Model selection in High-Dimensions: A Quadratic-risk based approach

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Summary. In this article we propose a general class of risk measures which can be used for data based evaluation of parametric models. The loss function is defined as generalized quadratic distance between the true density and the proposed model. These distances are characterized by a simple quadratic form structure that is adaptable through the choice of a nonnegative definite kernel and a bandwidth parameter. Using asymptotic results for the quadratic distances we build a quick-to-compute approximation for the risk function. Its derivation is analogous to the Akaike Information Criterion (AIC), but unlike AIC, the quadratic risk is a global comparison tool. The method does not require resampling, a great advantage when point estimators are expensive to compute. The method is illustrated using the problem of selecting the number of components in a mixture model, where it is shown that, by using an appropriate kernel, the method is computationally straightforward in arbitrarily high data dimensions. In this same context it is shown that the method has some clear advantages over AIC and BIC.

Keywords: Global comparison of models, high dimensional data, model selection, mixture models, quadratic distance, quadratic risk, spectral degrees of freedom.

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1. Introduction

In this article we consider data-based evaluation of statistical models, where by a statistical model we mean a parametric family of distributions. We will denote a parametric model by $M$, and an element of the model by $M_\theta$, for $\theta$ in some parameter space $\Theta$, so that $M = \{M_\theta; \theta \in \Theta\}$. A collection of a set of probability models $M_k$, $k = 1, 2, \ldots$ will constitute a model class, say $M$. We will focus on the problem of selecting one statistical model from the competing models in the class $M = \{M_k\}$, where $k$ is an index for the parametric model under consideration. In the example we consider in Section 4 $M$ is the class of all finite mixtures of multivariate Gaussians, and for each $k$, $M_k$ is the set of all $k$-component multivariate Gaussian mixtures. A particular model element $M_\theta \in M_k$ is a $k$-component mixture with specific values for the parameters $\theta$. Let us also use $F_\tau$ to denote the true distribution of the data.

In general, model selection can be approached from two main philosophical perspectives: (1) testing-based model assessment and (2) parsimony-based model assessment. The testing-based approach involves testing, for each $k$, $H_0 : F_\tau \in M_k$ vs $H_1 : F_\tau \in M_{k+1}$. The Likelihood Ratio Test (LRT) is often used to build a testing-based model selection method. However, we do not favor a simple testing approach, because, in the spirit of George Box, our prior belief is that every restricted model is flawed, in which case every model would be rejected by testing at some sample size. Under this belief, a suitable model selection theory should instead be based on the adequacy of the model approximation.

In parsimony-based model selection, we define a selection criterion, which usually involves a term accounting for the goodness of fit and a term penalizing richer models (models with more parameters). Then we choose as the best model among a given subset of models, i.e. $M_{best} \in M$, the model which optimizes our chosen criterion. The information criterion based approaches such as AIC (Akaike, 1973), BIC (Schwarz, 1978) and other model selection criteria based on approximations of Bayes factors (Haughton, 1988) all fall under this large class of parsimony-based model selection tools. These tools are usually designed under a specific probability structure or are designed to achieve specific goals. For example AIC is designed to achieve maximum predictive accuracy whereas the BIC criterion evaluates
the posterior probability of the competing models with specified priors. (Yang, 2005)

In practice the most parsimonious model is determined by the model associated with minimum risk under the specific loss function. For example, in case of the AIC criterion, the loss function of the risk is the Kullback-Leibler (KL) distance. We will here consider model selection from the same basic framework but we will replace Kullback-Leibler distance with quadratic distance (Lindsay et al., 2007). We do so because the family of quadratic distances allows for a very straightforward estimation of risk when the distance itself is used as the loss function. As evident later in this paper, the resulting quadratic risk has many desirable properties especially for high-dimensional data and for model comparisons in a non-regular parametric setup.

Before describing the quadratic risk we want to point out two underlying themes of this article. First, as our risk measure is in the spirit of AIC, we will draw parallel to AIC and wherever necessary, contrast our quadratic risk measures to AIC. Also, this research was originally motivated by the problem of model selection for high-dimensional data in the normal mixture model, a non-regular parametric class. We will use this important model to demonstrate and address pivotal mathematical and computational problems in model selection.

1.1. Quadratic risk based model selection

We will develop our model selection criteria within the following risk framework. The loss incurred in using a model element \( M_\theta \) (from a model \( \mathcal{M} \)) when the true distribution is \( F_\tau \) will be denoted by \( a(F_\tau, M_\theta) \). The function \( a \) should measure in some meaningful fashion the price of using \( M_\theta \) to approximate \( F_\tau \). The risk of using the model \( \mathcal{M} \), given a particular parameter estimator \( \hat{\theta} \), will be defined to be

\[
\rho_a(F_\tau, \mathcal{M}, m) = E(a(F_\tau, M_\hat{\theta})),
\]

where the \( m \) on the left side indicates that the estimate \( \hat{\theta} \) on the right side was based on a sample of size \( m \), and the expectation is taken over the true distribution. We alert the reader that we are retaining \( m \) as a risk argument because we will consider the estimation of risk for values of \( m \) other than the actual data size \( n \). Our goal here is to choose the
model that minimizes this risk, noting that the lowest risk model is likely to depend on
\( m \). That is, in this formal definition the problem is not to pick a true model, or even a
closest-to-true model, from \( M \): it is to pick a model for which our estimated model element
\( \hat{M}_\theta \) will be the most similar to \( F_\tau \), on average, in samples of size \( m \). Although models with
many parameters are likely to be closer to the true model, the estimation of the model
parameters creates extra variability that is penalized in the risk calculation.

The AIC model selection criterion arises in this context as follows. If we assume both
\( M_\theta \) and \( F_\tau \) to be continuous density functions, with densities \( m_\theta(x) \) and \( f_\tau(x) \) respectively,
the Kullback-Leibler (KL) loss function is

\[
\text{KL}(F_\tau, M_\theta) = \int \log \left( \frac{f_\tau(x)}{m_\theta(x)} \right) f_\tau(x) \, dx.
\]

Using twice the Kullback-Leibler as a loss function, we can split the risk into two pieces:

\[
\rho_{\text{KL}}(M, m) = -2E \left[ \int \log(m_\theta(x))f_\tau(x)dx + \int \log(f_\tau(x))f_\tau(x)dx \right]
\]

\[
= -2E \left[ \int \log(m_\theta(x))f_\tau(x)dx \right] + 2 \int \log(f_\tau(x))f_\tau(x)dx \quad (1)
\]

Here again \( m \) represents the sample size used for the estimator \( \theta \) and we will think of it as
a variable that changes the magnitude of the penalty function. Of course, the convention
is to replace \( m \) with \( n \), the actual sample size. The AIC criterion is based on estimation
of the first term on the right in \( (1) \). This can be done because the second term does not
depend on any of the models under consideration. As a consequence, one does not estimate
the full risk of using a model, but only its relative risk, which in turn depends on the other
models under consideration. That is, a model that is chosen as the best among a class of
models will still have an uncertain amount of total risk, and so could in fact be a poor fit.

Our quadratic risk is defined by using a quadratic distance (Lindsay et al., 2007) as
the loss function \( a(., .) \). A quadratic distance between the true distribution \( F_\tau \) and any
proposed distribution \( G \), where \( G \) can be either discrete or continuous, has the form

\[
d_K(F_\tau, G) = \iint K_G(s, t)d(F_\tau - G)(s)d(F_\tau - G)(t), \quad (2)
\]

where \( K_G \) is a kernel of appropriate dimensions (details in Section 2), that can be chosen
by the user to meet specific goals. Note that we will allow the kernel to depend on \( G \), the
second argument in distance \( d_K(F_\tau, G) \).
A familiar example of this type is the Pearson Chi-squared distance on a partitioned sample space.

