DETECTING BIMODALITY IN ASTRONOMICAL DATASETS

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ABSTRACT

We discuss statistical techniques for detecting and quantifying bimodality in astronomical datasets. We concentrate on the KMM algorithm, which estimates the statistical significance of bimodality in such datasets and objectively partitions data into sub-populations. By simulating bimodal distributions with a range of properties we investigate the sensitivity of KMM to datasets with varying characteristics. Our results facilitate the planning of optimal observing strategies for systems where bimodality is suspected. Mixture-modeling algorithms similar to the KMM algorithm have been used in previous studies to partition the stellar population of the Milky Way into subsystems. We illustrate the broad applicability of KMM by analysing published data on globular cluster metallicity distributions, velocity distributions of galaxies in clusters, and burst durations of gamma-ray sources. FORTRAN code for the KMM algorithm and directions for its use are available from the authors upon request.

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1. INTRODUCTION

Many astronomical systems exhibit some form of clustering in their constituents. This concept is most familiar in systems where the clustering is spatial, such as in clusters of galaxies, but clustering may be present in any variable. For instance, the metallicity bimodality in the Milky Way globular cluster system (e.g. Zinn 1985) can be viewed as clustering in metallicity.

Mixture modeling is a technique that can be used to detect clustering in datasets and assess its statistical significance. The fundamental idea in such an analysis is to fit models with different numbers of groups to a given dataset and establish which model provides the best description of the observations. A thorough overview of the mixture-modeling approach and clustering analysis is provided by McLachlan & Basford (1988). The technique has been described in an astronomical context by Nemec & Nemec (1991, 1993) who concentrated on the question of the number of distinct stellar populations in the Milky Way.

In this paper we concentrate on the use of mixture models to detect bimodality in univariate datasets. Most of our discussion also applies to the broader question of the detection of multimodality, but an extension to multivariate datasets is beyond the scope of the present paper. In particular, we will describe a mixture-modeling algorithm known as the KMM algorithm (Adams, McLachlan & Basford 1993) which can be used to detect the presence of two or more components in an observational dataset. We present results on the ability of KMM to correctly estimate the means and variances of two-Gaussian mixtures and on the sensitivity of the likelihood ratio test to detect such mixtures.

In addition to parameter estimation, the current version of the KMM code includes a calculation of the *likelihood ratio test statistic* (LRTS). Evaluation of the LRTS allows KMM to be used as a hypothesis test. We study the specific case in which the variable of interest for any single population has a Gaussian parent population. This is because in many astrophysical problems, the variables of interest are well-approximated by Gaussians.

Examples are given in Section 4. [Agha & Ibrahim (1984) present a maximum likelihood method of parameter estimation which allows a variety of functional forms of the parent populations to be tested.] Our null hypothesis is that a unimodal Gaussian parent population is a good description of the observational data. Use of the LRTS allows the evaluation of the improvement in goodness-of-fit for a two-component model relative to the unimodal; that is, to test the null hypothesis.

Strictly speaking, the hypothesis test defined above is not identical to testing for the presence of bimodality, at least in the case of finite datasets. There are datasets that are better fit by two-groups than a single Gaussian, for which a histogram of the data will not show two clear peaks. This can arise either because of the finite nature of the dataset, or because the parent population is comprised of two groups which are not widely separated in location. Since the presence of two distinct peaks in such a histogram is often dependent on the *binning* of the data, we regard our approach as more physically informative. From a statistical point of view, the subjective nature of binning is unattractive and it is preferable to search for quantifiable clustering in the data rather than attempting to locate two peaks in a histogram.

A related issue is the physical relevance that one places on bimodality. A distribution with two distinct peaks can sometimes be approximated by a quartic function, so one can always claim that such a bimodal distribution consists of a single population of objects with a probability density described by a quartic. From such a viewpoint, a mixture-model is nothing more than a mathematical tool for describing a particular distribution. Our assertion is that in many astronomical systems, key observable variables for individual populations of objects have distributions that are consistent with a Gaussian. Thus by demonstrating a significant improvement of a two-group fit to a one-group fit we claim to "detect" the presence of more than one group of objects in a given dataset.

The validity of this approach has been discussed by Nemec & Nemec (1991) in the

context of the stellar populations within the Milky Way. They recall a comment made by Eddington (1916) who noted that studying finite mixtures of Gaussian distributions to model stellar populations provides a crucial starting point for understanding the system. Having first analyzed the system in this manner, it is then possible to add refinements and study complications in the simple model. This is the spirit in which we present the combination of mixture-modeling and the LRTS that constitute the KMM algorithm.

A specific example may help to clarify this point. In the case of the Milky Way, the metallicity of the globular cluster system has been shown to be bimodal (e.g. Zinn 1985). Armandroff & Zinn (1988) fit two Gaussians to the overall metallicity distribution, as did Nemec & Nemec (1991) using a mixture-modeling approach (see also Ashman & Bird 1993). As noted above, fitting the metallicity distribution in this way can be viewed as nothing more than a mathematical convenience. However, studies of the kinematics and spatial distribution of the Milky Way globular cluster system (Zinn 1985; Armandroff & Zinn 1988; Armandroff 1989) have suggested that the two populations of globulars, as defined by the two-group fit to the metallicity distribution, are indeed two distinct populations. Thus verification of the presence of two populations of Milky Way globulars, as indicated by their metallicity distribution, is obtained through the study of additional variables. This result provides much of the basis for the separation of Milky Way globulars into disk and halo subsystems, as suggested by the earlier work of Kinman (1959).

In many astronomical systems, only one variable is easily accessible. In such cases, the detection of bimodality in that variable provides evidence for the presence of two distinct populations, but similar clustering in another variable is required to make the identification more secure. Alternatively, if there are strong theoretical reasons for believing that a variable should have a Gaussian distribution [for example, the distribution of line-of-sight velocities in a dynamically-relaxed cluster of galaxies (Bird 1993; see also Section 4.2 below)], then the presence of bimodality provides powerful evidence that two distinct populations are present.

The plan of this paper is as follows. In Section 2 we describe the KMM algorithm and its application to univariate datasets. We also discuss other statistical tests that can be used to explore a dataset for the presence of bimodality. In Section 3 we present a study of the sensitivity of KMM when applied to simulated bimodal datasets. KMM is applied to observational data in Section 4 to illustrate the practical implementation of the algorithm and its broad applicability to a range of astronomical systems. We briefly discuss the application of the KMM algorithm to multimodal models in Section 5. Conclusions are presented in Section 6.

