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BAYESIAN CLASSIFICATION USING GAUSSIAN MIXTURE MODEL AND EM ESTIMATION: IMPLEMENTATIONS AND COMPARISONS

Information Technology Project
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Lappeenranta, June 23, 2004

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ABSTRACT

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Bayesian Classification Using Gaussian Mixture Model and EM Estimation: Implementations and Comparisons

Information Technology Project

2004

35 pages, 10 figures, 1 table and 2 appendices.

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Keywords: Bayesian classification, Gaussian mixture, overfitting, expectation maximization, maximum likelihood, gmmbayes toolbox

The main purpose of this project was to develop a Bayesian classification toolbox with Gaussian mixture probability densities for Matlab. The toolbox has two parts: the training part estimates Gaussian mixture parameters from training samples and the classifier part classifies new samples according to the estimated parameters. Three different expectation maximization algorithms for Gaussian mixture estimation were implemented: the basic expectation maximization algorithm, an algorithm proposed by Figueiredo and Jain, and the greedy expectation maximization algorithm by Verbeek, Vlassis and Kröse.

The toolbox was tested with neighbor-bank transformed forest spectral color data, waveforms and noise data, and letter image recognition data. The basic expectation maximization algorithm produces the best classification accuracy, but requires tuning parameters by hand and is failure prone. Figueiredo-Jain algorithm produces better accuracy than the greedy algorithm, but requires a certain number of training data before it works at all. The greedy algorithm has much lower requirement for the amount of training data.

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ABBREVIATIONS AND SYMBOLS

CEM	Component-wise EM algorithm
EM	Expectation Maximization
FJ	Figueiredo-Jain algorithm
GEM	Greedy Expectation Maximization algorithm
GMM	Gaussian Mixture Model
ML	Maximum Likelihood
PDF	Probability Density Function
SCC	Sub-Cluster Classifier
c	(algorithmic) component index in a mixture
C	number of components in a mixture
C_{nz}	number of non-zero component weights in a mixture
D	number of data dimensions
$\mathrm{E}_{\mathsf{Y}}[\cdot]$	expectation of a function with Y as the random variable
k	(algorithmic) index of a class
K	number of classes
n	(algorithmic) index of a sample
N	number of samples
$p(\cdot)$	probability density function
$P(\cdot)$	probability (mass) function
V	number of parameters of a mixture distribution component
$\boldsymbol{x}$	a sample, data vector
X	a set of vectors
A^*	Adjoint matrix, complex conjugate matrix: $\mathsf{A} = (a_{ij}) \Leftrightarrow \mathsf{A}^* = (\overline{a_{ji}})$
$\aleph(\cdot)$	the size of a set (cardinal number)
α_c	weight of the cth component in a mixture
$\boldsymbol{\mu}$	mean vector of a Gaussian distribution
ω_k	kth class
Σ	(variance-)covariance matrix of a Gaussian distribution
$\lvert\Sigma\rvert$	determinant of a covariance matrix
$\boldsymbol{\theta}$	full set of mixture distribution parameters

1 INTRODUCTION

1.1 Background

When something is measured a piece of data is acquired. Naturally measurements are never exact, and at least some kind of noise is always present in the data. Getting the data itself is not in the focus but the problem is to understand what does the data mean. That is, we need to classify the data. For example, if the vibration of an electric motor is measured, how can one tell from the results if the bearings have gone bad? The data is usually so vague or complex that we cannot just say ”If it is like this, then the case is that.” We need to develop a classifier that takes the data, examines it and gives a meaning to it according to experience and knowledge of the phenomena.

Classification is a very common task in information processing, and it is not generally easy. Some of the application areas are industrial quality control, object recognition from a visual image, and separating different voices from hum of voices. While these tasks might be easy for human beings they are very hard for machines. Even with the simplest cases there are noise and distortions affecting the measurement results and making the classification task nontrivial.

Classifier algorithms do not usually work well with raw data, such as a huge array of numbers representing a digital image. Data have to be preprocessed to extract few pieces of valuable information, called features. Features are represented as a feature vector where the dimension of a vector is the number of scalar components of different features. Feature extraction is very important for achieving good classification results and it is typically application specific. Usually each known sample, i.e., feature vector, is labeled to belong to a known class.

Feature vectors with class labels can be used to estimate a model describing a class, provided that there are enough good samples available. Some assumptions have to be made about the structure of the estimating model because totally arbitrary models are difficult to handle. For example in the Bayesian classification it can be assumed that a class can be represented in feature space with a Gaussian probability density function (PDF). The classification of unknown samples is based on estimated class representations in a feature space. [1]

1.2 Objectives and Restrictions

The purpose of this study is to familiarize with Bayesian classifier, Gaussian mixture probability density function models, and several maximum likelihood parameter estimation methods. Gaussian mixture model is a weighted sum of Gaussian probability density functions which are referred to as Gaussian components of the mixture model describing a class. The goal is to implement a Bayesian classifier that can handle any feasible number of variables (data dimensions), classes and Gaussian components of a mixture model.

Feature extraction is a crucial part of recognition systems, but it is not considered here. Data used in classification are assumed to come from a proper feature extraction, to be real valued, and not to have any missing values in samples. Data used in a classifier construction are assumed to contain class labels. Now training of a classifier is actually supervised learning.

The project was supposed to be started by an implemention of a simple classifier system of two classes for one-dimensional data and a single Gaussian component. The classifier system should have contained two main components: a training function and a classification function, both implemented in Matlab. Additionally it may have been made to work with complex valued data. Purpose was to implement more than one expectation maximization (EM) algorithms in the training functionality.

The training methods should be evaluated by testing how well they learn artificially generated and real world data. Purpose was to integrate the classification system into the facial evidence detection system [2, 3] developed by Kämäräinen et al. where it should challenge the Mahalanobis-distance-based sub-cluster classifier (SCC) method.

The director of the project is professor Heikki Kälviäinen and the project was supervised by researcher Joni Kämäräinen. The work supports research areas of Laboratory of Information Processing, Department of Information Technology, Lappeenranta University of Technology.

1.3 Structure of the Report

This report is organized as follows: In Section 2 the classifier overfitting scenario and the Bayesian classification are presented. Also Gaussian mixture models are introduced and

complex valued data are discussed with respect to Gaussian mixtures. Section 3 presents the maximum likelihood principle and the basic EM algorithm, and describes the other two variations of the EM algorithm. In Section 4 some implementation details concerning the GMMBayes Matlab toolbox are revealed. Experiments and results are presented in Section 5, and the report is concluded in Section 6.

2 FUNDAMENTALS

2.1 Classifier

Classifier is an algorithm with features as input and concludes what it means based on information that is encoded into the classifier algorithm and its parameters. The output is usually a label, but it can contain also confidence values.

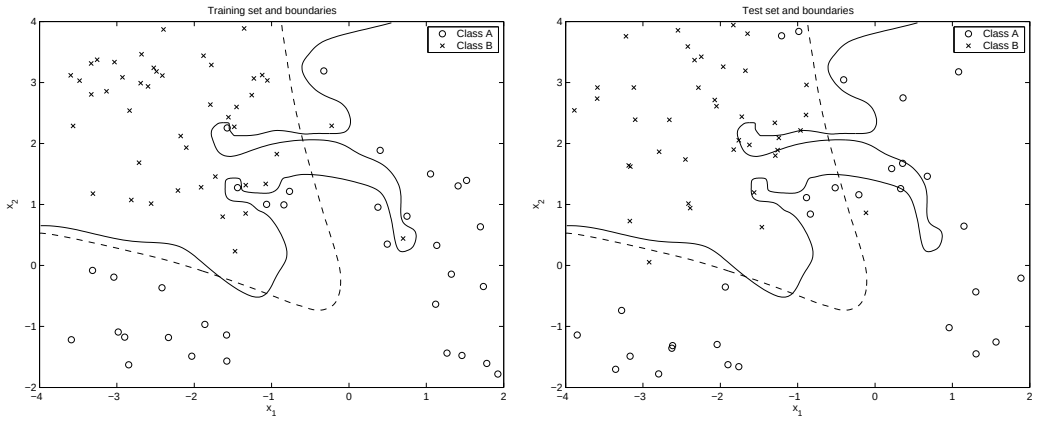
Knowledge of a classification task can be incorporated into a classifier by selecting an appropriate classifier type, for example a neural network, a distance transform or the Bayesian classifier. Knowledge is also required to determine a suitable inner structure for the classifier, for example the number of neurons and layers in a neural network classifier. For the Bayesian classifier the probability density models, or functions, need to be selected. The complexity of a classifier is determined mostly by these choices.

Classifier complexity is a tradeoff between representational power and generality for a task. A simple classifier may not be able to learn or represent classes well which yields poor accuracy. An overly complex classifier can lead to a situation shown in Figure 1: an overfitted classifier can classify the training data 100% correct, but when a different data set from the same task is presented, the accuracy can be poor. Therefore the training data is usually divided into two disjoint sets: an actual training set and a test set, so that the classifier performance can be estimated objectively.

A classifier can have numerous parameters that have to be adjusted according to the task. This is called training or learning. In supervised learning the training samples are labeled, and the training algorithm tries to minimize the classification error of the training set. In unsupervised learning or clustering the training samples are not labeled but the training algorithm tries to find clusters and form classes. In reinforcement learning the training samples are also not labeled, but the training algorithm uses feedback saying if it classifies a sample correctly or not. [1]

2.2 Bayesian Classification

Bayesian classification and decision making is based on probability theory and the principle of choosing the most probable or the lowest risk (expected cost) option [4].



(a) Training data plot.

(b) Test data plot.