**Example 1.** Let $A_1, ..., A_C$ be a partition of the sample space $S$ into $C$ bins and let $G$ be a target probability measure. Define the kernel by

$$K_G(x, y) = \sum_{i=1}^{C} \frac{I[x \in A_i] I[y \in A_i]}{G(A_i)},$$

where $I$ is the indicator function and $G(A_i) = \int_{A_i} dG(x)$. The resulting quadratic distance is the Pearson Chi-square, given by:

$$\sum_{i=1}^{C} \left[ F_{\tau}(A_i) - G(A_i) \right]^2 G(A_i).$$

We will be using the Pearson Chi-squared example throughout the paper as a way to exemplify our distance calculations in the simplest possible setting. In the example we introduce in Section 4, we will be using a Gaussian kernel.

**1.2. Why quadratic risk based model selection?**

Why do we propose this new measures of model selection? Here we discuss three key issues that played a role in the development of our methodology:

**1.2.1. Local vs global comparison of models**

Quadratic distance does not separate into two parts in the manner that Kullback Leibler does (see (1)). This means that one must estimate the absolute risk for a model. In the process, however, we can learn whether the models provide a low level of absolute risk, whereas for AIC we have no assurance that any model, even the best one, fits well in an absolute sense.

The absolute quadratic risk of a parametric model can be calibrated by comparing its risk with the risk of the empirical distribution function. The latter estimator has no lack of fit but, due to its flexibility, will have the highest variability. As we will see in our simulations, its risk provides a excellent benchmark for model quality. In effect, failure to meet this standard means that either more model building is needed, or nonparametric
Ray and Lindsay approaches should be used. In our application section we provide examples where the global comparison provides crucial decision making information in model selection.

1.2.2. The role of model regularity conditions

The approximations used to arrive at AIC, BIC and most other information criterion depend strongly on regularity conditions (boundary conditions, nested parameter structure among others) some of which are violated in important model selection exercises. For example, the regularity problems for nested mixture models are well known (see Section 4). Similar problems occur in the structural equations model (Bollen et al. 2006) and the multilevel model, where the boundary between nested models is irregular. All these makes the usual asymptotic expansions inappropriate.

On the other hand, our method is based on global tests of goodness of fit. As a result the test statistics that are used have asymptotic expansions that do not depend on regularity assumptions for nested models and so have wider validity.

1.2.3. Addressing computational challenges in high dimensions

A primary goal of our research was to devise model selection methods that would be practical for high dimensional problems. However, quadratic distances, such as the one we are proposing as the loss function of our risk, could require numerical integration of the same dimension as the data vector, which would defeat our purpose. For our mixture example we will show how to avoid this computational burden by using a “rational” kernel for the distance; this gives the needed integration in a closed form. A detailed description of construction of these kernels can be found in Lindsay et al. (2007).

An additional challenge in high dimensions is the construction of distances whose operating characteristics can be tuned to the dimension of the problem and the sample size. In a Chi-squared test this would be done by choosing the number and location of the bins. Lindsay et al. (2007) defined the degrees of freedom of a quadratic distance and discussed its use to select distances. The kernel we will use in the mixture example includes a “tuning parameter”, that allows us to select a suitable degrees of freedom for the distance and also
allows us to analyze the data at multiple resolutions.

1.3. Description of Paper

Section 2 provides a detailed description of our choice of the quadratic distance in defining the quadratic risk, the appropriateness of such a definition in the context of high dimensional datasets and the estimation of quadratic risk. In Section 3 we build model selection tools based on our quadratic risk. Next, in Section 4 we demonstrate how this model selection tool can be applied to select the number of components in a multivariate normal mixture. Application to real data and simulated datasets and comparison of our method with existing model selection tools are described in Section 5. Section 6 contains a discussion and the Appendix provides proofs of results stated in the article.

2. Quadratic Risk and estimation of Quadratic Risk

This section provides the foundational details and the estimation techniques for quadratic risk. We will start by defining the quadratic distance between two arbitrary probability measures. Then, after deriving an unbiased estimator of the quadratic distance we will use it to build an unbiased cross-validation based estimator for the quadratic risk measure. Although analytically attractive, this cross-validation method is computationally very expensive whenever parameter estimation is expensive, especially so for large datasets or when the dimensions are high. So, in the later part of this section we will derive an AIC-like approximation to the the risk measure, which is largely based on the decomposition of our quadratic risk and the asymptotics of quadratic distance. The definitions and results on quadratic distance that are discussed in this section are described in greater detail in Lindsay et al. (2007) and Ray (2003).

2.1. Quadratic Distance: Definition and empirical estimate

2.1.1. Quadratic Distance framework

First we provide the details of construction of the class of quadratic distance, which we use as the loss function of our risk measures. We define $d_K(F_\tau, G)$ to be the distance between
the true density, \( F \tau \) and any proposed distribution \( G \), provided that they are defined on the same sample space \( S \). The building block for our distance will be \( K(s, t) \), a bounded symmetric kernel function on \( S \times S \), which is conditionally non-negative (CNND)\(^{†}\) definite.

**Definition 1.** Given a CNND \( K_G(s, t) \), possibly depending on \( G \), the \( K \)-based quadratic distance between two probability measures \( F \tau \) and \( G \) is defined as

\[
d_K(F \tau, G) = \iint K_G(s, t) \, d(F \tau - G)(s)d(F \tau - G)(t). \quad (4)
\]

Note that by allowing \( K \) to depend on \( G \) we no longer have an inner product space, but we retain non-negativity due to CNND.

2.1.2. Estimation of Quadratic Distance

We now focus on the empirical estimation of the quadratic distance. We will later use these results for the estimation of quadratic risk. It will be useful to express our results in terms of the \( n \times n \) dimensional empirical kernel matrix \( K \) of a data set \( x_1, \ldots, x_n \), which we define to have \( ij \)-th element \( K_{ij} = K(x_i, x_j) \). Crucial to the estimation is the concept of the centered kernel defined as follows:

**Definition 2.** The \( G \)-centered kernel \( K \), denoted by \( K_{cen(G)} \), is defined as

\[
K_{cen(G)}(x, y) = K(x, y) - K(x, G) - K(G, y) + K(G, G), \quad (5)
\]

where \( K(x, G) = \int K(x, y)dG(y) \) and \( K(G, G) = \iint K(x, y)dG(x)dG(y) \).

For example, the \( G \)-centered kernel for the Pearson Chi-squared kernel in (3) simplifies to

\[
K_{cen(G)}(x, y) = \frac{\sum_i \mathbb{I}[x \in A_i]\mathbb{I}[y \in A_i]}{G(A_i)} - 1. \quad (6)
\]

Using the \( G \)-centered kernel we can rewrite the distance in form of a \( U \)-functional as

\[
d_K(F \tau, G) = \iint K_{cen(G)}(x, y)dF \tau(x)dF \tau(y). \quad (7)
\]

\(^{†}\)K is CNND if \( \iint K(s, t) \, d\sigma(s)d\sigma(t) \) is nonnegative for all bounded signed measures \( \sigma \), and if nonnegativity holds for all \( \sigma \) satisfying the condition \( \int d\sigma(s) = 0 \).
But as \( F_\tau \) is unknown we will use the empirical cdf \( \hat{F} \) to estimate \( d_K(F_\tau, G) \). Using (7), for any fixed \( G \), we arrive at the following two estimates for \( d_K(F_\tau, G) \). First, \( d_K(\hat{F}, G) = K\text{cen}(G)(\hat{F}, \hat{F}) := V_n \) is a \( V \)-statistic (Serfling, 1980) which is known to provide a biased estimate for the \( U \)-functional in (7). It can be calculated in matrix form as \( 1^T K\text{cen}(G)1/n^2 \).