2. THE STATISTICAL TESTS

2.1 The KMM Algorithm and the Likelihood Ratio Test

The KMM algorithm is an implementation of the EM (Expectation Maximization) algorithm of Dempster, Laird & Rubin (1977), described in detail by McLachlan & Basford (1988). Earlier work in this area is described by Orchard & Woodbury (1972) and includes the studies of Hasselblad (1966, 1969), Wolfe (1967, 1970) and Day (1969). KMM fits a user-specified number of Gaussian distributions to a dataset, calculates the maximum likelihood estimates of their means and variances and assesses the improvement of that fit over a single Gaussian. The KMM algorithm assumes that each of the N observed datapoints \mathbf{x}_j (j = 1, 2, ..., N) is independently drawn from a parent population which is a mixture of Gaussian probability densities. The mixture density may be represented as

$$f(\mathbf{x};\phi) = \sum_{i=1}^{g} \pi_i f_i(\mathbf{x};\theta). \tag{2.1}$$

Here π_i is the fraction of the parent population drawn from the *i*-th component (also called the mixing fraction), g is the total number of groups or components being fit, θ is the vector representing all the unknown model parameters for the g components, and

$$\phi = (\pi', \theta')' \tag{2.2}$$

is the vector transpose of the unknown model parameters and mixing fractions. User input into the program (in addition to the measurements being partitioned) is a first guess at the means and covariances of the Gaussian distributions to be fit, as well as an estimate of the mixing proportions. The user must also decide whether the routine should find groups with the same covariances (homoscedastic fitting) or allow the groups to have arbitrary, dissimilar covariances (heteroscedastic fitting).

An alternative option to providing the initial mixture of Gaussians is for the user to provide group membership for the individual datapoints. In this case, one can take advantage of techniques which estimate first splits of the dataset (e.g. Kaufman & Rousseeuw 1990). Based on this initial partition of the data, KMM calculates means and covariances of the corresponding Gaussian components and proceeds as described below. These two input options are essentially equivalent and we will only refer to the former in what follows.

In its first pass through the data, KMM finds the best fit single Gaussian for the given dataset (specifically, it finds the mean, μ , and variance, σ^2 , of the data). The unimodal log(likelihood) is defined as

$$L_C(1) = \sum_{j=1}^{N} \ln f(x_j; \theta)$$
 (2.3)

That is, it is the sum of the natural logarithms of the univariate Gaussian evaluated at x_j .

Next, KMM enters its iterative step, using the value of ϕ defined in the previous iteration (or specified by the user for the evaluation in the first pass). For each datapoint it calculates the *a posteriori* probability that the object belongs to each of the *g* groups. These probabilities are an estimate of the confidence that the algorithm places in its assignment of any particular object to any individual group. The datapoint is assigned to the group for which its probability of membership is the highest. After the assignments are made, the new vector ϕ is determined by finding the π_i , μ_i and σ_i^2 for each group. The log(likelihood) of

the q-group fit is

$$L_C(\phi) = \sum_{i=1}^g \sum_{j=1}^N z_{ij} \left(\ln \pi_i + \ln f_i(x_j; \theta) \right)$$
 (2.4)

Here z_{ij} is an indicator variable. In the ideal case, where the "true" external partition is known, $z_{ij} = 1$ if object j belongs to group i and 0 otherwise. KMM replaces this definition by the estimated posterior probability that object j belongs to group i. This procedure is repeated until the object assignments are stable and $L_C(\phi)$ has converged. The algorithm converges to a local maximum in the ϕ -parameter space, provided that the sequence of likelihood values is bounded above. This is always true for mixture models with equal covariance matrices for all components. In the heteroscedastic case, the sequence of likelihood values may not be bounded above.

The final value of $L_C(\phi)$ is used to determine whether or not the dataset is consistent with the null hypothesis. The *likelihood ratio test statistic* (hereafter LRTS) is

$$\lambda = L_C(\phi)/L_C(1) \tag{2.5}$$

and is an estimate of the improvement in going from a 1-mode to a g-mode fit. The significance of the LRTS may be estimated by comparing $-2\ln\lambda$ to a χ^2 distribution with a number of degrees of freedom equal to twice the difference between the number of parameters of the two models under comparison, not including the mixing proportions. However, this provides only an approximation of the statistical significance. For the homoscedastic, univariate case, this approximation has been shown to be adequate (McLachlan & Basford 1988 and references therein). However, for more complicated situations, the only way to reliably assess the statistical significance is a bootstrap estimation (McLachlan 1987; McLachlan & Basford 1988; Nemec & Nemec 1991; Bird 1993; see also Section 5 below). While bootstrapping individual moderate-sized datasets is trivial with current workstations, bootstrapping thousands of simulated datasets to test KMM sensitivity is too time-consuming. This is one reason why we restrict attention in the present paper to univariate, homoscedastic datasets since

we can exploit the χ^2 distribution to obtain reasonably reliable estimates of significance for large numbers of simulated datasets.

The current version of the KMM code (Adams, McLachlan & Basford 1993) incorporates an estimate of the statistical significance of the g-group fit over the unimodal case using the analytical technique described above. The resulting significance is expressed in terms of a P-value. The P-value is the probability that the likelihood ratio test statistic would be at least as large as the observed value if the null hypothesis were true. In our restricted case, the P-value represents the probability of determining the observed value of the LRTS from a sample distribution drawn from a unimodal Gaussian. The smaller the P-value, the less likely is the observed LRTS; that is, small P-values indicate that the null hypothesis is not a good description of the data. Conventionally, P < 0.05 indicates that the null hypothesis is strongly inconsistent with the data, whereas 0.05 < P < 0.1 indicates marginal inconsistency.

In addition to the P-value, the KMM algorithm returns values for the estimated means of the groups, μ_i , the estimated mixing fraction, π_i , and the estimated common covariance, σ^2 . (In the heteroscedastic case, the covariance for each group is calculated.) The algorithm also assigns individual datapoints to the groups for which their posterior probability is highest, and estimates a confidence value for each assignment. Thus KMM provides not only a powerful hypothesis test, it also allows objective partitioning of data into individual groups for a given g-group fit.