Figure 1: Too complex decision boundary (solid line) can separate the training set without any errors (Fig. (a)), but it can make many mistakes with another data set (Fig. (b)). Dashed line is a more general boundary that leads to lower average classification error.

Assume that there is a classification task to classify feature vectors (samples) to K different classes. A feature vector is denoted as $\boldsymbol{x} = [x_1, x_2, \ldots, x_D]^T$ where D is the dimension of a vector. The probability that a feature vector $\boldsymbol{x}$ belongs to class ω_k is $P(\omega_k|\boldsymbol{x})$, and it is often referred to as a posteriori probability. The classification of the vector is done according to posterior probabilities or decision risks calculated from the probabilities.

The posterior probabilities can be computed with the Bayes formula

$$P(\omega_k|\boldsymbol{x}) = \frac{p(\boldsymbol{x}|\omega_k)P(\omega_k)}{p(\boldsymbol{x})} \tag{1}$$

where $p(\boldsymbol{x}|\omega_k)$ is the probability density function of class ω_k in the feature space and $P(\omega_k)$ is the a priori probability, which tells the probability of the class before measuring any features. If prior probabilities are not actually known, they can be estimated by the class proportions in the training set. The divisor

$$p(\boldsymbol{x}) = \sum_{i=1}^{K} p(\boldsymbol{x}|\omega_i)P(\omega_i) \tag{2}$$

is merely a scaling factor to assure that posterior probabilities are really probabilities, i.e., their sum is one.

It can be shown that choosing the class of the highest posterior probability produces the

minimum error probability [1, 4]. However, if the cost of making different kinds of errors is not uniform, the decision can be made with a risk function that computes the expected cost using the posterior probabilities, and choose the class with minimum risk.

The major problem in the Bayesian classifier is the class-conditional probability density function $p(\boldsymbol{x}|\omega_k)$. The function tells the distribution of feature vectors in the feature space inside a particular class, i.e., it describes the class model. In practice it is always unknown, except in some artificial classification tasks. The distribution can be estimated from the training set with a range of methods.

2.3 Gaussian Mixture Probability Density Function

The Gaussian probability density function in one dimension is a bell shaped curve defined by two parameters, mean μ and variance σ^2. In the D-dimensional space it is defined in a matrix form as

$$\mathcal{N}(\boldsymbol{x}; \boldsymbol{\mu}, \Sigma) = \frac{1}{(2\pi)^{D/2}|\Sigma|^{1/2}} \exp\left[-\frac{1}{2}(\boldsymbol{x}-\boldsymbol{\mu})^T\Sigma^{-1}(\boldsymbol{x}-\boldsymbol{\mu})\right] \tag{3}$$

where $\boldsymbol{\mu}$ is the mean vector and Σ the covariance matrix. In Figure 2 is shown an example of 2-dimensional Gaussian PDF. Equiprobability surfaces of a Gaussian are $\boldsymbol{\mu}$-centered hyperellipsoids.

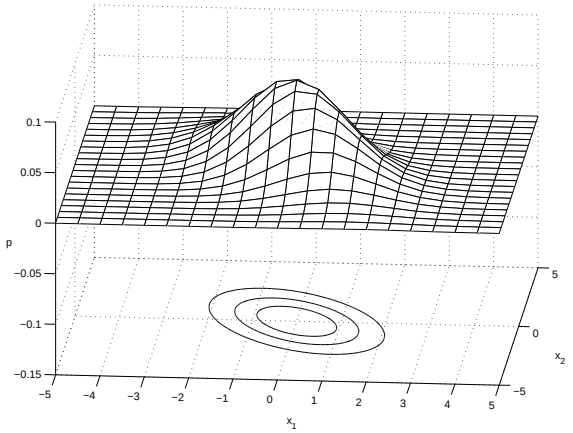


Figure 2: An example surface of two-dimensional Gaussian PDF with $\boldsymbol{\mu} = [0; 0]$ and $\Sigma = [1.56, -0.97; -0.97, 2.68]$ and contour plots (equiprobability surfaces) to emphasize the shape.

The Gaussian distribution is usually quite good approximation for a class model shape in a suitably selected feature space. It is a mathematically sound function and extends

easily to multiple dimensions. In the Gaussian distribution lies an assumption that the class model is truly a model of one basic class. If the actual model, the actual probability density function, is multimodal, it fails. For example, if we are searching for different face parts from a picture and there are several basic types of eyes, because of people from different races perhaps, the single Gaussian approximation would describe a wide mixture of all eye types, including patterns that might not look like an eye at all.

Gaussian mixture model (GMM) is a mixture of several Gaussian distributions and can therefore represent different subclasses inside one class. The probability density function is defined as a weighted sum of Gaussians

$$p(\boldsymbol{x};\boldsymbol{\theta}) = \sum_{c=1}^{C} \alpha_c \mathcal{N}(\boldsymbol{x};\boldsymbol{\mu}_c,\Sigma_c) \tag{4}$$

where α_c is the weight of the component c, $0 < \alpha_c < 1$ for all components, and $\sum_{c=1}^{C} \alpha_c = 1$. The parameter list

$$\boldsymbol{\theta} = \{\alpha_1, \boldsymbol{\mu}_1, \Sigma_1, \ldots, \alpha_C, \boldsymbol{\mu}_C, \Sigma_C\} \tag{5}$$

defines a particular Gaussian mixture probability density function. An example of Gaussian mixture model is shown in Figure 3. [5]

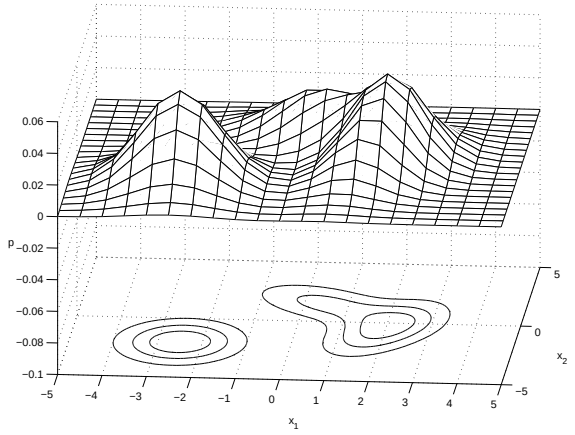


Figure 3: An example surface of a two-dimensional Gaussian mixture PDF with three components: $\alpha_1 = 0.40$, $\boldsymbol{\mu}_1 = [-2.5; -2]$, $\Sigma_1 = [0.81, 0; 0, 1.44]$, $\alpha_2 = 0.25$, $\boldsymbol{\mu}_2 = [0.5; 1.5]$, $\Sigma_2 = [1.30, -0.66; -0.66, 1.30]$ and $\alpha_3 = 0.35$, $\boldsymbol{\mu}_3 = [2.0; -0.5]$, $\Sigma_3 = [0.69, 0.61; 0.61, 2.36]$.

Estimation of the Gaussian mixture parameters for one class can be considered as unsupervised learning of the case where samples are generated by individual components of the mixture distribution and without the knowledge of which sample was generated by

which component. Clustering usually tries to identify the exact components, but Gaussian mixtures can also be used as an approximation of an arbitrary distribution.

2.4 Complex Valued Features

Some applications utilize complex valued features, for example describing the amplitude and phase of a sinusoidal signal. These features can be handled in three different ways. First, a single real value can be calculated from each complex attribute, by probably losing some information. Second, the complex value can be divided to two real values, which means that the length of feature vectors is doubled. Third, it might be possible to use the complex arithmetics directly.

The first approach is good in the sense that it reduces the dimensionality of a problem, which can lead to better performance even with small number of training data. If this is the case, it should have been done already in the feature extraction phase. On the other hand, combining two values into one can cause a loss of valuable information and the performance may degrade.

Dividing complex values into two parts, real and imaginary or modulus and argument, preserves all information, but increases the dimensionality of the problem. This can be a real problem with high dimensional complex valued data since the amount of training data may become insufficient or computation time increases too much.

Using the complex values directly is something between the two previous cases. It introduces a constraint to the Gaussian distribution model and requires little modifications in classifier training algorithms and the Gaussian PDF. If the transpose operation in Eq. 3 is changed to conjugate transpose, the resulting formula

$$\mathcal{N}(\boldsymbol{x}; \boldsymbol{\mu}, \Sigma) = \frac{1}{(2\pi)^{D/2}|\Sigma|^{1/2}} \exp\left[-\frac{1}{2}(\boldsymbol{x}-\boldsymbol{\mu})^{*}\Sigma^{-1}(\boldsymbol{x}-\boldsymbol{\mu})\right] \tag{6}$$

works also with complex valued $\boldsymbol{\mu}$ and Σ, assuming the covariance matrix is still positive definite. Changes in the training algorithms are explained later.

The constraint affects the shape of the distribution. It forces the shape of the density function to be spherical on each complex plane, eliminating the covariance between the real and imaginary part of a variable and making the variances equal.

The differences between approaches for using complex valued data in the Gaussian PDF are presented in Table 1. The degree of freedom here refers to an unknown value and the number of such values in the D-dimensional case are shown in the table. With the covariance matrix Σ the symmetry and real valued diagonal constraints are taken into account.

Table 1: Comparison of degrees of freedom in a single multivariate Gaussian density function with different approaches for using complex data.

	Degrees of Freedom	
Approach	$\boldsymbol{\mu}$	Σ
Convert to single real value	D	$\frac{1}{2}D^2 + \frac{1}{2}D$
Divide to two real values	$2D$	$2D^2 + D$
Use complex value	$2D$	D^2

3 GAUSSIAN MIXTURE DENSITY ESTIMATION

3.1 Maximum Likelihood Estimation

In construction of a Bayesian classifier the class-conditional probability density functions need to be determined. The initial model selection can be done for example by visualizing the training data, but the adjustment of the model parameters requires some measure of goodness, i.e., how well the distribution fits the observed data. Data likelihood is a such goodness value.