One can also construct an unbiased estimate using the corresponding \( U \)-statistic:

\[
U_n = \frac{1}{n(n-1)} \sum_{i \neq j} K\text{cen}(G)(x_i, x_j) = \frac{1}{n(n-1)} \left[ 1^T K\text{cen}(G)1 - \text{tr}(K\text{cen}(G)) \right], \tag{8}
\]

where \( \text{tr} \) denotes the usual matrix trace. Note that we will later use the notation \( \text{trace}_G(K) \) to refer to a functional version of the trace operation that is defined by

\[
\text{trace}_G(K) = \int K(x, x)dG(x). \tag{9}
\]

Note that for the Pearson Chi-squared distance, using the estimator \( V_n \) we get

\[
\sum_{i=1}^{C} \left( \hat{F}(A_i) - G(A_i) \right)^2 / G(A_i), \tag{10}
\]

which equals the Pearson Chi-squared statistic divided by \( n \), whereas the unbiased estimator using (8) gives

\[
\sum_{i=1}^{C} \left( \hat{F}(A_i) - G(A_i) \right)^2 / G(A_i) - \frac{(C-1)}{n}. \tag{11}
\]

Note that under the usual assumptions, \( n \) times (11) follows a \( \chi^2_{C-1} \) distribution, so its expectation is \( C - 1 \), whereas the unbiased estimator in (11) has expectation zero.

### 2.2. Quadratic Risk definition and unbiased estimation

Based on the quadratic distance we have already defined the quadratic risk of a parametric model \( \mathcal{M} \) as

\[
\rho_d(F_\tau, \mathcal{M}, m) = E(d_K(F_\tau, \hat{M}_\theta)). \tag{12}
\]

Here \( \hat{\theta} \) is an estimator of \( \theta \), based on a sample of size \( m \). In our subsequent analyses we will assume that \( \hat{\theta} \) is the maximum likelihood estimator of \( \theta \). Note also that \( \hat{M}_\theta \) is the second argument in \( d_K(\cdot, \cdot) \), so when we use a \( G \)-dependent kernel (see [4]) it will be playing the role of \( G \).
Next we construct an unbiased estimator of the risk given in (12). We start by showing how to unbiasedly estimate the quadratic risk of the empirical distribution function, a nonparametric estimator of $F_\tau$. As mentioned earlier, comparison of nonparametric risk and parametric risk gives a global assessment of model quality.

### 2.2.1. Unbiased estimation of empirical risk

For simplicity of notation, we define the risk of the nonparametric fit, based on $m$ observations, by $R_m$. A straightforward calculation shows that

$$R_m = E[d_K(F_\tau, \hat{F})] = \frac{1}{m} \text{trace}_F(K_{cen}(F_\tau)).$$

(13)

For example, for the Pearson Chi-squared example the above risk can be calculated as:

$$\frac{1}{m} \sum_{i=1}^{C} \left[ \frac{1}{F_\tau(A_i)} - 1 \right] F_\tau(A_i) = \frac{1}{m} \sum_{i=1}^{C} \left[ 1 - F_\tau(A_i) \right] = \frac{C - 1}{m}.$$

For most other kernels we will need to estimate $R_m$ because it will depend on $F_\tau$. Provided that $K$ does not depend on $G$, we can compute an unbiased estimator of $\text{trace}(K_{cen}(F_\tau))$, based on a sample of size $n$ using

$$\frac{1}{n} \sum_{i=1}^{n} K(x_i, x_i) - \frac{1}{n(n-1)} \sum_{i \neq j} K(x_i, x_j).$$

(14)

This immediately gives us the unbiased estimator of $R_m$ as

$$\hat{R}_m = \frac{1}{m} \left[ \frac{1}{n} \sum_{i=1}^{n} K(x_i, x_i) - \frac{1}{n(n-1)} \sum_{i \neq j} K(x_i, x_j) \right].$$

(15)

Note that $\hat{R}_m \xrightarrow{prob} 0$ as $n \to \infty$ and if we set $m = n$, then $\hat{R}_n = O_p(1/n)$. Hence any method of systematically selecting models with smaller estimated risk than $\hat{R}_n$ will give risk estimates converging to zero.

### 2.2.2. Unbiased estimation of risk of parametric models

We next build an unbiased estimator of the risk of the parametric model $M = \{M_\theta\}$, which is given in (12). This risk can be estimated unbiasedly at any sample size $m \leq n - 2$ as
follows: Let $A_m$ be a randomly selected subset of size $m$ from \{1, 2, ..., \$, and let the point estimator $\hat{\theta}(A_m)$ be the value of $\hat{\theta}$ based on \{x_i : i \in A_m\}. Also, we define

$$U(A_m) = \frac{1}{(n-m)(n-m-1)} \sum_{i,j \in A_m^2, i \neq j} K_{cen}(M_{\hat{\theta}(A_m)})(x_i, x_j),$$

(16)

$A^c$ being the complement of set $A$. As $\hat{\theta}$ is constructed from $m$ independent observations, $U(A_m)$ is an unbiased estimator of $\rho(M, m)$, for $m \leq n - 2$. Using (16) we can define an unbiased estimator by averaging over all possible subsets of size $m$,

$$\hat{\rho}(F, M, m) = \frac{1}{\binom{n}{m}} \sum_{i=1}^{\binom{n}{m}} U(A_{m}).$$

If one wishes to estimate $\rho(F, M, n)$, then $m = n - 2$ might be expected to generate the least bias. However, as we argue at the end of this section, other choices of $m$ might be made for the purposes of either consistency or of parsimony. Also, for computational reasons one might wish to use only a few selected subsets of size $m$, as in V-fold cross-validation (van der Laan et al., 2004), or randomly selected subsets of size $m$ (Blom, 1976).

Note that one can construct unbiased estimators of the AIC relative risk in a similar fashion. That is, one can estimate the first term on the right hand side of (11) as

$$\sum \log \left[ m(\hat{\theta}_{-i})(x_i) \right].$$

This estimator is unbiased for risk at sample size $m = n - 1$.

2.3. Decomposition of quadratic risk and approximate quadratic risk estimators

In many model selection problem, we may choose to simplify the unbiased estimates of risk, which can be both difficult and expensive to compute. The main difficulty is that the point estimators are traditionally obtained using the notoriously slow EM algorithm and therefore it is difficult to obtain them to sufficiently high precision in each of the many “leave-out” recalculations. For this reason, we derive an alternative estimate of the quadratic risk, based on asymptotic expansions, similar to those of the AIC derivation.

We start with the following decomposition of the distance:

$$d_K(F, M_{\theta}) = d_K(F, M_{\theta_{-i}}) + [d_K(F, M_{\theta}) - d_K(F, M_{\theta_{-i}})].$$

(17)

Here $\theta_{-i}$ denotes the parameters of the distribution (in the class of distributions denoted by $M_{\theta}$) closest in quadratic distance to the true model $F$. That is, $\theta_{-i} = \arg \min_{\theta} d_K(F, M_{\theta}).$
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We will call the first term on the right side of (17), the model lack of fit (MLF) because it assesses the distance between the best model element and the truth. In particular, it is zero if \( F_\tau \in M_\theta \). Notice that MLF does not depend on parameter estimation.