2.2 Double-Root Residuals

Double-Root Residuals (hereafter DRRs) provide an effective way of comparing any univariate dataset with a model distribution. Their use in an astronomical context has been described by Gebhardt & Beers (1991). Calculating residuals to compare a model with observed data and displaying the results as a difference plot (or hanging histogram) is a common

technique. However, the drawback of this method is that residuals in heavily-populated bins are often much larger than those in bins with few datapoints, simply because \sqrt{N} fluctuations are larger. Consequently, the distribution of residuals is often a poor diagnostic of the deviation of the observed data from the model distribution.

The DRR plot represents a simple refinement of the more familiar difference plot that overcomes the shortcomings inherent in ordinary residuals. By taking square-roots of both the number of observed datapoints per bin and the corresponding model prediction, the \sqrt{N} problem described above is effectively removed. Gebhardt & Beers (1991) note that an improvement over a comparison of simple square roots is provided by the expression:

$$DRR = \sqrt{2 + 4N_{data}} - \sqrt{1 + 4N_{model}} \quad (N_{data} \ge 1)$$
 (2.5a)

DRR =
$$1 - \sqrt{1 + 4N_{model}}$$
 $(N_{data} = 0)$ (2.5b)

(cf. Velleman & Hoaglin 1981). Here N_{data} is the number of datapoints in a given bin and N_{model} is the number of points in a given bin as predicted by the model under investigation.

The DRR plot illustrates clearly exactly where the observed data and model differ significantly from one another. In cases where the model provides an adequate fit to the data, DRRs also have the useful property of having numerical values roughly equivalent to normal deviates. Thus DRRs can be used to test the fit of a model to a given dataset. If the DRR has a local value of 2 or greater, this indicates a discrepancy between the model and the data at the 2σ (95%) level. We illustrate these properties explicitly in Sections 3 and 4.

Using DRRs to test the validity of a unimodal versus bimodal distribution is a relatively straightforward procedure. If, as in the KMM case, one is testing the hypothesis that the data is well-fit by a single Gaussian, one calculates the best-fit Gaussian to the data, bins that Gaussian, and calculates the DRRs using equation (2.5). It is a simple matter to modify the model distribution against which the data is to be tested. One way this can be exploited in the detection of bimodality is to compare the data with a uniform distribution.

The rationale here is that "boxy" distributions (which have fewer datapoints in the tails of the distribution relative to a Gaussian) are generally better fit by a mixture of Gaussians than a single Gaussian. Thus there is a concern when fitting Gaussian mixtures that a two-group model will be preferred over a one-group model not because the parent population is comprised of two components, but because it is intrinsically light-tailed. As we illustrate in Section 4, calculating the DRRs for a uniform model can help determine whether the parent distribution is genuinely bimodal or simply boxy.

The primary drawback of the DRR technique is that it relies on binning of the data. The likelihood ratio test exploited by the KMM algorithm is free of this weakness. Nevertheless, it is also apparent that DRRs are a useful addition to the arsenal of statistical weapons that can be used to detect or reject the presence of bimodality.

2.3 Shape Estimators and ROSTAT

The ROSTAT statistics package (Beers et al. 1990; Bird & Beers 1993) is designed to determine robust estimates of the location, scale, and shape of univariate datasets. ROSTAT contains an array of statistical tests, some of which can be exploited to detect bimodality and mixtures of distributions in a dataset.

We retain our earlier assumption that individual components in a dataset can be approximated by Gaussian distributions. A mixture of two (or more) Gaussians in which the individual means of the two components differ produces a distribution that is light-tailed. If, in addition, the individual components of a distribution contain significantly different numbers of datapoints, the result is usually an asymmetric distribution in which more points lie on one side of the mean than the other. Examples of datasets with these properties are discussed in Sections 3 and 4.

Traditionally, the shape of a distribution is described by its kurtosis and skewness (cf. Bird & Beers 1993 and references therein). The skewness, which is the third moment about

the mean of a distribution, measures the degree of asymmetry of the distribution and is given by:

$$a_3 = \frac{\int (x-\mu)^3 f(x) dx}{\sigma^3} \tag{2.6}$$

where f(x) is the probability density function under study, μ is its mean, and σ is its standard deviation. The kurtosis is the fourth moment about the mean of a distribution:

$$a_4 = \frac{\int (x - \mu)^4 f(x) dx}{\sigma^4} - 3 \tag{2.7}$$

With these definitions, the skewness and kurtosis are both equal to zero for a Gaussian distribution.

Bird & Beers (1993) have compared the skewness and kurtosis with robust shape estimators known as the asymmetry and tail indices. They find that, while the asymmetry and tail indices are more powerful for comparing the shapes of univariate distributions, the skewness and kurtosis are preferable if one is primarily concerned with testing the hypothesis that a given distribution is consistent with Gaussian. In the context of the present discussion, we suggest that skewness and kurtosis provide a useful diagnostic in the search for possible bimodality. The ROSTAT package returns the probability that the dataset under study is consistent with a Gaussian distribution, as determined by these quantities. This complements the other methods described earlier in this Section, although we emphasize that of these three techniques only the likelihood ratio test combined with mixture modeling directly addresses the issue of multiple components in a dataset.

It is important to stress that the techniques described above represent only a fraction of the tests that can be applied when investigating the presence of bimodality. A fuller discussion is provided by McLachlan & Basford (1988), Hartigan & Hartigan (1985) and Nemec & Nemec (1991). However, we have found that the KMM algorithm, with support from DRRs and the normality tests of the ROSTAT package, is a powerful tool for studying the question in practice.

3. TESTING THE SENSITIVITY OF KMM

We have carried out a series of experiments to study the sensitivity of the KMM algorithm to bimodality. Specifically, we have generated realizations of bimodal distributions consisting of two equal-variance Gaussians in which the mixing proportions are equal. For computational convenience, we fixed the mean of group 1 at $\mu_1 = 0.0$ and varied μ_2 between 1.75 and 3.25 in steps of 0.25. The common variance of the groups was set at $\sigma^2 = 1.0$ and the total number of data points, N, varied from 50 to 500.