Assume that there is a set of independent samples $\mathsf{X} = \{\boldsymbol{x}_1, \ldots, \boldsymbol{x}_N\}$ drawn from a single distribution described by a probability density function $p(\boldsymbol{x}; \boldsymbol{\theta})$ where $\boldsymbol{\theta}$ is the PDF parameter list. The likelihood function

$$\mathcal{L}(\mathsf{X}; \boldsymbol{\theta}) = \prod_{n=1}^{N} p(\boldsymbol{x}_n; \boldsymbol{\theta}) \tag{7}$$

tells the likelihood of the data X given the distribution or, more specifically, given the distribution parameters $\boldsymbol{\theta}$. The goal is to find $\hat{\boldsymbol{\theta}}$ that maximizes the likelihood:

$$\hat{\boldsymbol{\theta}} = \arg\max_{\theta} \mathcal{L}(\mathsf{X}; \boldsymbol{\theta}). \tag{8}$$

Usually this function is not maximized directly but the logarithm

$$L(\mathsf{X}; \boldsymbol{\theta}) = \ln \mathcal{L}(\mathsf{X}; \boldsymbol{\theta}) = \sum_{n=1}^{N} \ln p(\boldsymbol{x}_n; \boldsymbol{\theta}), \tag{9}$$

called the log-likelihood function which is analytically easier to handle. Because of the monotonicity of the logarithm function the solution to Eq. 8 is the same using $\mathcal{L}(\mathsf{X}; \boldsymbol{\theta})$ or $L(\mathsf{X}; \boldsymbol{\theta})$. [4]

Depending on $p(\boldsymbol{x}; \boldsymbol{\theta})$ it might be possible to find the maximum analytically by setting the derivatives of the log-likelihood function to zero and solving $\boldsymbol{\theta}$. It can be done for a Gaussian PDF, which leads to the intuitive estimates for a mean and variance [1], but usually the analytical approach is intractable. In practice an iterative method such as the expectation maximization (EM) algorithm is used. Maximizing the likelihood may in some cases lead to singular estimates, which is the fundamental problem of maximum likelihood methods with Gaussian mixture models [5].

Recall the task of classifying vectors into K classes. If different classes can be seen as independent, i.e., training samples belonging to one class tell nothing about other classes, the estimation problem of K class-conditional PDFs can be divided into K separate estimation problems.

3.2 Basic EM Estimation

The expectation maximization (EM) algorithm is an iterative method for calculating maximum likelihood distribution parameter estimates from incomplete data (some elements missing in some feature vectors). It can also be used to handle cases where an analytical approach for maximum likelihood estimation is infeasible, such as Gaussian mixtures with unknown and unrestricted covariance matrices and means.

Assume that each training sample contains known features and missing or unknown features. Mark all good features of all samples with X and all unknown features of all samples with Y. The expectation step (E-step) for the EM algorithm is to form the function

$$Q(\boldsymbol{\theta}; \boldsymbol{\theta}^i) \equiv \mathrm{E}_{\mathsf{Y}}[\, \ln \mathcal{L}(\mathsf{X}, \mathsf{Y}; \boldsymbol{\theta}) \,|\, \mathsf{X};\, \boldsymbol{\theta}^i \,] \tag{10}$$

where $\boldsymbol{\theta}^i$ is the previous estimate for the distribution parameters and $\boldsymbol{\theta}$ is the variable for a new estimate describing the (full) distribution. $\mathcal{L}$ is the likelihood function (Eq. 7). The function calculates the likelihood of the data, including the unknown feature Y marginalized with respect to the current estimate of the distribution described by $\boldsymbol{\theta}^i$. The maximization step (M-step) is to maximize $Q(\boldsymbol{\theta}; \boldsymbol{\theta}^i)$ with respect to $\boldsymbol{\theta}$ and set

$$\boldsymbol{\theta}^{i+1} \leftarrow \arg\max_{\boldsymbol{\theta}} Q(\boldsymbol{\theta}; \boldsymbol{\theta}^i). \tag{11}$$

The steps are repeated until a convergence criterion is met. [1]

For the convergence criterion it is suggested in [1] that

$$Q(\boldsymbol{\theta}^{i+1}; \boldsymbol{\theta}^i) - Q(\boldsymbol{\theta}^i; \boldsymbol{\theta}^{i-1}) \leq T \tag{12}$$

with a suitably selected T and in [4] that

$$||\boldsymbol{\theta}^{i+1} - \boldsymbol{\theta}^i|| \leq \epsilon \tag{13}$$

for an appropriately chosen vector norm and ϵ. Common for both of these criteria is that iterations are stopped when the change in the values falls below a threshold. A more sophisticated criterion can be derived from Eq. 12 by using a relative rather than absolute rate of change.

The EM algorithm starts from an initial guess $\boldsymbol{\theta}^0$ for the distribution parameters and the log-likelihood is guaranteed to increase on each iteration until it converges. The convergence leads to a local or global maximum, but it can also lead to singular estimates, which is true particularly for Gaussian mixture distributions with arbitrary covariance matrices. The description of the general EM algorithm and also its application for the Gaussian mixture model can be found in [6, 1, 4].

The initialization is one of the problems of the EM algorithm. The selection of $\boldsymbol{\theta}^0$ (partly) determines where the algorithm converges or hits the boundary of the parameter space producing singular, meaningless results. Some solutions use multiple random starts or a clustering algorithm for initialization. [7]

The application of the EM algorithm to Gaussian mixtures according to [7] goes as follows. The known data X is interpreted as incomplete data. The missing part Y is the knowledge of which component produced each sample $\boldsymbol{x}_n$. For each $\boldsymbol{x}_n$ there is a binary vector $\boldsymbol{y}_n = \{y_{n,1}, \ldots, y_{n,C}\}$, where $y_{n,c} = 1$, if the sample was produced by the component c, or zero otherwise. The complete data log-likelihood is

$$\ln \mathcal{L}(\mathsf{X}, \mathsf{Y}; \boldsymbol{\theta}) = \sum_{n=1}^{N} \sum_{c=1}^{C} y_{n,c} \ln \left(\alpha_c \, p(\boldsymbol{x}_n | c; \boldsymbol{\theta}) \right). \tag{14}$$

The E-step is to compute the conditional expectation of the complete data log-likelihood, the Q-function, given X and the current estimate $\boldsymbol{\theta}^i$ of the parameters. Since the complete data log-likelihood $\ln \mathcal{L}(\mathsf{X}, \mathsf{Y}; \boldsymbol{\theta})$ is linear with respect to the missing Y, the conditional expectation $\mathsf{W} \equiv \mathrm{E}[\mathsf{Y} \,|\, \mathsf{X}, \boldsymbol{\theta}]$ has simply to be computed and put it into $\ln \mathcal{L}(\mathsf{X}, \mathsf{Y}; \boldsymbol{\theta})$. Therefore

$$Q(\boldsymbol{\theta}, \boldsymbol{\theta}^i) \equiv \mathrm{E}\left[\ln \mathcal{L}(\mathsf{X}, \mathsf{Y}; \boldsymbol{\theta}) \,|\, \mathsf{X}, \boldsymbol{\theta}^i \right] = \ln \mathcal{L}(\mathsf{X}, \mathsf{W}; \boldsymbol{\theta}) \tag{15}$$

where the elements of W are defined as

$$w_{n,c} \equiv \mathrm{E}\left[y_{n,c} \,|\, \mathsf{X}, \boldsymbol{\theta}^i \right] = \Pr\left[y_{n,c} = 1 \,|\, \boldsymbol{x}_n, \boldsymbol{\theta}^i \right]. \tag{16}$$

The probability can be calculated with the Bayes law

$$w_{n,c} = \frac{\alpha_c^i \, p(\boldsymbol{x}_n | c; \boldsymbol{\theta}^i)}{\sum_{j=1}^{C} \alpha_j^i \, p(\boldsymbol{x}_n | j; \boldsymbol{\theta}^i)} \tag{17}$$

where α_c^i is the a priori probability (of estimate $\boldsymbol{\theta}^i$) and $w_{n,c}$ is the a posteriori probability that $y_{n,c} = 1$ after observing $\boldsymbol{x}_n$. In other words, $w_{n,c}$ is the probability that $\boldsymbol{x}_n$ was produced by component c. [7]

Applying the M-step to the problem of estimating the distribution parameters for C-component Gaussian mixture with arbitrary covariance matrices, the resulting iteration formulas are as follows:

$$\alpha_c^{i+1} = \frac{1}{N} \sum_{n=1}^{N} w_{n,c} \tag{18}$$

$$\boldsymbol{\mu}_c^{i+1} = \frac{\sum_{n=1}^{N} \boldsymbol{x}_n w_{n,c}}{\sum_{n=1}^{N} w_{n,c}} \tag{19}$$

$$\Sigma_c^{i+1} = \frac{\sum_{n=1}^{N} w_{n,c} (\boldsymbol{x}_n - \boldsymbol{\mu}_c^{i+1})(\boldsymbol{x}_n - \boldsymbol{\mu}_c^{i+1})^T}{\sum_{n=1}^{N} w_{n,c}}. \tag{20}$$

The new estimates are gathered to $\boldsymbol{\theta}^{i+1}$ (Eq. 5). If the convergence criterion (Eqs. 12 or 13) is not satisfied, $i \leftarrow i + 1$ and Eqs. 17–20 are evaluated again with new estimates. [1]

The interpretation of the Eqs. 18–20 is actually quite intuitive. The weight α_c of a component is the portion of samples belonging to that component. It is computed by approximating the component-conditional PDF with the previous parameter estimates and taking the posterior probability of each sample point belonging to the component c (Eq. 17). The component mean $\boldsymbol{\mu}_c$ and covariance matrix Σ_c are estimated in the same way. The samples are weighted with their probabilities of belonging to the component, and then the sample mean and sample covariance matrix are computed.