We will call the second term on the right side of (17), \( [d_K(F_\tau, M_\hat{\theta}) - d_K(F_\tau, M_{\theta_\tau})] \), the parameter estimation error because it measures the deviation of \( \hat{\theta} \) from the best parameter \( \theta_\tau \). We observe that it is always non-negative, by definition of \( \theta_\tau \), and its magnitude increases as \( \hat{\theta} \) deviates from \( \theta_\tau \). In fact, it is shown in the appendix (equation (36)) that this term is approximately a quadratic form in \( (\hat{\theta} - \theta_\tau) \), which implies that the parameter estimation cost is a monotonic function of \( (\hat{\theta} - \theta_\tau) \). Based on the interpretation of the decomposition of the distance we can rewrite (17) as

\[
d_K(F_\tau, M_\hat{\theta}) = \text{MLF} + \text{Parameter Estimation Error.}
\]

For the risk calculation we take expectations in (18) to get

\[
E(d_K(F_\tau, M_\hat{\theta})) = \text{MLF} + \text{PEC}_m,
\]

where \( \text{PEC}_m = E [d_K(F_\tau, M_\hat{\theta}) - d_K(F_\tau, M_{\theta_\tau})] \) represents the parameter estimation cost when \( \hat{\theta} \) comes from a sample of size \( m \).

This decomposition is essential both for finding an approximation to the overall risk and for providing a useful interpretation of the different errors driving the risk. The approximation and the estimates for the two terms, MLF and PEC, will be directly based on the asymptotic theory of quadratic distance (Lindsay et al., 2007) and the unbiased estimators of quadratic distance.

Now we will state a few results from Lindsay et al. (2007) and use these results to justify our approximation and finally provide an appropriate estimator for the quadratic risk.

2.3.1. Kernel projection operator and score centered kernel

Crucial to these approximations of quadratic risk are the concept of scored centered kernel and the score based projection operators which we now define.

For a parametric model given by \( G_\theta \), with density given by \( g(x; \theta) \), let us denote the set of score functions by \( \nabla \log g(x_i; \theta) = s(x_i; \theta) \), where \( \nabla \) is the vector differential with respect
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Let \( \theta \) be every element of \( \theta \). Note the MLE \( \hat{\theta} \) is obtained as a solution to \( \sum s(x_i; \theta) = 0 \). Further, we define the extended score vector \( u^*_{\theta}(x) = (1, s(x, \theta)^T)^T \) and the extended information matrix for a single observation to be:

\[
\mathbb{J}^*_{\theta} = E_{\theta}[u^*_{\theta}u^*_{\theta}^T].
\]

We will then let \( P^* \) be the kernel operator defined by

\[
P^*_{\theta}(x, y) = u^*_{\theta}(x)^T \cdot \mathbb{J}^{-1} \cdot u^*_{\theta}(y).
\] (20)

That is, \( P^*_{\theta} \) acts as a projection operator on the likelihood scores \( u^*_{\theta} \). The score centered kernel \( K_{\text{scen}(G_{\theta})}(x, y) \), as centered under \( G_{\theta} \), is defined to be

\[
K_{\text{scen}(G_{\theta})} = (I - P^*_{\theta}) \cdot K \cdot (I - P^*_{\theta}) = \int K(x, z)P^*_{\theta}(z, y)dG_{\theta}(z) + \int P^*_{\theta}(x, z)K(z, w)P^*_{\theta}(w, y)dG_{\theta}(z)dG_{\theta}(w). \] (21)

Similar to the matrix form of \( K \), we define the \( n \times n \) matrix \( P_{\theta} = u_{\theta}J_{\theta}^{-1}u_{\theta}^T \), where \( u_{\theta} \) is the \( n \times p \) matrix with entries \( \partial_{\theta_j}[\log g_{\theta}(x_i)], x_i \) being the \( i^{th} \) data point and \( \theta_j \) being the \( j^{th} \) component of \( \theta \). Similarly we represent the matrix version of the scored centered kernel as \( K_{\text{scen}(\theta)} \) which can be calculated as

\[
K_{\text{scen}(\theta)} = (I - P^*_{\theta}) \cdot K \cdot (I - P^*_{\theta}) = (I - P_{\theta}) \cdot K_{\text{scen}(\theta)} \cdot (I - P_{\theta}).
\]

The first important property of score centering is the following alternative representation for the empirical distance between the data and the estimated model:

\[
d_K(\hat{F}, G_{\hat{\theta}}) = \int \int K_{\text{scen}(\theta)}(x, y)\ d\hat{F}(x)d\hat{F}(y),
\]

which has the following asymptotic property:

**Theorem 1.** \cite{Lindsay et al. (2007)} Given the regularity assumptions stated in \cite{Lindsay et al. (2007)}, under \( G_{\theta} \) we have

\[
n \left[ d_K(\hat{F}, G_{\hat{\theta}}) - \int \int K_{\text{scen}(\theta)}(x, y)\ d\hat{F}(x)d\hat{F}(y) \right] \overset{prob}{\rightarrow} 0.
\] (22)
This result can then be used to show that \( nd_K(\hat{F}, G_{\hat{\theta}}) \) has an asymptotic distribution that can be represented as \( \Sigma_{i=1}^{\infty} \lambda_i \chi_1^2 \), where the \( \lambda_i \)’s are the eigenvalues of the spectral decomposition of kernel \( K_{\text{scen}(G_{\theta})} \). The asymptotic mean is therefore \( \sum_{i=1}^{\infty} \lambda_i = \text{trace}(K_{\text{scen}(G_{\theta})}) \) (see Lindsay et al., 2007, for details).

### 2.3.2. Approximate quadratic risk estimators

We now return to our original purpose of approximating the different terms of our quadratic risk. These approximations will be based on asymptotic calculations for each model, assuming that the model is correct. This same technique is used in the AIC calculation, where it clearly produces great simplification in risk estimation. We start with the asymptotic approximation to PEC:

**Proposition 2.1.** Suppose that \( M_\theta \) has the density function \( m_\theta \) and that the true model \( F_\tau \) is in the model space \( M_\theta \), having parameter \( \theta_\tau \). In this case \( d_K(F_\tau, M_\theta) = 0 \). Define

\[
V(x, y) = \int \int P(x, z)K(z, w)P(w, y) \, M_{\theta_\tau}(z)M_{\theta_\tau}(w)
\]

where \( P(x, y) = u(x)^T \Psi^{-1} u(y) \). Then as \( m \), the sample size for \( \hat{\theta} \), goes to infinity,

\[
md_K(F_\tau, M_{\hat{\theta}}) - m \int \int V(x, y) \hat{F}(x)\hat{F}(y) \xrightarrow{\text{prob}} 0.
\]

It follows that the asymptotic mean of \( md_K(F_\tau, M_{\hat{\theta}}) \) is

\[
\text{tr}_{\theta_\tau}(V) = \int \int V(x, y) \, M_{\theta_\tau}(x)M_{\theta_\tau}(y).
\]

**Proof.** See Appendix.

As a simple example, for the Pearson Chi-squared kernel the PEC is simply \( \text{dim}(\hat{\theta})/m \), where \( \text{dim}(\hat{\theta}) \) denotes the number of parameters being estimated. In general we have to estimate PEC and for an estimator of \( \text{trace}(P_\theta^*K\hat{P}_\theta^*) \), we use its empirical version \( \frac{1}{n}\text{tr}(P_\theta^*K\hat{P}_\theta^*) \) based on the full sample. This yields the following estimator:

\[
\hat{\text{PEC}}_{(m)} = \frac{1}{m} \left( \frac{1}{n} \text{tr}(P_\theta^*K\hat{P}_\theta^*) \right).
\]
Now we turn to the estimation of $\text{MLF}=d_K(F_\tau, M_{\theta_\tau})$, a term not depending on hypothetical sample size $m$. We start with its sample equivalent given by

$$d_K(\hat{F}, M_{\hat{\theta}}) = \int \int K_{\text{scen}(M_{\hat{\theta}})}(x,y) d\hat{F}(x) d\hat{F}(y) = \frac{1}{n^2} \mathbf{1}^T K_{\text{scen}(M_{\hat{\theta}})} \mathbf{1}. \quad (24)$$