We define a dimensionless separation of the means:

$$\Delta \mu = \frac{(\mu_2 - \mu_1)}{\sigma} \tag{3.1}$$

With our assumed values, it is apparent that $\Delta \mu = \mu_2$. Thus varying μ_2 as described above corresponds to varying $\Delta \mu$. For each pair of $(N, \Delta \mu)$ we generated 100 simulated datasets. The KMM algorithm was then applied to these distributions.

Before discussing our results, it is worth stressing the analogy between our numerical experiments and the application of KMM to observational data. First, there are analytic results concerning the detectability of bimodality for idealized double-Gaussian distributions with equal mixing proportions. One of the simplest and most useful is that such a distribution only shows two peaks if:

$$\Delta \mu > 2.0 \tag{3.2}$$

(cf. Everitt & Hand 1981). In other words, in the case of infinite N, a distribution will have two peaks if equation (3.2) is satisfied. With the exception of the cases with $\Delta \mu = 1.75$, all of the simulated distributions are drawn from such idealized parent populations. However, we expect KMM to return different significance levels of bimodality on distributions even when they are drawn from a parent population with the same $(N, \Delta \mu)$, simply because of the finite number of datapoints. The important point to note here is that observation of a

finite number of objects drawn from some parent population is directly analogous to simulating distributions. Thus studying the performance of KMM on our simulations provides a direct measure of the detectability of bimodality using KMM on observed astronomical datasets, provided of course that the observed datasets have similar statistical properties to the simulated ones.

As described in Section 2, the KMM algorithm requires user-specified starting values for the estimated means and common variance of the groups to be fit. When running KMM on the simulated datasets, we provided it with the values used to produce the simulated datasets. We have found that for two-group homescedastic fitting, KMM is insensitive to these input values and will converge to the "correct" 2-group fit even when its starting values are far removed from the true means and variance (see also Everitt 1981, Bird 1993). (The only exceptions are starting values in which either the means are very close together or the variance is very large.) Thus while using these values as input speeds up the convergence of KMM, it does not affect the results we obtain. When applying KMM to real datasets it does not hurt to try a range of starting values, but in our experience the two-group homoscedastic fit is forgiving of poor initial choices.

The results of running KMM on these simulated distributions are summarized in Tables 1 and 2 and Figures 1 to 3. For our present study, the most important quantity returned by the KMM algorithm is the P-value of the hypothesis test that a two-group fit is an improvement over a one-group fit (see Section 2.1 above). In Table 1 we present the median P-value, $\langle P \rangle$, based on 100 simulations for each parameter pair $(N,\Delta\mu)$. The median value of P provides a more robust estimate of the "characteristic" P-value than a straight mean, primarily because the distribution of P-values for any given parameter pair tends to be highly skewed (see Section 3.1 below). The information in Table 1 is displayed graphically in Figure 1.

Our experiments revealed that for N < 50 the likelihood ratio test used in the KMM

algorithm does not provide a reliable method for detecting bimodality. For N=50 it is apparent that large separations in the means of the two components are required for KMM to "typically" return a strongly significant (P < 0.05) rejection of the unimodal hypothesis. As N gets larger, the likelihood of rejecting the unimodal hypothesis increases. Note that for the parameter pair $(N=500, \Delta\mu=1.75)$ we obtain $\langle P \rangle < 0.05$, despite the fact that this value of $\Delta\mu$ lies below the bimodality constraint in equation (3.2). This partly reflects the fact that with finite N one can be fortunate and draw a sample that is bimodal even when the parent distribution does not satisfy (3.2). However, this also reflects the fact that KMM can accurately partition data into two groups and demonstrate the improvement of fit over a unimodal distribution even when the parent distribution is not bimodal. Thus while it is not entirely accurate to describe such distributions as bimodal, one can test the likelihood that the parent distribution is comprised of two distinct groups. In astronomical applications, the presence of two components is of more physical significance than the presence of two distinct peaks (cf. our comments in Section 1 above).

In Table 2a and 2b we present the fraction of simulations for each parameter pair in which P < 0.05 and P < 0.1, respectively. Figures 2a and 2b display this information graphically. Since the distributions are generated from double-Gaussian parent populations, these results can be viewed as the efficiency with which KMM correctly identifies the presence of two Gaussian components. (Note that one reason this efficiency is not 100% is because in some of these finite realizations the double-Gaussian characteristics are washed out. Again, this is analogous to the process of observation when, with finite datasets, one can simply be unlucky.)

In Figure 3 we display the information contained in Tables 2a and 2b in the $(N,\Delta\mu)$ plane. The four lines represent loci of the fixed fractions of simulations (99% and 95%) for
which P < 0.05 and P < 0.1. The lines are simple linear interpolations of the results given
in Tables 2a and 2b.

As one would intuitively expect, KMM becomes more efficient at detecting bimodality as N and $\Delta\mu$ increase (see also McLachlan 1987; Mendell et al. 1992, 1993). The quantitative results can be exploited when planning observational strategies. For instance, if one is attempting to test a model in which bimodality is predicted to exist in an observable quantity at some $\Delta\mu$, Table 2a and Figure 2a give the number of datapoints required to detect such bimodality with a given probability.

These figures and tables can also be used in the interpretation of analyses of real data. This may be particularly important when the user has been forced to throw out datapoints in an attempt to remove a background or other contamination of the dataset. Such clipping of the data is often justified for physical or statistical reasons and is sometimes necessary to obtain reliable results with KMM. For instance, a " 3σ -clipping" routine was proposed by Yahil & Vidal (1977) to identify galaxies as cluster members based on their redshifts. While their iterative technique has been shown to be unreliable (Beers et al. 1990), redshift filters are regularly applied to galaxy cluster velocities to reduce foreground and background contamination (cf. Malumuth et al. 1992, Bird 1994).

If one retains a constant background in a dataset, the result is usually a distribution with artificially extended tails. In such datasets, KMM will attempt to fit these tails (as well as potentially-significant deviations) when finding the optimum one- and two-group fit, thereby producing spurious results. In fact, under such conditions, the significance of the two-group fit will usually be reduced, since a single, broad unimodal typically provides a better fit to the long tails. The potential hazard in clipping univariate data is that such truncation tends to make a dataset more boxy. This generates the opposite effect to a constant background contamination, and in some instances it is possible that the likelihood of the two-group fit will be artificially increased.

