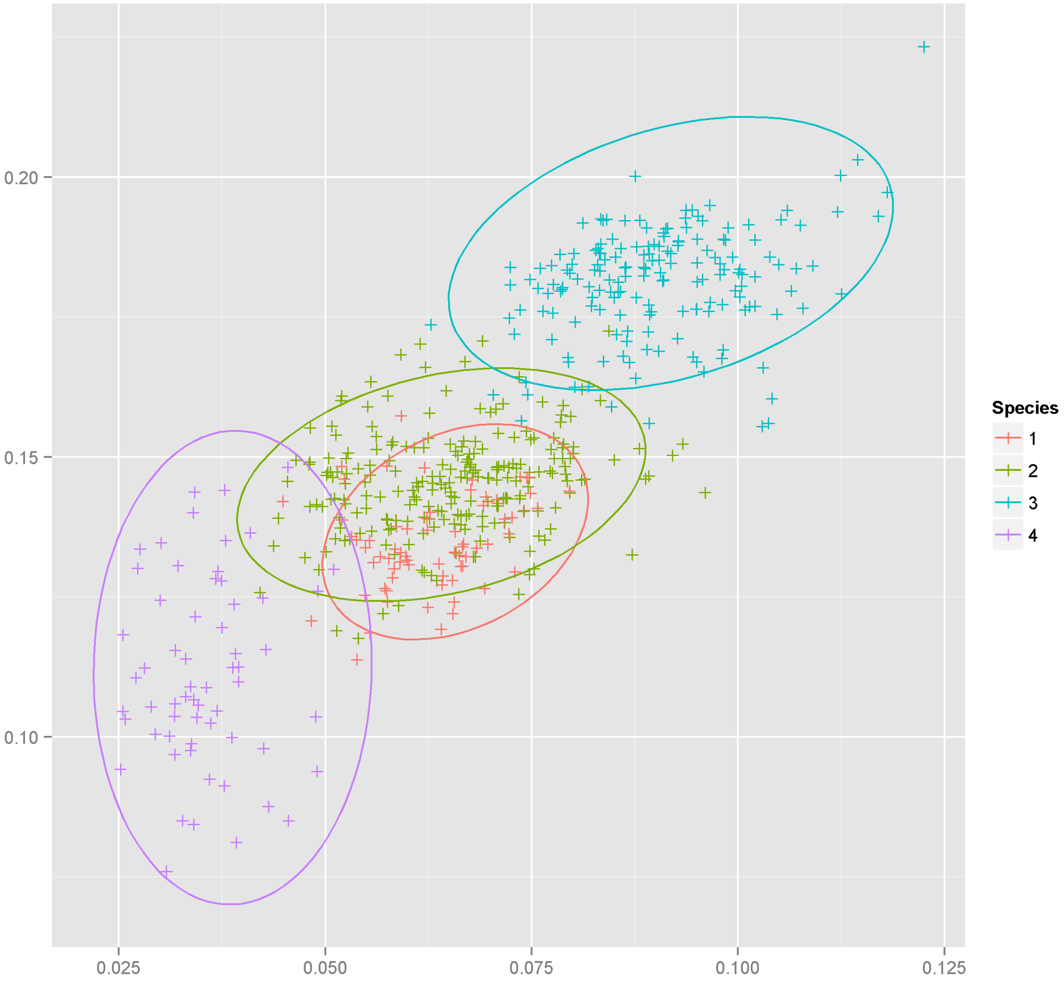


Figure 6.14. Spatial–EM BIC Cluster Plot

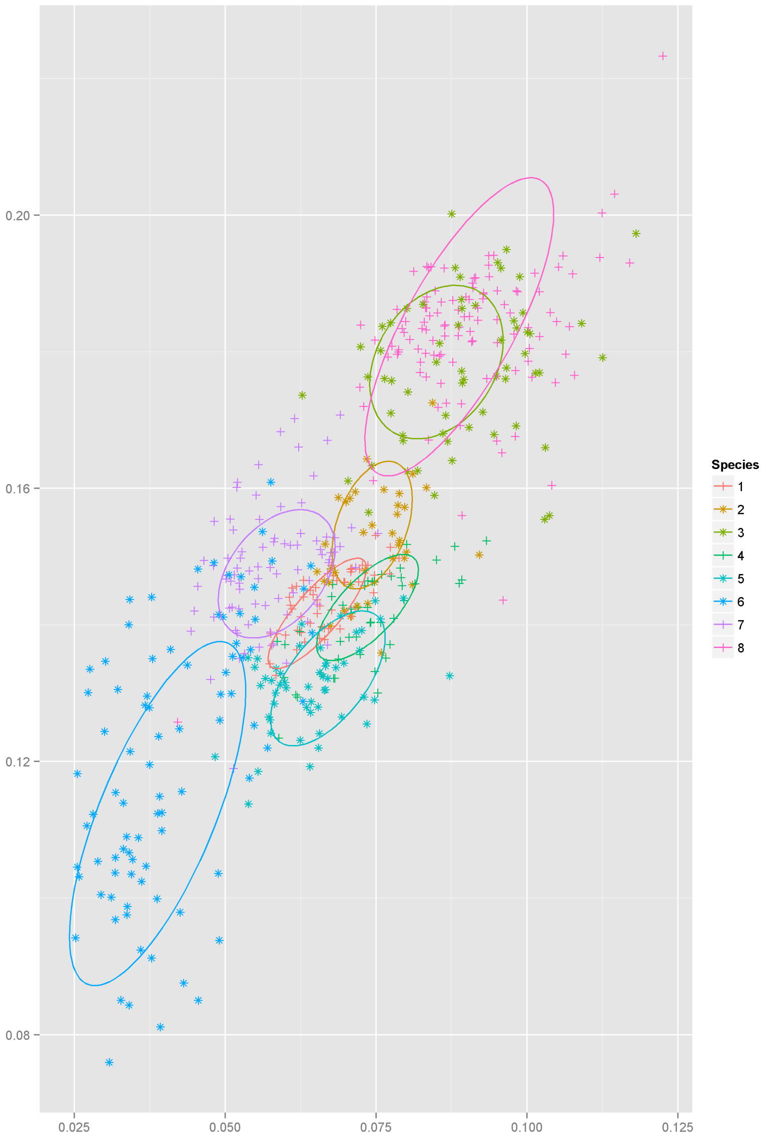


Figure 6.15. Kotz–EM BIC Cluster Plot

We perform outlier detection for the fish dataset using the optimal number of components.