This estimator has bias $E(d_K(\hat{F}, M_{\hat{\theta}})) - \text{MLF}$. To do bias correction we again use an asymptotic approximation assuming that $F_\tau = M_{\theta_\tau}$, so that $\text{MLF} = 0$. Applying the remarks following Theorem 1 we obtain the following approximation to the bias term:

$$E(d_K(\hat{F}, M_{\hat{\theta}})) - \text{MLF} \approx \frac{1}{n} \text{trace}_{\theta_\tau}(K_{\text{scen}(M_{\hat{\theta}})}). \quad (25)$$

The right side of (25) can be estimated by its sample equivalent

$$\frac{1}{n^2} \text{trace}_{\hat{\theta}}(\mathbf{I} - P_{\hat{\theta}}^*) K_{\text{scen}(M_{\hat{\theta}})} K_{\text{scen}(M_{\hat{\theta}})}^* \mathbf{I} - P_{\hat{\theta}}^*). \quad (26)$$

Thus, we have the bias corrected estimator of MLF,

$$\hat{\text{MLF}} = \left[ d_K(\hat{F}, M_{\hat{\theta}}) - \frac{1}{n^2} \text{trace}_{\hat{\theta}}(\mathbf{I} - P_{\hat{\theta}}^*) K_{\text{scen}(M_{\hat{\theta}})} K_{\text{scen}(M_{\hat{\theta}})}^* \mathbf{I} - P_{\hat{\theta}}^* \right]. \quad (27)$$

For example, in the Pearson Chi-squared case (26) reduces to $(C - 1 - \text{dim}(\hat{\theta}))/n$ and thus the MLF can be estimated as:

$$\sum_{i=1}^{C} \left[ \frac{\hat{F}(A_i) - G_{\hat{\theta}}(A_i)}{G_{\hat{\theta}}(A_i)} \right]^2 - \frac{C - 1 - \text{dim}(\hat{\theta})}{n}. \quad (28)$$

Since $(C - 1 - \text{dim}(\hat{\theta}))$ gives the residual degrees of freedom for the $C$-cell Pearson Chi-squared test it is clear how the correction removes the bias inherent in the Chi-square limiting distribution.

Finally combining the estimators of $\text{PEC}_{(m)}$ and MLF given in (23) and (27) we have the following estimator for the quadratic risk:

$$\rho_{d_K(M,m)} = \left[ d_K(\hat{F}, M_{\hat{\theta}}) - \frac{1}{n^2} \text{trace}(\mathbf{I} - P_{\hat{\theta}}^*) K_{\text{scen}(M_{\hat{\theta}})} K_{\text{scen}(M_{\hat{\theta}})}^* \mathbf{I} - P_{\hat{\theta}}^* \right] + \frac{1}{nm} \text{trace}_{\hat{\theta}}(P_{\hat{\theta}}^* K_{\text{scen}(M_{\hat{\theta}})} K_{\text{scen}(M_{\hat{\theta}})}^* P_{\hat{\theta}}^*). \quad (28)$$

Note that for the Pearson Chi-squared example the risk estimator, when calculated at $m = n$ simply becomes:

$$\sum_{i=1}^{C} \left[ \frac{\hat{F}(A_i) - G_{\hat{\theta}}(A_i)}{G_{\hat{\theta}}(A_i)} \right]^2 / G_{\hat{\theta}}(A_i) - \frac{(C - 1) + 2\text{dim}(\hat{\theta})}{n}. \quad (29)$$
Observe that the risk estimator given by (28) is numerically less expensive than the cross validation based exact estimator given in (16). Unlike the unbiased risk estimator, it does not require repeated parameter estimation. Moreover, the matrix operations involved in the calculation are also inexpensive, making (28) a promising risk estimator.

For model comparison purposes we will also want to estimate the risk of the empirical distribution function \( \hat{F} \), in which case \( P^*_\theta = I \). The estimated distance \( d_K(\hat{F}, \hat{F}) \) is zero. So a biased estimator of \( R_m \), the risk of the \( \hat{F} \), at sample size \( m \), may be calculated using

\[
\hat{R}_m^b = \frac{1}{nm} tr \left( \mathbb{K}_{cen}(\hat{F}) \right). \tag{30}
\]

We will later see that if we use an appropriately scaled kernel \( K^* \), \( \hat{R}_m^b \) is exactly equal to the degrees of freedom corresponding to the scaled kernel \( K^* \). In fact for the Pearson Chi-squared kernel \( \hat{R}_m^b = C - 1 \), which is the degrees of freedom for a \( C \)-cell Chi-squared goodness of fit test.

In the special case that the estimated risk is evaluated at \( m = n \) we will call it the Quadratic AIC risk or in short QAIC, where AIC reflects commonality with the AIC derivation. We will now show how to mimic the BIC criterion by using a different value of \( m \). Recall that for the usual AIC with KL loss function, the relative MLF, after subtracting \( \int \log(f_\tau(x)) f_\tau(x) dx \) common to all models corresponds to \( -\int \log(m_{\theta}) f_\tau(x) \) (see [1]), which has the approximately unbiased estimator (under the model):

\[
\hat{MLF} = -2\frac{\hat{l}}{n} + \frac{\dim(\hat{\theta})}{n}. \tag{31}
\]

The parameter estimation cost, \( PEC_{(m)} = \frac{\dim(\hat{\theta})}{m} \), giving us the estimated risk,

\[
-2\frac{\hat{l}}{n} + \frac{\dim(\hat{\theta})}{n} + \frac{\dim(\hat{\theta})}{m}. \tag{31}
\]

For AIC risk we use \( PEC_{(n)} \), which gives us \( AIC/n = -2\hat{l}/n + 2\dim(\hat{\theta})/n \). Note the similarity of this risk to the Pearson risk estimator in [20]. The essential difference is that the latter estimates absolute risk, not relative risk. If one uses \( m = n/(\log n - 1) \) in (31), one arrives at the standard BIC formula:

\[
\frac{BIC}{n} = -2\frac{\hat{l}}{n} + \frac{\log(n)\dim(\hat{\theta})}{n}. \tag{31}
\]

\( ^4 \) \( K^* = K/c \), where \( c = tr(K)/tr(K^2) \)
For this reason the estimated risk \( (28) \) evaluated at \( m = n/(\log n - 1) \) will be called QBIC, and can be written as

\[
QBIC = \hat{MLF} + (\log(n) - 1) \times \hat{PEC}(n).
\]

\[
= \left[ d_k(\hat{F}, \hat{M}_\theta) - \frac{1}{n^2} tr(\mathbb{I} - \hat{P}^*_\theta)K(\mathbb{I} - \hat{P}^*_\theta) \right] + \left[ \frac{(\log(n) - 1)}{n^2} tr(\hat{P}^*_\theta K\hat{P}^*_\theta) \right]. \quad (32)
\]

Along with a recipe for estimation of the risk, the decomposition in (28) provides an excellent tool for deeper understanding and analysis of the interplay of model misspecification and the effective parameter cost of using the model. This provides us with the ingredients for constructing alternative model selection tools and tools for accessing global fits which we discuss in the following section.

### 2.4. Consistency and choice of \( m \)

It seems very natural to assess the risk of a model at the sample size \( m = n \). This risk indicates how well the chosen model, along with the current parameter estimates, might be expected to perform when used to approximate the true distribution. Unfortunately, estimating the risk at \( m = n \) is a hard problem: one cannot estimate this risk well enough to discriminate consistently between two true models with different numbers of parameters.