One way to guard against this problem is to use the results of the sensitivity tests presented above. If one only obtains a strong bimodal signal after clipping a dataset, a

comparison of the value of N and the derived value of $\Delta\mu$ with Figures 2 and 3 may help determine whether the bimodality signal is an artifact of the clipping procedure. If the observed values lie in a region of the $(N, \Delta\mu)$ -plane with a low expectation of rejecting the unimodal hypothesis, it is likely that clipping has artificially introduced the bimodal signal. We return to this point in Section 4.

3.1 Distribution of P-values, Means, and Variances

To illustrate the typical dispersion in the parameters returned by KMM, we now study one set of simulations in more detail. Specifically, we look at the 100 simulated datasets with N=300 and $\Delta\mu=2.25$. Inspection of other datasets reveals that the distribution of the KMM output parameters becomes more concentrated around the input values as one goes to larger N and $\Delta\mu$, as expected.

In Figure 4 we show that distribution of P-values returned by KMM for the simulations with N=300 and $\Delta\mu=2.25$. While most of the values strongly reject the unimodal hypothesis, there is a tail of high P-values which do not reject the unimodal model.

Figures 5(a)–(e) show the distributions of the other parameters returned by KMM. Recall that the input parameters for the simulations here have the mean of the first group $\mu_1 = 0.0$, the mean of the second group $\mu_2 = 2.25$, the common variance $\sigma^2 = 1.0$ (so that $(\mu_2 - \mu_1)/\sigma^2 = 2.25$) and the ratio of mixing proportions, $\pi_1/\pi_2 = 1.0$. Thus these figures can be viewed as a summary of how well KMM is doing in returning the input values (although, as noted in Section 2, much of the variation in the returned parameter values reflect the finite nature of the simulated datasets).

Figures 5(a) and 5(b) show the distribution of μ_1 and μ_2 , respectively. More than half the returned values lie within 0.1 of the input value. In Figure 5(c) we show the distribution of σ^2 returned by KMM, which is clearly sharply peaked around the input value of 1.0. Figure 5(d) shows the distribution of separation of the means normalized to the value of σ returned

by KMM. In Figure 5(e) we show π_1/π_2 returned by KMM. These figures show that the parameter values calculated by KMM are reliable estimates of the parameters describing the parent populations.

3.2 A Case Study

We now look in detail at one randomly selected dataset drawn from the 100 simulations of the N=300, $\Delta\mu=2.25$ set discussed in the previous subsection. The purpose is to compare the results returned by KMM with other statistical tests and to illustrate the application of the ROSTAT package and DRRs to such datasets. A histogram of this dataset is given in Figure 6, where the best-fitting single Gaussian ($\mu=1.21$, $\sigma=1.5$) is also shown.

One of the most striking aspects of Figure 6 is that the histogram does not look particularly bimodal! This is somewhat surprising, given the large number of points and respectable separations of the means of the two groups. Despite the appearance of the histogram, the KMM algorithm separates the distribution into two groups at a high degree of confidence. Specifically, KMM returns $\mu_1 = -0.074$, $\mu_2 = 2.250$, $\sigma^2 = 0.914$, and $\pi_1/\pi_2 = 128/172$. The rejection of the unimodal hypothesis is strongly significant with P = 0.001. Comparison with the results summarized in Section 3.1 above show that this is an unexceptional dataset from the N = 300, $\Delta \mu = 2.25$ set of simulations. The ratio π_1/π_2 is on the low side, but the other results are typical for these input parameters.

Perhaps the most notable result is that KMM correctly identifies, at strong significance, the presence of two groups in this dataset, even though the histogram of the distribution does not have two obvious peaks. This illustrates the superiority of an objective algorithm such as KMM over binning the data and assessing the results by eye. However, it is worth noting that Figure 6 reveals the boxiness which is characteristic of some two-group mixtures.

The normality tests contained in the ROSTAT package return interesting information on the dataset, which further supports the results of the KMM analysis. Firstly, the skewness has a value of -0.104, indicating a deficiency of datapoints with values less than the mean. This level of skewness does *not* reject the single Gaussian hypothesis. (This is encouraging since although the parent population is not Gaussian it *is* symmetric.) On the other hand, the kurtosis for this datset has a value of -0.665, corresponding to a rejection of the single Gaussian hypothesis at a confidence level of P < 0.001. Negative kurtosis is expected for a bimodal dataset and supports the rejection of the single Gaussian model by KMM.

Finally, we apply the DRR technique to the dataset in Figure 6. In Figure 7(a) we plot the DRRs of the dataset when compared to the best-fitting single Gaussian model. The residuals creep above the 2σ level on each side of the single Gaussian mean, in the manner expected if the distribution is bimodal. Thus the DRR plot rejects the single Gaussian model at 95% confidence. In Figure 7(b) we plot DRRs for a model with a uniform distribution. Here one has a certain flexibility in deciding how far the uniform distribution extends. However, the presence of highly significant DRRs with both negative and positive sign indicates that a uniform distribution is inconsistent with this dataset.

In other datasets, particularly when N is small, we have found that uniform distributions are often acceptable fits to genuine bimodal distributions, according to the DRR technique. This is primarily because of the boxy nature of bimodal distributions when binned. In Figure 7(b), the largest positive DRR is produced by the heavily-populated bin at x = 2.0. Creative binning can significantly reduce this bin and hence the associated DRR, although for this particular dataset we have not been able to find a sensible binning that reduces all DRRs below 2σ . As noted earlier, this dependence on binning is an unattractive aspect of the DRR method. We therefore advocate the use of KMM as the primary diagnostic unless there are good reasons for believing that the parent distribution of the variable of interest for a single population is non-Gaussian.

3.3 Playing Devil's Advocate

The results discussed above indicate that the likelihood ratio test, using KMM parti-

tions, can correctly identify bimodality in univariate datasets. However, it is also of interest to establish the frequency with which KMM erroneously "detects" bimodality in datasets drawn from single Gaussian parent distributions. To investigate this possibility we simulated unimodal Gaussian distributions with N varying from 50 to 500 as before. The mean of the Gaussian was set at 0.0, with a dispersion of 1.0. For each value of N we generated 100 simulations and ran KMM on the datasets. We provided KMM with the input values: $\sigma^2 = 1.0$, $\mu_1 = -0.5$, $\mu_2 = 0.5$. The results of this exercise are presented in Figure 8, which shows the fraction of the simulations f_{05} and f_{10} which returned P-values less than 0.05 and 0.10, respectively.