It is worthwhile to note that so far the number of components C was assumed to be known. Clustering techniques try to find the true clusters and components from a training set, but our task of training a classifier only needs a good enough approximation of the distribution of each class. Therefore, C does not need to be guessed accurately, it is just a parameter defining the complexity of the approximating distribution. Too small C prevents the classifier from learning the sample distributions well enough and too large C may lead to an overfitted classifier. More importantly, too large C will definitely lead to singularities when the amount of training data becomes insufficient.

3.3 Figueiredo-Jain Algorithm

The Figueiredo-Jain (FJ) algorithm tries to overcome three major weaknesses of the basic EM algorithm. The EM algorithm presented in Section 3.2 requires the user to set the number of components and the number will be fixed during the estimation process. The FJ algorithm adjusts the number of components during estimation by annihilating components that are not supported by the data. This leads to the other EM failure point, the boundary of the parameter space. FJ avoids the boundary when it annihilates components that are becoming singular. FJ also allows to start with an arbitrarily large number of components, which tackles the initialization issue with the EM algorithm. The initial guesses for component means can be distributed into the whole space occupied by training samples, even setting one component for every single training sample. [7]

The classical way to select the number of mixture components is to adopt the "model-class/model" hierarchy, where some candidate models (mixture PDFs) are computed for each model-class (number of components), and then select the "best" model. The idea behind the FJ algorithm is to abandon such hierarchy and to find the "best" overall model directly. Using the minimum message length criterion and applying it to mixture models leads to the objective function

$$\Lambda(\boldsymbol{\theta}, \mathsf{X}) = \frac{V}{2} \sum_{c:\, \alpha_c > 0} \ln(\frac{N\alpha_c}{12}) + \frac{C_{\mathrm{nz}}}{2} \ln \frac{N}{12} + \frac{C_{\mathrm{nz}}(V+1)}{2} - \ln \mathcal{L}(\mathsf{X}, \boldsymbol{\theta}) \qquad (21)$$

where N is the number of training points, V is the number of free parameters specifying a component, and C_{nz} is the number of components with nonzero weight in the mixture ($\alpha_c > 0$). $\boldsymbol{\theta}$ in the case of Gaussian mixture is the same as in Eq. 5. The last term $\ln \mathcal{L}(\mathsf{X}, \boldsymbol{\theta})$ is the log-likelihood of the training data given the distribution parameters $\boldsymbol{\theta}$ (Eq. 9). [7]

The EM algorithm can be used to minimize Eq. 21 with a fixed C_{nz} [7]. It leads to the M-step with component weight updating formula

$$\alpha_c^{i+1} = \frac{\max\left\{0, \left(\sum_{n=1}^{N} w_{n,c}\right) - \frac{V}{2}\right\}}{\sum_{j=1}^{C} \max\left\{0, \left(\sum_{n=1}^{N} w_{n,j}\right) - \frac{V}{2}\right\}}. \qquad (22)$$

This formula contains an explicit rule of annihilating components by setting their weights to zero. Other distribution parameters are updated as in Eqs. 19 and 20. [7]

The above M-steps are not suitable for the basic EM algorithm though. When initial C is high, it can happen that all weights become zero because none of the components have enough support from the data. Therefore a component-wise EM algorithm (CEM) is adopted. CEM updates the components one by one, computing the E-step (updating W) after each component update, where the basic EM updates all components "simultaneously". When a component is annihilated its probability mass is immediately redistributed strengthening the remaining components. [7]

When CEM converges, it is not guaranteed that the minimum of $\Lambda(\boldsymbol{\theta}, \mathsf{X})$ is found, because the annihilation rule (Eq. 22) does not take into account the decrease caused by decreasing C_{nz}. After convergence the component with the smallest weight is removed and the CEM is run again, repeating until $C_{\mathrm{nz}} = 1$. Then the estimate with the smallest $\Lambda(\boldsymbol{\theta}, \mathsf{X})$ is chosen. [7]

The implementation of the FJ algorithm uses a modified cost function instead of $\Lambda(\boldsymbol{\theta}, \mathsf{X})$. The derivation of the modified cost function is presented in Appendix 1.

Hitherto the only things assumed for the mixture distribution are that an EM algorithm can be written for it and all components are parameterized the same way (number of parameters V for a component). With Gaussian mixture model the number of parameters per component $V = D + \frac{1}{2}D^2 + \frac{1}{2}D$ in the case of real valued data and arbitrary covariance matrices. With complex valued data the number of real free parameters $V = 2D + D^2$ where D is the dimensionality of the (complex) data. It would seem logical to choose this value for V instead of the previous one defined with real valued data. As seen in Eq. 22 this amplifies the annihilation which makes sense because there are more degrees of freedom in a component. On the other hand there are more training data with the same number of training points, because the data is complex (two values in one variable as opposed to one value). The nature of complex data with Gaussian PDF has been discussed in Section 2.4.

3.4 Greedy EM Algorithm

The greedy algorithm starts with a single component and then adds components into the mixture one by one. The optimal starting component for a Gaussian mixture is trivially computed, optimal meaning the highest training data likelihood. The algorithm repeats two steps: insert a component into the mixture, and run EM until convergence. Inserting

a component that increases the likelihood the most is thought to be an easier problem than initializing a whole near-optimal distribution. Component insertion involves searching for the parameters for only one component at a time. Recall that EM finds a local optimum for the distribution parameters, not necessarily the global optimum which makes it initialization dependent method.

Let p_C denote a C-component mixture with parameters $\boldsymbol{\theta}_C$. The general greedy algorithm for Gaussian mixture is as follows [8]:

1. Compute the optimal (in the ML sense) one-component mixture p_1 and set $C \leftarrow 1$.
2. Find a new component $\mathcal{N}(\boldsymbol{x}; \boldsymbol{\mu}', \Sigma')$ and corresponding mixing weight α' that increase the likelihood the most:

$$\{\boldsymbol{\mu}', \Sigma', \alpha'\} = \arg \max_{\{\boldsymbol{\mu}, \Sigma, \alpha\}} \sum_{n=1}^{N} \ln[(1-\alpha)p_C(\boldsymbol{x}_n) + \alpha \mathcal{N}(\boldsymbol{x}_n; \boldsymbol{\mu}, \Sigma)] \qquad (23)$$

   while keeping p_C fixed.
3. Set $p_{C+1}(\boldsymbol{x}) \leftarrow (1-\alpha')p_C(\boldsymbol{x}) + \alpha'\mathcal{N}(\boldsymbol{x}; \boldsymbol{\mu}', \Sigma')$ and then $C \leftarrow C+1$.
4. Update p_C using EM (or some other method) until convergence. [optional]
5. Evaluate some stopping criterion; go to Step 2 or quit.

The stopping criterion in Step 5 can be for example any kind of model selection criterion, wanted number of components, or a minimum message length criterion.

The crucial point is of course Step 2. Finding the optimal new component requires a global search, which is performed by creating CN_{cand} candidate components. The number of candidates will increase linearly with the number of components C, having N_{cand} candidates per each existing component. The candidate resulting in the highest likelihood when inserted into the (previous) mixture is selected. The parameters and weight of the best candidate are then used in Step 3 instead of the truly optimal values. [8].

The candidates for executing Step 2 are initialized as follows: the training data set X is partitioned into C disjoint data sets $\{\mathsf{A}_c\}$, $c = 1 \ldots C$, according to the posterior probabilities of individual components; the data set is Bayesian classified by the mixture components. From each A_c number of N_{cand} candidates are initialized by picking uniformly randomly two data points $\boldsymbol{x}_l$ and $\boldsymbol{x}_r$ in A_c. The set A_c is then partitioned into two using the

smallest distance selection with respect to $\boldsymbol{x}_l$ and $\boldsymbol{x}_r$. The mean and covariance of these two new subsets are the parameters for two new candidates. The candidate weights are set to half of the weight of the component that produced the set A_c. Then new $\boldsymbol{x}_l$ and $\boldsymbol{x}_r$ are drawn until N_{cand} candidates are initialized with A_c. The partial EM algorithm is then used on each of the fresh set of candidates. The partial EM differs from the EM and CEM algorithms by optimizing (updating) only one component of a mixture, it does not change any other components. In order to reduce the time complexity of the algorithm a lower bound on the log-likelihood is used instead of the true log-likelihood. The lower-bound log-likelihood is calculated with only the points in the respective set A_c. The partial EM update equations are as follows:

$$w_{n,C+1} = \frac{\alpha \mathcal{N}(\boldsymbol{x}_n; \boldsymbol{\mu}, \Sigma)}{(1-\alpha)p_C(\boldsymbol{x}) + \alpha \mathcal{N}(\boldsymbol{x}; \boldsymbol{\mu}, \Sigma)} \tag{24}$$

$$\alpha = \frac{1}{\aleph(\mathsf{A}_c)} \sum_{n \in \mathsf{A}_c} w_{n,C+1} \tag{25}$$

$$\boldsymbol{\mu} = \frac{\sum_{n \in \mathsf{A}_c} w_{n,C+1} \boldsymbol{x}_n}{\sum_{n \in \mathsf{A}_c} w_{n,C+1}} \tag{26}$$

$$\Sigma = \frac{\sum_{n \in \mathsf{A}_c} w_{n,C+1} (\boldsymbol{x}_n - \boldsymbol{\mu})(\boldsymbol{x}_n - \boldsymbol{\mu})^T}{\sum_{n \in \mathsf{A}_c} w_{n,C+1}} \tag{27}$$

where $\aleph(\mathsf{A}_c)$ is the number of training samples in the set A_c. These equations are much like the basic EM update Eqs. 18–20. The partial EM iterations are stopped when the relative change in log-likelihood of the resulting $C+1$ -component mixture drops below threshold or maximum number of iterations is reached. When the partial EM has converged the candidate is ready to be evaluated. [8]

4 GMMBAYES TOOLBOX

4.1 GMMBayes Matlab Toolbox Interface

The developed Matlab functions for different algorithms and the Bayesian classifier were wrapped into a common function interface and packaged as the GMMBayes Matlab Toolbox which is available from the web site [9]. The basic interface consists of the functions `gmmb_create` (create and train GMM) and `gmmb_classify` (classify samples with the Bayesian or Mahalanobis distance classifier). There is also a higher level interface of the functions `gmmb` and `newgmmb`, but it is just a simple wrapper for the basic interface functions that provides an abstraction layer to allow the use of other classification tools in a portable way. The function (or m-file) call graph is shown in Figure 4.