In this section we will consider the meaning of consistency under several asymptotic scenarios. We will use the AIC method to illustrate our points because of its simple form. In all of them, we will suppose that the true distribution is in one of the models, i.e. \( F^*_\tau \in \mathcal{M} \).

First, if one leaves \( m \) fixed as \( n \to \infty \), then the best model, in terms of risk, need not contain the true distribution, and consistency would mean selection of this (possibly false) best model. This might be desirable for reasons of parsimony, as the true models may be too complex to be useful.

In a formal sense, methods like AIC cannot be consistent in this asymptotic scenario because they use asymptotic approximations for the cost of estimating parameters, and those approximations assume the model is true. If one replaces the exact risk with the asymptotic approximation, however, consistency is achieved. See, for example, the AIC in (31), where the \( \hat{MLF} \) term is consistent for MLF, and the approximate parameter estimation cost is just a function of parameter dimension when \( m \) is fixed.
A second way to view consistency is to let \( m = m_n \) increase with \( n \). In this case, the parameter estimation costs shrink to zero, and so consistency would involve selecting a true model. A stringent form of consistency, but natural, would require the method to select the smallest true model with probability approaching one. We will call this smallest-true-model (STM) consistency.

It is well known that AIC, with \( m_n = n \), lacks this form of consistency. When two true models \( M_1 \subset M_2 \) are nested (and regularity conditions hold), the probability that AIC picks the larger of the two models corresponds to using a likelihood ratio test with the constant critical value \( 2(\dim(M_2) - \dim(M_1)) \). For example if the difference of dimension is 1, with probability 0.16(= \( Pr(\chi^2_1 > 2) \)) we choose the larger model.

It turns out that STM consistency holds when \( m/n \) goes to zero. The proportional case, when \( m_n \approx \gamma n \), for constant \( \gamma > 0 \), is at the cutting edge of consistency. It is easily checked that for the AIC criterion, it is equivalent to using the critical value \( (1 + \gamma^{-1})(\dim(M_2) - \dim(M_1)) \). For example if the difference of dimension is 1, the probability of overshooting is around .045, .025, .01, .001 for the proportion \( \gamma = \frac{1}{3}, \frac{1}{4}, \frac{1}{5}, \frac{1}{10} \) respectively. Thus as \( \gamma \) approaches zero, the probability of overshooting goes to zero.

Although one might choose to use a BIC type criterion for its familiarity, we think it would be very useful to also describe the null probability of rejection for the corresponding likelihood ratio critical value.

3. Model Selection using Quadratic Risk

Now, we provide a short description of how one might use quadratic risk as a model selection tool. First, one needs to understand the interplay of the terms in the risk decomposition. Please see Figure 11 for an illustration. It shows the relevant quantities for an example in Model(3) with \( n = 300 \), described later in Section 5. Suppose we have a sequence of models \( M_k \) that are nested with increasing \( k \). As model complexity \( k \) increases the empirical distance \( d_K(\hat{F}, \hat{M}_k) \) decreases but must stay non-negative. We also know that \( \hat{\text{MLF}} \), for any model that contains \( F_\tau \), will tend to zero in probability. The estimated parameter estimation cost \( \hat{\text{PEC}} \) starts near zero and increases with model complexity. However it never will be larger than the risk of the empirical estimate, which is the parameter estimation cost.
of a non-parametric fit. By construction, the total quadratic risk is the simple addition of the MLF and the PEC. Thus models with low estimated risk arise as a compromise between the decreasing MLF and the increasing PEC. A simple model selection rule is to pick the model having the minimum value of QAIC.

The QBIC form of the risk, given in (32) introduces a larger penalty for parameter estimation than QAIC. In Figure 1(b) one can see how this alteration has created a much sharper minimum in the risk function. Both for QAIC and QBIC, we will say that the model with the minimum estimated risk is the best model.

Just like AIC and BIC, quadratic risks need not attain an absolute minimum in the range of models considered. However, there is an important benchmark, given by the empirical risk, for evaluating the performance of a model when using quadratic risk measures. Note that for the empirical distribution there is no model lack of fit, because the model is nonparametric, but there is the maximal possible parameter estimation cost. Models that don’t meet this benchmark clearly suffer from substantial model lack of fit and so we will label them as “inadequate models,” while the rest will be called “adequate”. Even in the presence of a minimum risk model, if all our proposed models are “inadequate” it indicates that more model building in the same class, or exploration in a larger class of models might be necessary. For example, based on the QAIC risk for proposed models and empirical
model in Figure 1(b), if we had explored only the 5 smallest models, then QAIC and QBIC would have selected model 3. However based on the MRA criterion no model would have been found adequate, thus providing the crucial global framework for model selection.

On the other hand if we have more than one “adequate models” we will call the smallest model in this set the minimal-risk-adequate model (henceforth denoted as MRA). Note that the consistency of the empirical risk (shown in Section 2.2.1) ensures that this model selection method would have estimated risk going to 0 as \( n \to \infty \). Now inspecting Figure 1(b) for the whole range of 10 components model, we see that all models from 6 onwards are adequate. Thus model 6 is the MRA model, even though the QAIC selects model 9 as the minimum risk model.

We will provide illustrations of these criteria in the application section.

4. Application: Selecting the number of components in mixture models

Now we apply our quadratic risk model selection methodology to the problem of selecting the number of components in a multivariate normal mixture model. We start by introducing the following notation and definitions for mixture models.

A random variable \( X \in \mathbb{R}^D \) is said to follow a \( k \)-component normal mixture model if its density \( f^{(k)} \) can be written as

\[
f^{(k)}(x; \mu, \Sigma, \pi) = \sum_{j=1}^{k} \pi_j \phi(x; \mu_j, \Sigma_j) \quad \text{for} \ x \in \mathbb{R}^D,
\]

where \( \phi(x; \mu_j, \Sigma_j) \) denotes a normal density with mean \( \mu_j \) and variance \( \Sigma_j \), and \( \pi_j < 1 \forall j \) and \( \sum_{j=1}^{k} \pi_j = 1 \). For compactness we denote \( \theta = \{ \mu, \Sigma, \pi \} \), with the above restrictions and denote the density in (33) as \( f^{(k)}_\theta \).

According to the general framework, now \( \mathcal{M} \) denotes the class of all \( D \)-dimensional finite mixtures with normal mixing components; i.e. for a fixed \( D \), our \( \mathcal{M} = \{ \mathcal{M}_1, \mathcal{M}_2, \ldots \} \), where \( \mathcal{M}_k \) denotes the \( k \)-component normal mixture models, and for a particular model element \( M_\theta \in \mathcal{M}_k \), more precisely denoted as \( M^{(k)}_\theta \) we have \( dM^{(k)}_\theta = f^{(k)}_\theta \).

The complexity of the null distribution makes a testing theory for the number of components rather more difficult. It also means that the standard regularity assumptions behind
the derivations of the AIC and BIC are false. For a description of the previous approaches to selecting the number of components of mixture models see McLachlan and Peel (2000).

4.1. Risk-based analysis of mixture complexity

We now develop a strategy for selecting the number of components using our quadratic risk assessment approach. First, we will specify the kernel in order to specify the loss function. We will then outline the steps for estimating the risk function and finally illustrate the use of the risk measure in choosing a mixture model.

4.1.1. Specifying the kernel

In principle, any nonnegative definite kernel can be used to build the distance measure. However, from the results in Section 2 it is clear that the key to the calculation of the distance, and hence the risk, are the integrals required in the definition of the quadratic distance. These will involve high dimensional numerical integration for arbitrary choice of the kernel $K$. For this reason it is desirable to use kernels for which the integrations $\int K(x, y)dM(y)$ and $\int \int K(x, y)dM(x)dM(y)$ can be carried out explicitly.