It is apparent from Figure 8 that KMM occasionally identifies bimodality in samples drawn from a Gaussian parent population. However, even in low-N datasets, the false-positive frequency is never greater than 10%. Such a level is expected on the basis of the definition of the P-value. About 50% of the false bimodality detections in these simulations can be rejected using the kurtosis returned by ROSTAT. That is, for about half of these distributions the kurtosis indicates consistency with a single Gaussian. Thus using KMM in conjunction with the kurtosis of the dataset leads to \sim 5% false detection of bimodality for N=50, with the fraction dropping at higher N. Given the power of the KMM algorithm in correctly identifying bimodality, we conclude that this low level of false detections is acceptable.

4. APPLICATION TO DATA

4.1 The Color Distribution of Globular Clusters around NGC 5128

Broad-band colors of old globular clusters can be used to deduce their metallicities (e.g., Harris 1991 and references therein). The shape of such metallicity distributions contains valuable information about the formation of globular cluster systems and the early chemical and dynamical evolution of their host galaxies. Of interest to the present discussion is the

suggestion that a merger origin for elliptical galaxies leads to a globular cluster metallicity distribution which is bimodal (Ashman & Zepf 1992). More generally, two or more populations of globular clusters around a galaxy indicates that the formation of these objects probably occurred in discrete bursts rather than through some continuous process.

In the Milky Way, the halo and disk globular cluster systems individually have metallicity distributions that are well-approximated by Gaussians (cf. Armandroff and Zinn 1988; Nemec & Nemec 1991). As noted in Section 1, kinematic and spatial distributions of Milky Way globulars confirm this separation of the system into two subsystems. It is therefore reasonable to hypothesize that individual populations of globular clusters have a distribution in [Fe/H] that is Gaussian-distributed. In metallicity distributions derived from broad-band photometry, errors in [Fe/H] (arising from internal photometric errors) are also Gaussian. This is therefore an ideal situation to use the KMM algorithm and its assumption that individual populations have Gaussian-distributed variables (in this case, [Fe/H]).

The Washington $(C - T_1)$ index has good sensitivity to metallicity variations and has been used to derive metallicity distributions for a number of extragalactic globular cluster systems. As an example, we consider the color distribution of globulars around NGC 5128 presented by Harris et al. (1992). [A summary of the results from a KMM study of this system was given by Zepf & Ashman (1993).]

In Figure 9(a) we show the distribution of $(C-T_1)$ colors for the globular clusters around NGC 5128. These are the colors presented by Harris et al. (1992) without any correction for reddening. It is apparent that two of the datapoints are somewhat removed from the main distribution. Both these extreme points are flagged as uncertain by Harris et al. (1992), the blue object having a close neighbor and the red one being near the NGC 5128 dust lane. Moreover, both colors are beyond the range for which the metallicity-color relationship is calibrated. Since the foundation of the Gaussian hypothesis here is that *metallicity* is Gaussian-distributed, these two extreme points could compromise the analysis. We therefore

exclude them from the following discussion. The curve shown in Figure 9(a) is the best-fit single Gaussian to the remaining 60 datapoints.

A KMM study yields the following results. The P-value for the dataset is 0.093, representing a marginally significant rejection of the unimodal hypothesis. The means of the two groups are 1.53 and 1.95, respectively, with a common variance of $\sigma^2 = 0.024$. KMM assigns 33 objects to the blue group and 27 to the red. We noted in Section 3 that comparing KMM output with the results from simulated datasets provides a useful check of whether the KMM output is reasonable. This has additional merit in cases such as the present one where a couple of points have been excluded from the KMM analysis. The KMM output parameters imply $\Delta\mu = 2.7$ for this N = 60 dataset. From Figures 1 and 2 it is apparent that a P-value of 0.093 is typical for a dataset with these values of $\Delta\mu$ and N. This provides added support that KMM is accurately partitioning this dataset and that the exclusion of the two extreme datapoints is reasonable.

Zepf & Ashman (1993) have suggested that the blue colors of some clusters in NGC 5128 may be indicative of youth rather than low metallicity. In particular, Zepf & Ashman (1993) noted that the metallicity-radius relation for globulars in this galaxy is more consistent with other systems if the blue globulars at small projected radii are young rather than metalpoor. The two bluest clusters in the 60-point dataset both have small projected radii. If they are removed from the analysis, the bimodality signal in this system is much stronger. A KMM analysis of this 58-point dataset returns a P-value of 0.004, corresponding to a strong rejection of the single-Gaussian hypothesis. The means and mixing proportions are not significantly affected by this further clipping (the variance of the two groups drops somewhat), providing some evidence that the partitions are reasonable. However, this does illustrate the subjective element that inevitably creeps in to such analyses, as well as the slightly unstable performance of KMM in datasets with small N. On a more optimistic note, the KMM analysis has provided direction for future observations which could definitively

establish whether this globular cluster color distribution is bimodal.

In Figure 9(b) and 9(c) we show the DRR plots of the best uniform and Gaussian model, respectively. The Gaussian model is consistent at the 2σ level with the data. This result agrees with the KMM analysis where the rejection of the single Gaussian was at less than 95% confidence. The uniform distribution formally is rejected at greater than 2σ , although it is apparent from Figure 9(c) that the discrepancy is caused by the tails of the dataset. Since it is possible that datapoints could be scattered into outlying bins through observational uncertainties, this is not a compelling reason to reject the uniform distribution. However, the arguments given above that individual globular cluster populations have Gaussian metallicity distributions suggest to us that the bimodal interpretation of this data is more reasonable.

The kurtosis of this dataset is -0.737, corresponding to a P-value of 0.072 and a marginally significant rejection of the Gaussian hypothesis. This is encouragingly similar to the KMM result. Note that the kurtosis is negative, as expected for a bimodal distribution. The skewness shows no significant departure from Gaussian, indicating a symmetric dataset (as expected for a bimodal distribution with a similar number of points in each peak). Other examples of the application of the KMM algorithm to globular cluster color distributions are given by Ashman & Zepf (1993), Ashman & Bird (1993), Lee & Geisler (1993), Ostrov et al. (1993), Zepf & Ashman (1993) and Zepf, Ashman & Geisler (1994).