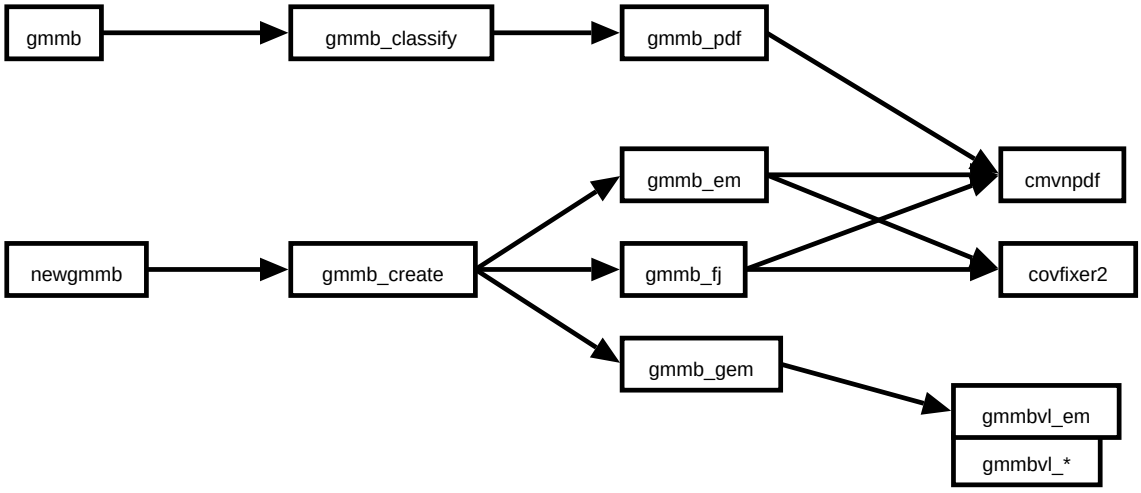


Figure 4: Function call graph of the GMMBayes Matlab Toolbox.

Under the `gmmb_create` interface there are the implementations of three introduced algorithms. Each one of them uses different parameters, so the parameter list should be built individually consulting the desired function. All function m-files contain usage documentation and parameter descriptions.

All `gmmbvl_*` functions have been downloaded from the home page of Dr. Nikos Vlassis (link provided in [9]).

4.2 Avoiding Covariance Matrix Singularities

The EM algorithm tends to converge to a singular solution, especially when training data is (nearly) insufficient. The FJ algorithm does not suffer from this, but still the training data may sometimes lead to an invalid covariance matrix.

Function `covfixer2` takes a candidate covariance matrix and returns a slightly modified matrix that fulfills the requirements for a valid covariance matrix (semipositive definite, complex conjugate symmetric). If the input matrix is already valid, it is returned as is.

In the function the matrix is forced to complex conjugate symmetric as follows:

$$\Sigma \leftarrow \Sigma - \frac{\Sigma - \Sigma^*}{2}. \tag{28}$$

Possible imaginary components are removed from the diagonal, which results in a Hermitian matrix. Then it is tested for positive definiteness (Cholesky factorization), and while the test fails one of two things is done: i) If there is a negative element in the diagonal, then one percent of the maximum element in the diagonal is added to all diagonal elements; ii) Otherwise all the diagonal elements are increased by one percent.

By growing the covariance matrix diagonal we try to get rid of singular matrices. The iterative algorithm, which called the `covfixer2` function, is supposed to fix the possible ill effects of the matrix modifications on next iterations, but it may also lead again to a singular covariance matrix; algorithm starts to oscillate and may jam.

4.3 Algorithm Implementation Details

The Gaussian probability density function is evaluated in `cmvnpdf` function, which is a modified version of the Matlab R13 `mvnpdf` function, since it does not handle complex valued data correctly.

The `gmmb_classify` function can additionally classify samples according to Mahalanobis distance, where the distance is computed to each component of each trained class. This method ignores all a priori and component weight information. When using the function to classify using the Bayesian rule, the function can output either only a class label or all posterior probabilities for each sample.

The EM implementation uses fuzzy c-means clustering for initializing the component means. Component covariance matrices are initialized to diagonal part of the whole data covariance matrix. Weights are set to equal. The `covfixer2` function is used on every iteration. The algorithms stops when relative change[1] of the log-likelihood of the data falls below a threshold. The implementation can compute with complex data directly.

In the Figueiredo-Jain algorithm implementation component mean vectors are initialized to random data points. Covariance matrices are initialized to $\sigma^2 I$, where I is the unitary matrix and σ^2 is one tenth of the maximum of the diagonal of the whole data covariance matrix. Initial component weights are equal. The `covfixer2` function is used on every iteration of the component-wise EM algorithm. The stopping criteria for the component-wise EM is a threshold in the relative change of the data log-likelihood, and the whole algorithm stops when the minimum number of components is reached and CEM has converged. The FJ implementation also computes with complex data.

The greedy EM implementation contains a trivial initialization step, because it starts from a single Gaussian component; the standard mean and covariance of the data. The stopping condition for the partial EM when creating candidates is the relative change in data log-likelihood falling below 0.01 or number of iterations reaching 20. After all candidates are created one of the candidate components is selected and then it is updated again with partial EM with relative log-likelihood change threshold 10^{-5}. The change in the log-likelihood when inserting the new component is checked and the component is inserted if the log-likelihood increases. Otherwise the algorithm stops. The whole mixture updating EM is stopped when the relative change in log-likelihood falls below 10^{-5}.

[1] Originally it was the absolute change, but it was changed in gmmb_em.m revision 1.7.

5 EXPERIMENTS

Three different data sets were used in the experiments: forest spectral colors, artificial waveforms and noise, and letter image recognition data. The tests were run with the following parameters:

EM

relative log-likelihood change threshold:	10^{-5}
number of mixture components:	1 to 8

Figueiredo-Jain

relative log-likelihood change threshold:	10^{-5}
maximum number of mixture components:	4, 8, 16, 32, 64

Greedy EM

maximum number of mixture components:	4, 8, 16, 32, 64
number of candidates per existing component:	8

For each algorithm the number of components was varied.

In a test round a data set was randomly divided into three: the test data, the training data and unused data. The test data was always 30% of the data set and the training data was varied from 20% to 70% with ten percent unit steps. The division algorithm assures that the training and test data sets are non-overlapping and the class proportions remain the same in the three subsets and the data set.

A test round produced an accuracy ratio (correctly classified samples in the test data set), the estimated Gaussian mixture model and miscellaneous data about the used algorithm. One test round was repeated three times with the same parameters and data sets. For each set of parameters the training and test sets were randomly created five times. This method totals to 15 test rounds per a test run with each fixed parameters, algorithm and data set. Description of the result file format is in Appendix 2.

Because the FJ and GEM can produce different number of components for different classes within a single test round, the maximum number of components of class models is used to describe the result of a round. The crashed runs are taken into account as zero accuracy.

An algorithm crash is a situation where the algorithm did not produce a final mixture estimate and cannot continue. For example in the EM algorithm a covariance matrix becomes undefined, or in the FJ algorithm all mixture components get annihilated.

Test runs were executed for every combination of data set, parameter and algorithm mentioned in this section.

5.1 Forest Spectral Colors

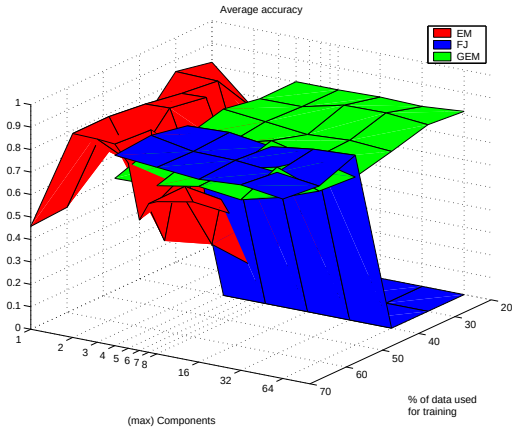
The forest colors set contains samples of reflectance spectra of pine, spruce and birch. The spectra is recorded in wavelength interval 390 nm – 850 nm with 5 nm resolution which leads to 93-element sample vectors. There are 349 samples from spruce, 337 from birch and 370 from pine. [10]

The data is too high-dimensional to be used directly, and it was thus transformed with neighbor-bank projection [11] to 23, 15 and 10-dimensional data sets with $\cos^2$ bank shape. The 23-dimensional case was near the classification accuracy optimum in [11], and 15 and 10-dimensional cases were created in case 23 dimensions would be too much for the algorithms considering the amount of training data.