When the model is a finite mixture of normals, the multivariate normal kernel meets this goal. The $D$-dimensional normal kernel, in its most general form, is defined as

$$K_{\Sigma}(x, y) = \frac{1}{(2\pi)^{D}|\Sigma|^{1/2}} \exp \left( -\frac{1}{2}(x - y)'\Sigma^{-1}(x - y) \right).$$

We will take $\Sigma = h^2I$, $h$ being a “smoothing parameter” and henceforth denote the corresponding kernel as $K^h$. This constant $h$ can be thought of as a “tuning” parameter, something analogous to the bin-width in the construction of a histogram. We will discuss its role further in the next subsection.

4.1.2. Role of tuning parameter “h” and its empirical estimation

Lindsay et al. (2007) developed a tool for the understanding of the operating characteristics of a quadratic distance they called the spectral degrees of freedom of the kernel (sDOF). It is a generalization of the degrees of freedom of the chi-squared distance (itself a quadratic distance) to other kernels by examining their limiting distributions. With this tool one can
roughly equate the degree of smoothing that comes from a choice of \( h \) to that of the chi-squared test having the same degrees of freedom, which in turn corresponds to the number of cells used in its construction. The tuning parameter \( h \) is analogous to choosing the bin-width of each cell (or, equivalently choosing the number of cells) in a Chi-squared goodness of fit test.

The spectral degrees of freedom of the kernel depend on the true sampling distribution and the kernel \( K \) (whether centered or score centered) through the formula

\[
s_{\text{DOF}} = \left( \frac{\int K^h(x,x)dF_\tau(x)}{\int (K^h(x,x))^2 dF_\tau(x)} \right)^2.
\] (34)

In this paper, we will base our selection of \( h \) on the empirical estimate of \( s_{\text{DOF}} \) given by

\[
\hat{s}_{\text{DOF}} = \left( \frac{\text{tr}(K^h_{\text{cen}}(\hat{F}))}{\text{tr}(K^h_{\text{cen}})^2} \right)^2,
\] (35)

where the centered kernel matrix based on the empirical distribution has the \( ij^{th} \) element

\[
K_{\text{cen}}^h(x_i,x_j) = K_h(x_i,x_j) - \frac{1}{n} \sum_i K_h(x_i,x_j) - \frac{1}{n} \sum_j K_h(x_i,x_j) + \frac{1}{n^2} \sum_i \sum_j K_h(x_i,x_j).
\]

Just as in a Chi-squared goodness of fit test, there are choices for the spectral degrees of freedom that are clearly too small and others that are clearly too large. As a rough rule of thumb for selecting the number of cells for \( D = 1 \) we suggest that the degrees of freedom should be more than 5 and less than \( n/5 \), \( n \) being the total number of observations. For \( D > 1 \) dimensions one needs to increase the lower bound of 5 because the goodness of fit test now must assess fit in several directions. We find that if \( s_{\text{DOF}} \) is smaller than \( \left( \frac{D+1}{2} \right) \), it is likely to be too much smoothing, whereas if \( s_{\text{DOF}} > n/5 \) it would mean too little smoothing. See our simulation section for more on the role of the smoothing parameter on model selection.

4.2. Constructing the risk estimators for mixture model selection

Till now we have focused on the form and the smoothing parameter of the kernel for our problem. Using this kernel we will now illustrate the steps in estimating the risk of each parametric mixture model \( M_k, \ k = 1, 2, \ldots \) along with the risk of the empirical model. First, we compute the estimates of the parameters \( \theta_k \) for each parametric model
Simultaneously, we construct a projection matrix $\mathbb{P}^*_{\hat{\theta}}$ for each model, which is strictly based on the estimates $\hat{\theta}_k$ and the observations. We also calculate the score-centered kernel $\mathbb{K}_{\text{acen}(\mathcal{M}_{\hat{\theta}})}$. Then we calculate the risk estimate of each model using (28) and (32).

5. Simulation results and Applications

Now we apply our model selection tool to select the number of components in mixtures. The following steps were used for choosing models in all the examples of this section. First, we standardized the data (i.e. the variance of each variable was scaled to unity). This step was done because we used the same $h$ for all the variables. In this simulation study we restrict ourselves to normal kernels based on the discussion in 4.1.1. Using the results in Section 4.1.2 we estimated the $sDOF$, which gives us a range of interesting smoothing parameter values. The simulation results reported in this section used one representative value from this range, though the results were quite stable across our suggested range. The ML estimates for the range of models under consideration are calculated using an EM Algorithm and the projection matrices $\mathbb{P}^*_{\hat{\theta}}$ based on this estimate. Note that for analysis at different levels of smoothing we only need to recalculate the distance and computationally simple matrix $\mathbb{K}$, and not the projection matrix $\mathbb{P}^*_{\hat{\theta}}$.

5.1. Simulation experiment

Given a mixture parameter set and a fixed sample size, we generated 100 sets of random samples from the true mixture distribution. We have tabulated the frequency of selection...
Table 1. Model Selection results for a set of 2 dimensional simulated datasets. Boldface * indicates selection of true model.

| Estimated number of Components | 1   | 2   | 3   | 4   | 5   | 6   | 7   | 8   | 9   | >10 |
|-------------------------------|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| Model (1): 2 moderately overlapping clusters, 2D, n=1000 |
| AIC                           | -   | -   | 52* | 17  | 8   | 12  | 3   | 3   | 5   |     |
| QAIC                          | -   | -   | -   | -   | -   | -   | -   | -   | -   | -   |
| MRA                           | 62* | -   | -   | -   | -   | -   | -   | -   | -   | -   |
| BIC                           | -   | -   | -   | -   | -   | -   | -   | -   | -   | -   |
| QBIC                          | -   | -   | -   | -   | -   | -   | -   | -   | -   | -   |
| Model (2): 4 distinct clusters, 2D, n=1000 |
| AIC                           | -   | -   | 66* | 18  | 6   | 4   | 4   | 1   |     |     |
| QAIC                          | -   | -   | -   | -   | -   | -   | -   | -   | -   | -   |
| MRA                           | 100*| -   | -   | -   | -   | -   | -   | -   | -   | -   |
| BIC                           | -   | -   | 100*| -   | -   | -   | -   | -   | -   | -   |
| QBIC                          | -   | -   | 98* | 2   | -   | -   | -   | -   | -   | -   |
| Model (3): 6 distinct clusters, 2D, n=1000 |
| AIC                           | -   | -   | -   | -   | 43* | 34  | 12  | 4   | 7   |     |
| QAIC                          | -   | -   | -   | -   | -   | 64* | 31  | 9   | 4   | 2   |
| MRA                           | -   | -   | -   | -   | -   | 100*| -   | -   | -   | -   |
| BIC                           | -   | -   | 5   | -   | -   | 95* | -   | -   | -   | -   |
| QBIC                          | -   | -   | 94* | 5   | -   | -   | -   | -   | -   | -   |
| Model (3): 6 distinct clusters, 2D, n=300 |
| AIC                           | -   | -   | -   | -   | -   | -   | -   | -   | -   | -   |
| QAIC                          | -   | -   | -   | -   | -   | 1   | 28* | 38  | 17  | 10  |
| MRA                           | 3   | 25  | 13  | 12  | 1   | 28* | 38  | 17  | 10  | 6   |
| BIC                           | -   | 50  | 12  | 12  | 12  | -   | -   | -   | -   | -   |
| QBIC                          | 11  | 17  | 49* | 17  | 1   | -   | -   | -   | -   | -   |

of the number of components by each of the 5 model selection methods (AIC, QAIC, MRA, BIC, and QBIC) under different examples, in an experimental design that varies by dimension, sample size and separateness of the components. For some example we also vary the range of models in the model space.