4.2 Galaxy Velocities in the Cluster A548

The line-of-sight velocities of galaxies in a dynamically-relaxed cluster are expected to be Gaussian-distributed (Bird 1993 and references therein). Deviations from a Gaussian distribution may indicate that the cluster is unrelaxed, that substructure is present, or the three-dimensional velocity distribution is anisotropic. A double-Gaussian distribution is suggestive of two gravitationally-distinct groups of galaxies. Clearly, this situation is another example where the KMM algorithm can provide useful information about the physical state

of the system, since the assumption of individual populations having Gaussian-distributed velocities has a firm foundation. While the positions of galaxies also provide important insight into the dynamical structure of these massive systems, for the purposes of this paper we will discuss the application of KMM to velocity distributions only. KMM has been applied simultaneously to velocity and position information for clusters of galaxies by Bird (1994) and Davis et al. (1994).

The KMM algorithm and other techniques have been applied to velocity datasets of many clusters of galaxies (Yahil & Vidal 1977; Beers et al. 1990; Beers et al. 1992; Bird & Beers 1993; Zabludoff, Franx and Geller 1993). To demonstrate the application of KMM to a cluster velocity dataset, we consider the cluster A548, which was observed by Dressler & Shectman (1988) in their study of substructure in rich clusters of galaxies. In Figure 10(a) we show the velocity distribution of 133 galaxies along with the best-fitting Gaussian to the dataset. Velocities are given relative to the cluster recessional velocity of 12394 km/s (Davis et al. 1994). The dataset is clearly somewhat more boxy than a Gaussian, providing a hint that bimodality might be present.

The results of applying the KMM algorithm provide strong evidence that the galaxy velocities have at least a bimodal distribution. The P-value of 0.003 rejects the single Gaussian model. The parameters calculated by KMM for the two-group homoscedastic model include individual group means of -629 km/s and +771 km/s and a common variance of $(517 \text{ km/s})^2$. The two groups are similarly populated with 71 points assigned to the low-velocity group and 62 to the high-velocity group.

Figures 10(b) and 10(c) show the DRRs for the best-fitting Gaussian and a uniform distribution, respectively. The Gaussian model has both negative and positive DRRs in excess of 2, ruling out the model at the 2σ level. In an attempt to fit a uniform distribution, we excluded the tails of the dataset (which would give large negative DRRs). Even with this helping-hand, the DRRs for the uniform distribution shown in Figure 10(c) clearly rule out

the uniform model.

The kurtosis of this dataset confirms its boxy appearance with a value of -0.860 and a P-value less than 0.001, strongly rejecting the Gaussian model. The skewness shows consistency with a symmetric distribution, again reflecting the roughly equal number of points in the two groups.

Although the dataset shown in Figure 10(a) does not look strongly bimodal, the results of these tests indicate clearly that a two-group fit is preferred over a single group fit. The larger number of points in this dataset relative to the one considered in the previous subsection is an important factor in producing this higher level of confidence in the analysis.

The combination of velocities and positions for galaxies in A548, presented along with ROSAT X-ray observations of this system in Davis et al. (1994), suggest that its physical structure is even more complex than the KMM analysis indicates. When the location of gas density peaks are used to constrain the number of groups that KMM fits, A548 is found to possess at least four physically-distinct subunits, of which three are probably gravitationally-bound. In this case, the use of KMM provides a powerful addition to the gas and galaxy diagnostics provided directly by the observations.

4.3 The Duration of Gamma-Ray Bursts

Recent work by Kouveliotou et al. (1993) has shown that the duration of gamma-ray bursts (hereafter GRBs) has a bimodal distribution. These authors further show that the burst durations are anticorrelated with spectral hardness, adding support to the claim of two distinct populations. Since the nature of GRBs remains controversial, we do not have strong theoretical reasons for assuming any particular form for the distribution of burst durations. However, the logarithmic distribution of T_{90} has the appearance of two roughly Gaussian distributions [see Figure 11(a) of this paper and Figure 1(a) of Kouveliotou et al. (1993)]. Here, T_{90} is the time in seconds during which the cumulative BATSE (Burst and Transient

Source Experiment on the *Compton Gamma-Ray Observatory*) background-subtracted signal increases from 5% to 95% of the total counts. Like Kouveliotou et al. (1993) we use the data contained in the First BATSE Catalog (Fishman et al. 1994). This contains 222 datapoints with reliable duration measurements.

We ran the KMM algorithm on $\log(T_{90})$ and obtained a rejection of a single Gaussian with P < 0.001. The means of the two groups occur at $\log(T_{90}) = -0.346$ and 1.462 (or 0.45s and 28.9s, respectively). KMM assigns 63 points to the short duration group and 159 to the long duration group. This is consistent with the visual appearance of Figure 11(a) that the two groups contain a significantly different number of objects. The variance in $\log(T_{90})$ is $(0.242s)^2$.

DRR plots are shown in Figures 11(b) and 11(c). Both the Gaussian and uniform model fits are strongly rejected. The kurtosis of the dataset is -0.692, corresponding to P < 0.001 for the single Gaussian model. The skewness also rejects a single Gaussian. Its value of -0.606 reflects the smaller number of objects in the short duration group.

5. DISCUSSION

In the above Sections we have demonstrated the ability of KMM to evaluate the presence of two-group mixtures of Gaussians. There are many astronomical applications where the two-group homoscedastic model is theoretically and/or empirically plausible. However, there are also situations where there is little empirical or theoretical motivation for believing the homoscedastic assumption is valid. In such cases it may be useful to drop the equal variance requirement and use KMM to look for heteroscedastic groups. In galaxy cluster applications, for instance, heteroscedastic fits can be very helpful for isolating small foreground and background groups [e.g., the cluster A85, Bird (1994)].

One disadvantage of heteroscedastic mixture models is the lack of a reliable analytic approximation to the significance level. As discussed in Section 2, the χ^2 distribution is only a

good approximation to the *P*-value distribution for bimodal homoscedastic fits (McLachlan & Basford 1988). In other cases, the bootstrap technique must be employed. Generally speaking, any bootstrap algorithm generates non-independent random datasets under the null hypothesis of the statistic being evaluated. It allows a determination of the significance of a statistic (in the present case, the likelihood ratio test statistic) based on the sampling fluctuations and distribution properties of the observed dataset. [See Efron (1981), McLachlan & Basford (1988); Beers et al. (1990) and Bird (1993) for detailed discussions of bootstrapping techniques.]