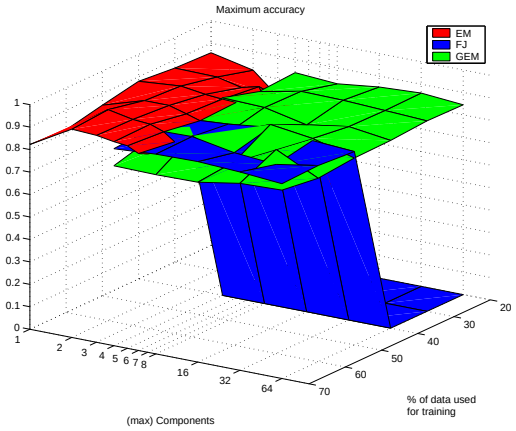
The results are presented as follows: Figure 5 with the 23-dimensional forest colors data, Figure 6 with the 15-dimensional data and Figure 7 with the 10-dimensional data. With these data sets the EM algorithm provides the best classification accuracy with two components though in Figure 7(d) the performance remains steady up to seven components. The FJ and GEM algorithms perform comparably with the 23-d and 15-d sets, GEM little worse with the 10-d set. GEM chose always only one component so its stable performance is not a surprise. FJ also chose only one component with the 23-d data, but produced also two-component estimates with 15-d and 10-d data (Figs. 6(d), 7(d)). The two-component estimates of FJ were not better than the one-component estimates.

In Figures 5(c), 6(c) and 7(c) it is shown that the EM algorithm is quite unstable and crashes more often with higher a number of mixture components. Why it crashes with one component (Fig. 5(c)) is a mystery. The FJ algorithm has a clear limit of how much training data is required before it works at all, and it depends on the data dimension. This can be traced back to the annihilation step in Eq. 22. Below this limit all mixture components are annihilated and the FJ algorithm crashes. The GEM algorithm did not

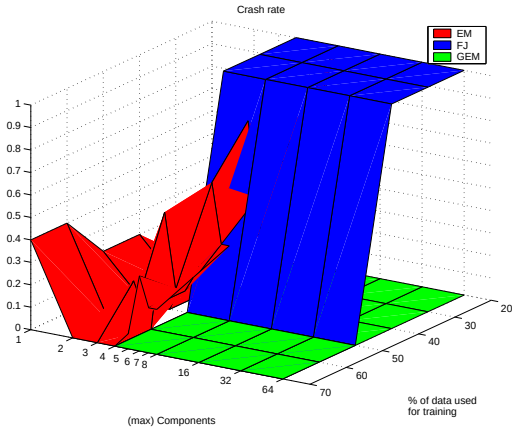
crash at all.



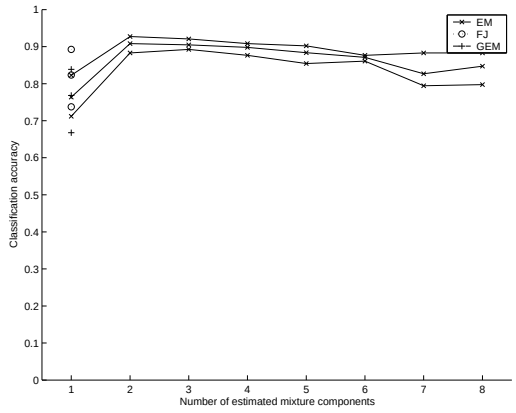
(a) Average classifi cation accuracy.



(b) Maximum classifi cation accuracy.

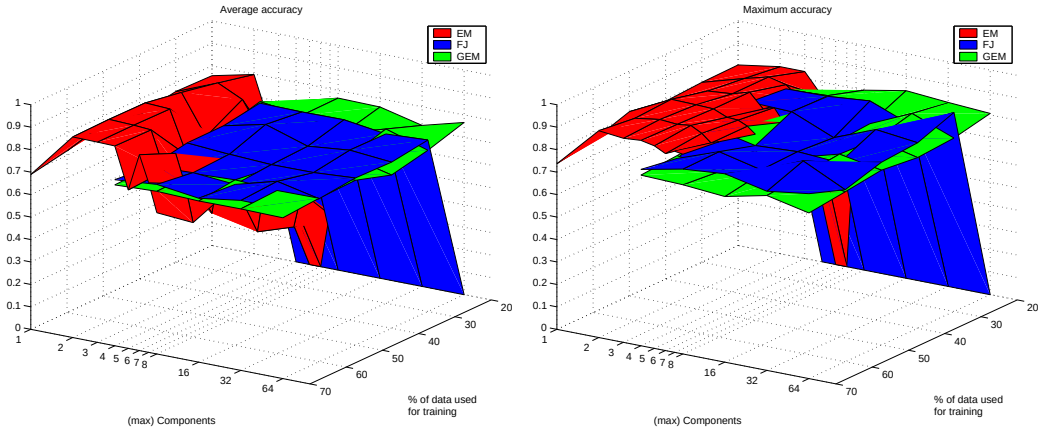


(c) Crash rates.



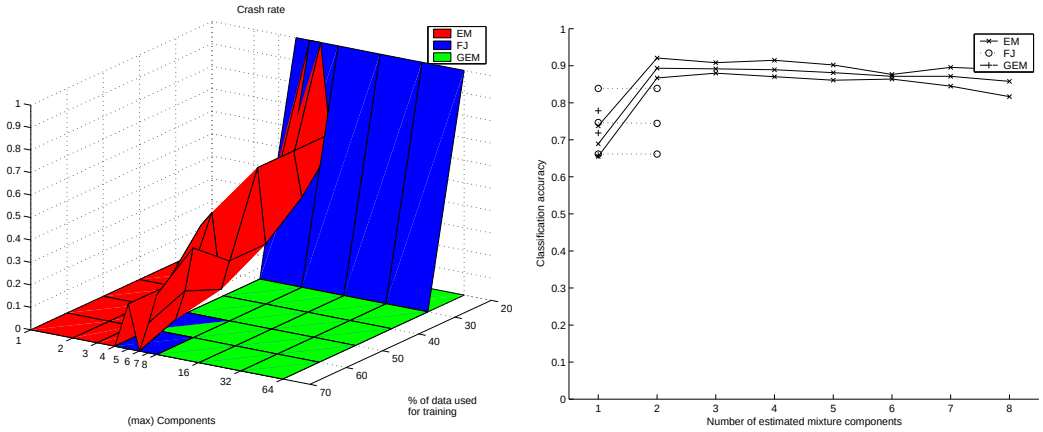
(d) Maximum, average and minimum classifi cation accuracy vs. produced mixture estimate complexity.

Figure 5: Results for the 23-dimensional forest colors data. In (a)–(c) each point is a statistic of 15 test rounds. Plot (d) is made with 70% of data used for training.



(a) Average classifi cation accuracy.

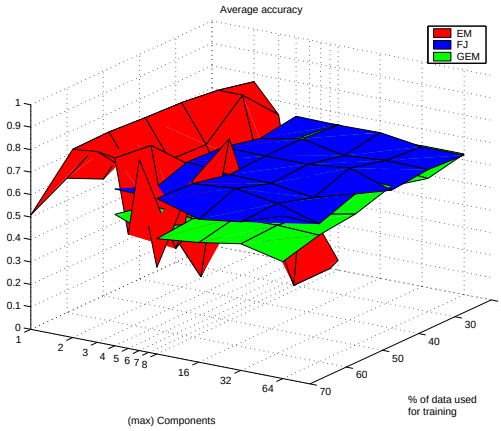
(b) Maximum classifi cation accuracy.



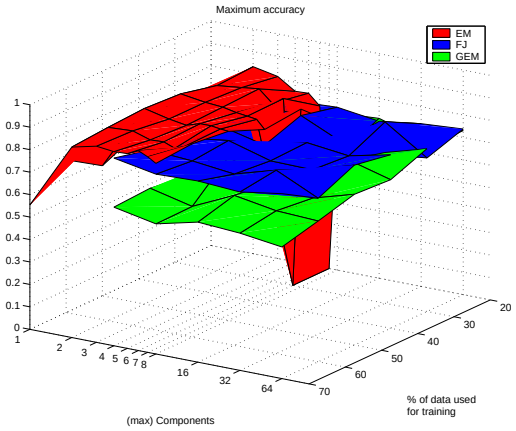
(c) Crash rates.

(d) Maximum, average and minimum classifi cation accuracy vs. produced mixture estimate complexity.

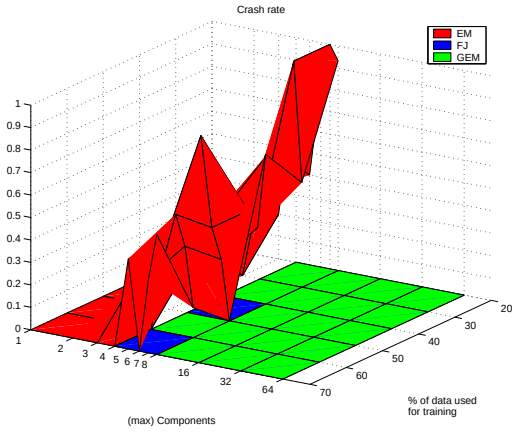
Figure 6: Results for the 15-dimensional forest colors data. In (a)–(c) each point is a statistic of 15 test rounds. Plot (d) is made with 70% of data used for training.