Species	Regular–EM	Spatial–EM	Kotz–EM
Carpiodes Carpio	0.050000000	0.05000000	0.01666667
Carpiodes Cyprinus	0.05263158	0.18421053	0.00000000
Catostomus Commersoni	0.23333333	0.01666667	0.00000000
Carpiodes Velifer	0.12500000	0.31250000	0.06250000
Erimyzon Tenuis	0.01666667	0.01666667	0.00000000
Hypentelium Nigricans	0.06666667	0.05000000	0.01666667
Ictiobus Bubalus	0.02325581	0.13953488	0.04651163
Minetrema Melanops	0.56666667	0.28333333	0.03333333
Moxostoma Poecilurum	0.48333333	0.58333333	0.00000000
Pantosteus Discobolus	0.13333333	0.03333333	0.00000000
Average	**0.1750887**	**0.1669579**	**0.01756783**

Table 6.2. Table showing Type II errors in outlier detection using the Estimated Component

6.1.3 Discussion of Results

To perform the outlier detection, we remove one specie as the unknown data and perform a model selection on the remaining data using the trimmed BIC. The trimmed BIC model produces worse results for the Spatial–EM algorithm, and the Kotz–EM algorithm, but does not change the average result for the Regular–EM. The Kotz–EM performs particularly well with the lowest average error rate. The Spatial–EM performs better than the Regular–EM but does not perform as well as the Kotz–EM.

CHAPTER 7

THE SPATIAL–EM R PACKAGE

7.1 Module Relationship

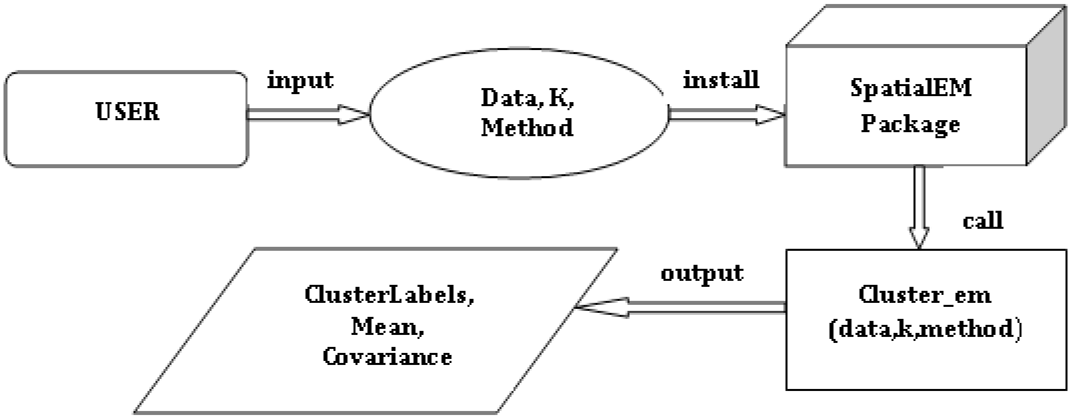


Figure 7.1. Visual representation of the Spatial–EM package

7.2 Package Design

To build the package, the R package manager **Rtools** is used. The package is built using the following command

R CMD build SpatialEM

SpatialEM is the package name and the command builds a package tarball which can be converted to a zip folder for distribution and installation.

The SpatialEM folder consisting of the following subfolders:

R This folder contains all the .R files that are to be included in the package. The .R files are the files containing the functions used for the implementation of the algorithm.

man This folder contains all the .Rd file which are documentationsl for all the functions that are to be exported. An exported function is a function that is visible to users.

src This folder consists of all compiled codes. In the Spatial–EM package, the only compiled code is the weighted rank function, which is implemented as a FORTRAN subroutine.

The R package also contains the following text files:

DESCRIPTION As implied, this file gives a general description of the package. It consists of information such as the author's name, author's email, maintainer's name, maintainer's email, package description, to list a few.

NAMESPACE The namespace file is analogous to a permission file. It contains the functions to be exported and other packages whose functionalities need to be imported for use by some functions in the package. Only functions declared with the export command in the namespace file is visible to the user.

LICENSE In addition to the above files, a License file is included that explains the terms of agreement for using the package.

There are currently three functions accessible to the users. These functions include:

cluster_em This function accepts as input the data, the number of components of the distribution, and the type of algorithm to be used. The algorithms available include the Spatial–EM, the Regular–EM, and the Kotz–EM. It returns as output the predicted labels of the data, and the parameter estimates i.e. the mean and the covariance of the distribution.

k_means This function uses the K-means library in the e1071 R package to perform a K-means clustering of the data provided. It accepts as input the data, and the number of components, and returns as output the centroids of each component.

confusionMatrix This function accepts as input the true labels, and the predicted labels, and returns as output the confusion matrix.

To access the package in R, we use the syntax **library(SpatialEM)** where SpatialEM is the name of the package.

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