Extensive experimentation with stellar and galaxy cluster datasets suggests that the estimated P-value provided by the KMM algorithm usually underestimates the significance of a given model (Bird 1993). That is, in most cases the bootstrap P-value is even lower (i.e., more significant) than the analytically estimated value. Thus the analytic approximation is useful when one is exploring a dataset by fitting different heteroscedastic models, in that it provides a guide to preferred models. Such studies can avoid the time-consuming process of bootstrapping P-values for a large number of different models.

Using KMM to detect multimodality (g > 2) in homoscedastic datasets suffers from similar limitations. The analytic P-value is often a useful guideline to the significance of a given model, but bootstrapping is generally required to obtain an accurate value. Comparing a g-group homoscedastic fit to a unimodal Gaussian can be carried out in a fashion analogous to the 2-group versus unimodal fit described in earlier Sections. The main uncertainty is the determination of the optimum number of groups for a given dataset. This question has been the focus of extensive statistical research in recent years [see, for instance, Rozál & Hartigan (1994) and references therein]. Unfortunately, no single powerful technique has yet emerged for determining how many groups are present in a dataset.

Nemec & Nemec (1991) advocate an Occam's razor approach in which the optimum number of groups is determined by the smallest number of groups that is consistent with the data. These authors discuss various techniques of how the goodness-of-fit of such mixture models can be assessed and illustrate these techniques by applying them to stellar populations within the Milky Way.

A similar method has been suggested by Bird (1994) who obtains analytic P-values for g-group fits versus the unimodal case for a range of g. If a number of models return strongly significant rejections of the unimodal hypothesis, Occam's razor suggests that the fit with the smallest number of groups be preferred. Other criteria can be added, such as rejecting models where one or more of the groups contains a small fraction of the total number of datapoints. (For example, this may be applicable if small groups are deemed unlikely on physical grounds.) It is, of course, still possible to use the LRTS to directly compare the significance of two competing models by bootstrapping P. In practice, observed datasets frequently do not strongly point to a unique solution. Ultimately, there is no substitute for additional empirical information to determine a physically preferable partition.

There are statistical techniques that address some of these issues more directly, many of which are described by McLachlan & Basford (1988). Of particular interest is the procedure proposed by Hawkins (1981) which tests simultaneously for homoscedasticity and normality of the components of a mixture model. Since our primary aim in this paper is to present the KMM algorithm, we refer the interested reader to McLachlan & Basford (1988), Hawkins (1981) and Fatti, Hawkins & Raath (1982) for further information on Hawkins' test and other techniques. More recently, Roeder (1994) has introduced a graphical technique for identifying the number of groups in a mixture of Gaussians.

The above comments and caveats indicate that KMM has many uses beyond the bimodality hypothesis test discussed in earlier Sections. However, it is also apparent that in the univariate, homoscedastic, bimodal case, the hypothesis test is relatively straight-forward and easy to implement. With more complicated models, more care must be used when applying KMM, but even in such cases much can be gleaned by exploring the clustering within a dataset using KMM.

6. CONCLUSIONS

We have discussed a variety of tests for detecting and quantifying bimodality in astronomical datasets. The most important of these is a mixture-modeling technique implemented using the KMM algorithm. Our simulations indicate that this algorithm provides a powerful means to explore bimodality in univariate datasets. We have illustrated the practical use of KMM by applying it to data from three astrophysical systems. The primary goal of this paper is to introduce the astronomical community to the KMM algorithm as applied to univariate datasets. FORTRAN code for the KMM algorithm is available electronically from the authors upon request, along with further instructions on the use of the algorithm.

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FIGURE CAPTIONS

- Figure 1. Median P-value versus $\Delta \mu$ for a range of N, as determined by the KMM algorithm when testing for a 2-group fit over a 1-group fit.
- Figure 2. The fraction of simulations for which KMM returns: (a) P < 0.05; (b) P < 0.1 plotted against $\Delta \mu$. The different lines represent different values of N. Symbols are the same as in Figure 1.
- **Figure 3.** The frequency of strongly significant (P < 0.05) and marginally significant (P < 0.1) rejection of the unimodal hypothesis in favor of a 2-group fit. Loci are shown for 95% and 99% rejection frequencies.
- Figure 4. The distribution of P-values as returned by KMM for 100 simulations with N=300 and $\Delta\mu=2.25$. The range of P-values shown is: (a) 0.000 < P < 0.01; (b) 0.01 < P < 0.25.
- Figure 5. The distribution of parameters returned by KMM for 100 simulations with N=300 and $\Delta\mu=2.25$: (a) mean of first Gaussian, μ_1 ; (b) mean of second Gaussian, μ_2 ; (c) common variance, σ^2 ; (d) $(\mu_2-\mu_1)/\sigma$; (e) ratio of mixing fractions, π_1/π_2 .
- Figure 6. A histogram showing one realization of the N = 300, $\Delta \mu = 2.25$ simulations. This is the dataset studied in detail in Section 3.2. The best-fitting single Gaussian for this dataset is superimposed.
- **Figure 7.** DRR plots for the dataset shown in Figure 6 when compared to (a) a Gaussian; (b) a uniform distribution.
- **Figure 8.** Fraction of simulations of unimodal distributions in which KMM returns P < 0.1 (f_{10}) and P < 0.05 (f_{05}) . Only partitions with at least 20% of the datapoints in each group are included.
- Figure 9. (a) The $(C T_1)$ colors of globular clusters around NGC 5128 from the data of Harris et al. (1992). The superimposed curve is the best-fitting Gaussian to the 60-point

dataset in which the two outliers have been removed. (b) The DRRs of the the best-fitting Gaussian to the 60-point dataset. (c) The DRRs of a uniform model distribution.

Figure 10. (a) The velocity distribution of galaxies in the cluster A548 from Dressler & Shectman (1988). The best-fitting Gaussian is superimposed. (b) The DRRs of the best-fitting Gaussian model. (c) The DRRs of a uniform model distribution with the two high-velocity datapoints removed.

Figure 11. The distribution of $log(T_{90})$ of BATSE gamma-ray burst durations from the data of Fishman et al. (1994). The best-fitting Gaussian is also shown. (b) The DRRs of the best-fitting Gaussian model. (c) The DRRs of a uniform model distribution.