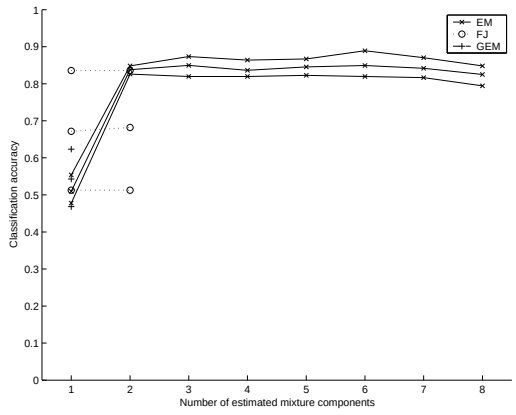
(a) Average classifi cation accuracy.



(b) Maximum classifi cation accuracy.



(c) Crash rates.



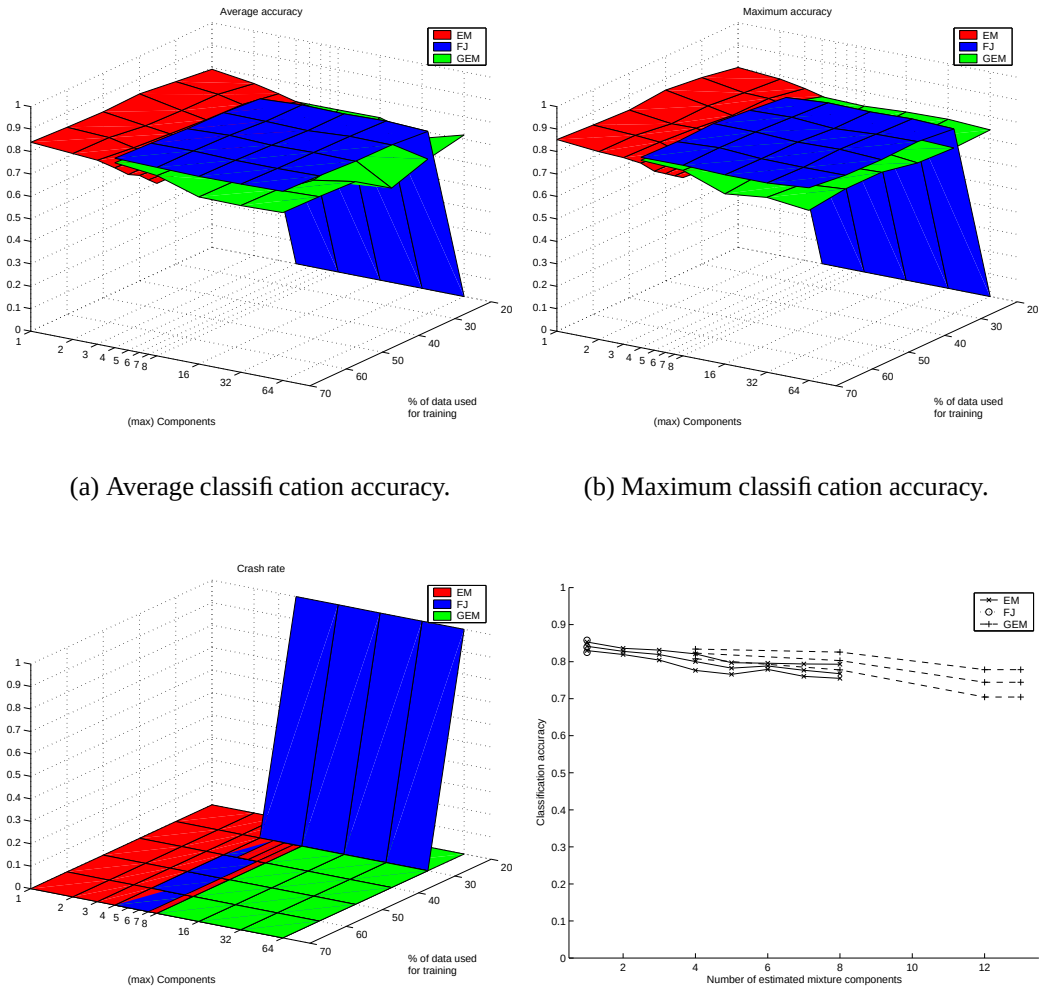
(d) Maximum, average and minimum classifi cation accuracy vs. produced mixture estimate complexity.

Figure 7: Results for the 10-dimensional forest colors data. In (a)–(c) each point is a statistic of 15 test rounds. Plot (d) is made with 70% of data used for training.

5.2 Waveforms and Noise

Waveforms and noise data is an artificial data set from three classes of waves [12]. The data set was retrieved from the UCI Machine Learning Repository [13] and it contained 5000 samples with equal class distributions. A sample is a 40-element vector, where the first 21 elements are real attributes with added noise (zero mean, unity variance) and the last 19 elements are pure noise. All vector elements are real valued. The optimal Bayes classification accuracy is 86% [12].

The results with the waveforms and noise data set are in Figure 8.



(a) Average classification accuracy.

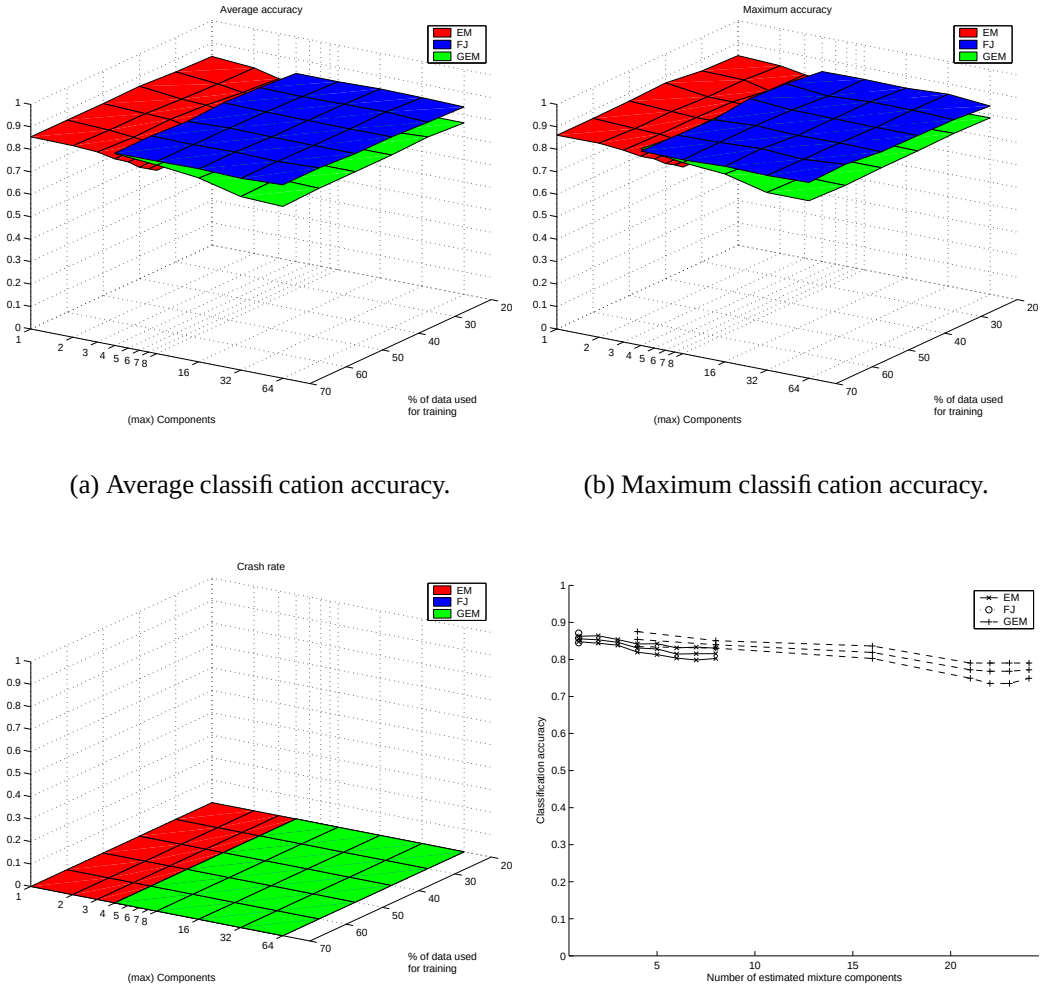
(b) Maximum classification accuracy.

(c) Crash rates.

(d) Maximum, average and minimum classification accuracy vs. produced mixture estimate complexity.

Figure 8: Results for the waveforms and noise data. In (a)–(c) each point is a statistic of 15 test rounds. Plot (d) is made with 70% of data used for training.

Another test was executed with the pure noise components excluded, using only the first 21 elements of the sample vectors. The results with that data set are in Figure 9.



(a) Average classification accuracy.

(b) Maximum classification accuracy.

(c) Crash rates.

(d) Maximum, average and minimum classification accuracy vs. produced mixture estimate complexity.

Figure 9: Results for the waveforms data without pure noise components. In (a)–(c) each point is a statistic of 15 test rounds. Plot (d) is made with 70% of data used for training.

The performance of all algorithms is quite near the reported optimum with these data sets and only FJ crashes for too little training data in the 20% case with the 40-dimensional data. The FJ algorithm always chooses just one component into mixtures which makes it the best and most stable algorithm for these data sets. GEM produces too complex estimates with the 40-dimensional data set and overfitting shows as degrading performance as the complexity grows. The EM algorithm shows also the effect of overfitting. Surprisingly GEM estimates with four components per mixture manage to reach the same accuracy as FJ with the 21-dimensional data.

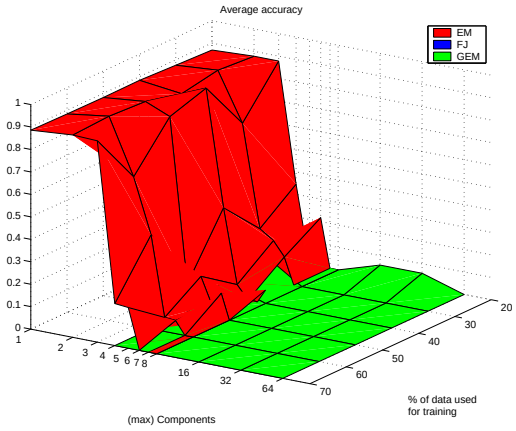
5.3 Letter Image Recognition Data

The letter image recognition data is an artificial data set containing 20,000 16-element sample vectors. The black-and-white letter images were generated from 20 different fonts using 26 different uppercase letters and adding random distortions. The sample vectors were calculated from those images, and include attributes such as mean x and y variance of pixels. [14]

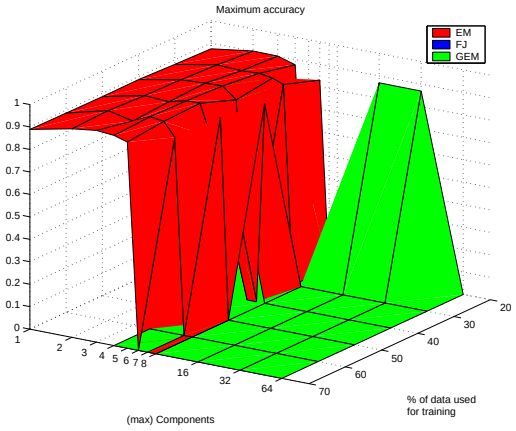
The data set was retrieved from the UCI Machine Learning Repository [13]. All attributes were already transformed to integers in the range $[0, 15]$ which makes this data set difficult, because the algorithms were coded for real valued, not integer, data. The class distribution of the 26 classes (letters) ranged from 734 to 813 samples per class. The best classification accuracy obtained in [14] was a little over 80%.

The results with the letter image recognition data set are shown in Figure 10.

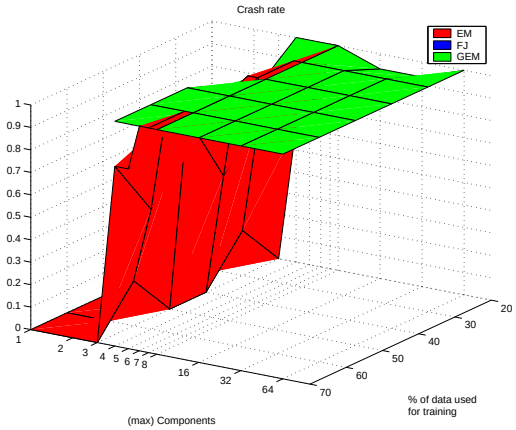
The data set proved to be very difficult indeed, only the EM implementation produced results. FJ did not finish a single test round within reasonable time and thus there are no results from FJ, and only in few test rounds GEM did not crash (Fig. 10(c)). The EM implementation is quite reliable with one, two and even three components for mixtures and produces classification accuracies near 90% (Fig. 10(d)).



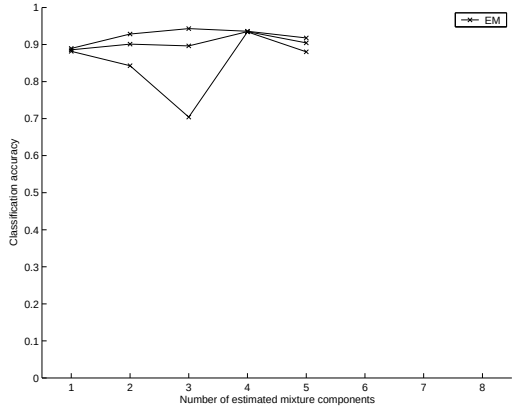
(a) Average classifi cation accuracy.



(b) Maximum classifi cation accuracy.



(c) Crash rates.



(d) Maximum, average and minimum classifi cation accuracy vs. produced mixture estimate complexity.

Figure 10: Results for the letter recognition data. In (a)–(c) each point is a statistic of 15 test rounds. Plot (d) is made with 70% of data used for training. The FJ algorithm did not produce any results.

6 CONCLUSIONS

The goal for this project is well achieved, although it took over a year to complete. The Bayesian classifier using Gaussian mixtures is functional and the three different Gaussian mixture estimation algorithms are available in the developed GMMBayes Matlab Toolbox. The experiments show that the toolbox is working well and that there are differences in the behavior of the three implemented estimation algorithms.

There are some projection errors in the 3-dimensional graphs due to the way Matlab and PostScript handle the vector graphics, but they should not obscure the results. Corretly projected bitmap images can found at [9].

The EM implementation requires the user to set the number of components a priori for each mixture, but seems to outperform the other algorithms if a good number is found. Another downside of EM is its crash rate, but as the letter image recognition data experiments proved, it can work in situations where the other algorithms fail.

The FJ implementation determines the number of components by itself, going down from the user defined maximum. FJ also produced better classification accuracies than the GEM implementation, but FJ has a failure mode too: its minimum requirement for the number of training samples is higher than with the other algorithms. For some reason FJ could not produce a single mixture estimate with the letter image recognition data, although in preliminary tests during the development FJ did produce results.

The GEM implementation also determines the number of components by itself, inserting components one by one. GEM was the most stable implementation on average, looking at the crash rates, but produced generally a little worse classification accuracies than FJ. GEM produced results where the FJ implementation failed, except with the letter image recognition data, where they both failed.

The EM and FJ implementations work also with complex valued data, using complex arithmetics. The effects of the different approaches to using complex valued data described in Section 2.4 were not tested, but it would be an interesting topic, though the behavior might be application dependent.

The GMMBayes Toolbox was incorporated in the facial evidence detection system [2, 3] developed by Kämäräinen et al. where it outperformed the SCC method. The results can

be found in [15].

The GMMBayes Matlab Toolbox is already in use or to be used in several other projects at the Laboratory of Information Processing in Lappeenranta university of Technology.

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APPENDIX 1. Derivation of the FJ Cost Function

The objective function was defined in Eq. 21 as

$$\Lambda(\boldsymbol{\theta}, \mathsf{X}) = \frac{V}{2} \sum_{c:\, \alpha_c > 0} \ln\left(\frac{N\alpha_c}{12}\right) + \frac{C_{\mathrm{nz}}}{2} \ln\frac{N}{12} + \frac{C_{\mathrm{nz}}(V+1)}{2} - \ln \mathcal{L}(\mathsf{X}, \boldsymbol{\theta}).$$

The log-likelihood is not of interest here and it is discarded during the deriving. By decomposing the logarithms of products into sums of logarithms we get

$$\frac{V}{2} \sum_{c:\, \alpha_c > 0} (\ln N + \ln \alpha_c - \ln 12) + \frac{C_{\mathrm{nz}}}{2}(\ln N - \ln 12) + \frac{C_{\mathrm{nz}}(V+1)}{2}.$$

The only thing dependent on c inside the sum is $\ln \alpha_c$ so the other terms can be taken out. C_{nz} is defined as the number of summables.

$$\frac{V}{2} \sum_{c:\, \alpha_c > 0} \ln \alpha_c + \frac{VC_{\mathrm{nz}}}{2}(\ln N - \ln 12) + \frac{C_{\mathrm{nz}}}{2}(\ln N - \ln 12) + \frac{C_{\mathrm{nz}}(V+1)}{2}$$

Rearranging the terms and adding the log-likelihood back we get

$$\frac{V}{2} \sum_{c:\, \alpha_c > 0} \ln \alpha_c + \frac{C_{\mathrm{nz}}(V+1)}{2} \ln N + (V+1)(1 - \ln 12) - \ln \mathcal{L}(\mathsf{X}, \boldsymbol{\theta}).$$

Recalling the message length interpretation of Eq. 21 the term $(V+1)(1-\ln 12)$ can be discarded because it is an irrelevant additive constant which does not depend on the data or component weights of the mixture (V is the parameter count for one component). Therefore the final cost function to be minimized is

$$\Lambda'(\boldsymbol{\theta}, \boldsymbol{X}) = \frac{V}{2} \sum_{c:\, \alpha_c > 0} \ln \alpha_c + \frac{C_{\mathrm{nz}}(V+1)}{2} \ln N - \ln \mathcal{L}(\mathsf{X}, \boldsymbol{\theta}).$$

APPENDIX 2. Experiment Save File Format

The result save file is a MAT-file with two variables: `desc` and `results`. It is produced by the `testrun` function which takes the `desc` as argument.

The `desc` is a structure with fields:

`datafile`	the input data file name
`method`	EM, FJ or GEM
`params`	cell array of algorithm specific parameters
`trainsizes`	vector of relative training set sizes
`redivs`	number of division repetitions
`iters`	number of test run repetitions
`savefile`	the result save file name

The `results` variable is a `length(trainsizes)` long cell array of structures:

`sets{redivs}`	cell array of data division label vectors
`rounds{redivs}`	cell array of arrays of the `round` structures
`trainsize`	the training set size used

The `round[iters]` array of structures:

`bayesS`	structure describing the estimated Gaussian mixture model
`stats`	miscellaneous information about the test run
`accuracy`	the test set classification accuracy

The `stats` field is a number of classes long cell array of structures with fields depending on the used algorithm and logging level:

`iterations`	algorithm iterations, all algorithms
`covfixer2`	covariance fixer running counts, EM and FJ
`loglikes`	history of the log-likelihood, all algorithms
`initialmix`	the initial guess, EM and FJ, extra logging
`mixtures`	history of the mixture model, EM and FJ, extra logging
`costs`	development of the FJ cost function
`annihilations`	FJ component annihilation history