Here, we have fixed the variance structure, so our model selection only refers to selecting the number of components. Readers familiar with the MCLUST software should note that Fraley and Raftery (1999) provide a unified strategy to select both the number of components and the variance structure, but only with a single criterion, the BIC. We now discuss the results of our simulation experiment.

5.1.1. Two dimensional simulation

In our first study we held the data dimension to two and varied the normal mixture model as well as the sample size (for some cases). The scatterplot of a representative sample from
the simulation of each of the 4 models is given in Figure 2.

First we consider simulations from the first 3 models which are generated from 2, 4 and 6 component normal mixtures respectively. From Table 1 it is clear that AIC and QAIC are the more liberal methods- in the sense of favoring models larger than the true model. Although QBIC and BIC are both potentially conservative, QBIC is slightly less so and made model selection errors on both sides of the true value. The MRA criterion (here using the $m = n$ risk) was fairly conservative in some cases (e.g. Simulation 1) but otherwise fairly competitive. Like BIC it never overshot the true model.

Next we explore the effect of sample size on model selection in Model (3). Decreasing the sample size from 1000 to 300 tended to increase the underestimation of the three conservative methods, but did not greatly degrade the liberal estimates of AIC and QAIC, reflecting their lack of consistency.

Overall QAIC performed much better than AIC. Though QAIC overestimated the complexity, in comparison to AIC the distribution of the the number of components was much more peaked at the true number while the right tail tapered off very quickly. Also, if the components had high degree of overlap, in the sense of not displaying distinct modes for distinct components, then QBIC performed better than BIC, which most often underestimated the number of components.

Note also that the quadratic risk based methods are more stable with change of sample size. In those cases where the sample size was small and BIC badly underestimated, the QBIC and MRA methods were distinctly better. Finally, the simulation study revealed that adequacy is a very useful measure. In many examples it provided extra information about the minimal number of components that would be needed to explain the data in hand. Often the minimal adequate model had a considerably smaller number of components than the one with minimum risk QAIC model.

5.2. Quadratic risk as global measure of risk

Next we explore two examples where the true model is beyond our model space and show how the quadratic risk measures provides an excellent global model selection criterion in identifying the scenario. We have already observed that with n=1000 in Model (3) with
Table 2. Model selection results demonstrating global risk measure

| Model (3): 6 components, 2D, n=1000 (limited to 5 components) | Estimated number of Components |
|---------------------------------------------------------------|--------------------------------|
|                                                               | 1    | 2    | 3    | 4    | >5   |
| AIC                                                           | -    | -    | 52   | 9    | 39   |
| QAIC                                                          | -    | -    | 58   | 6    | 36   |
| MRA                                                           | -    | -    | -    | -    | -    |
| BIC                                                           | -    | -    | 100  | -    | -    |
| QBIC                                                          | -    | -    | 87   | -    | 13   |

six distinct normal components, QAIC, QBIC, MRA and BIC all overwhelmingly select six components. But what happens if we explore only up to 5 components, i.e. we do not include the true model in the model class? Table 2 summarizes the results for the 5 different criteria when we explore only up to 5 components. We immediately observe that BIC selects the 3 component model in 100% of the cases. Independently our quadratic measures also selected this model in 52% and 87% of the cases, but the MRA criterion shows that none of the models are adequate. Thus if we based our conclusion on BIC alone we would have failed to recognize that we are trapped in a local minima. But if we use the quadratic risk measure along with the MRA criterion we are forced to explore models beyond 3 components as we have a clear indication that even the 5 component model is not adequate.

We now explore an example where the model is not a normal mixture, but rather when the scatter of the distribution has the shape of the letter U, as given in Figure 2 (Model 4). These datasets were simulated by first generating the $x$ coordinate uniformly between -1.5 and 1.5 and then generating $y$ uniformly between $x^2 - 1$ and $x^2 + 1$. By design, this density is very hard to capture with a few normal components. So we explored up to 14 normal components. BIC and QBIC mostly choose 8-10 components. Even using the liberal measure QAIC, 51% of the times we choose a model with less than 14 components. But the MRA criterion overwhelmingly (70% of the cases) shows that even a 14 component model is not adequate. This suggests that we should either explore beyond 14 component model or we should explore beyond normal mixtures.

In both these examples it can be easily seen that BIC, which is the most widely used model selection method for mixtures, does not provide the best result, simply because it is a relative rather than a global measure of risk. On the other hand in each of these simulations the MRA criterion clearly points out, that the minimum risk model does not
### Table 3. Model selection results for the U Example (simulation (4))

| Estimated number of Components | 1  | 2  | 3  | 4  | 5  | 6  | 7  | 8  | 9  | 10 | 11 | 12 | 13 | >14 |
|--------------------------------|----|----|----|----|----|----|----|----|----|----|----|----|----|-----|
| AIC                           | -  | -  | -  | -  | -  | -  | -  | 2  | 16 | 82 |
| QAIC                          | -  | -  | -  | -  | -  | -  | 1  | 5  | 7  | 19 | 19 | 49 |
| MRA                           | -  | -  | -  | -  | -  | -  | 1  | 3  | 7  | 8  | 3  | 8  |
| BIC                           | -  | -  | -  | -  | -  | -  | 16 | 50 | 24 | 6  | 3  | 1  |
| QBIC                          | -  | -  | -  | -  | -  | -  | 12 | 30 | 28 | 9  | 10 | 7  | 4  |

### Table 4. High dimensional simulation results

| Estimated number of Components | 1  | 2  | 3  | 4  | 5  | 6  | 7  | 8  | 9  | >10 | Estimated number of Components (search limited to 5 components) | 1  | 2  | 3  | 4  | >5 |
|--------------------------------|----|----|----|----|----|----|----|----|----|----|---------------------------------------------------------------|----|----|----|----|----|
| Model (5): 6 components, n=1000 in 4 dimensions             |    |    |    |    |    |    |    |    |    |    | Model (5): 6 components, n=1000 in 4 dimensions             |    |    |    |    |    |
| AIC               | -  | -  | -  | -  | -  | 23 | 40 | 14 | 15 | 8  | -  | -  | -  | -  | 100 |
| QAIC             | -  | -  | -  | -  | -  | 56 | 27 | 11 | 3  | 3  | -  | -  | 8  | -  | 92  |
| MRA              | -  | -  | -  | -  | -  | 96 | -  | -  | -  | -  | -  | -  | -  | -  | 4   |
| BIC              | -  | 20 | 3  | 77 | -  | -  | -  | -  | -  | -  | -  | -  | 88 | -  | 12  |
| QBIC             | -  | 3  | 3  | 95 | -  | -  | -  | -  | -  | -  | -  | -  | 49 | -  | 51  |
| Model (6): 6 components, n=1000 in 8 dimensions             |    |    |    |    |    |    |    |    |    |    | Model (6): 6 components, n=1000 in 8 dimensions             |    |    |    |    |    |
| AIC               | -  | -  | -  | -  | -  | 17 | 32 | 22 | 16 | 13 | -  | -  | -  | -  | 100 |
| QAIC             | -  | -  | -  | -  | -  | 54 | 34 | 10 | 2  | -  | -  | 33 | 1  | 66  |
| MRA              | -  | -  | -  | -  | 8  | 92 | -  | -  | -  | -  | -  | -  | -  | 8   |
| BIC              | -  | 25 | 5  | 69 | -  | -  | -  | -  | -  | -  | -  | 71 | 0  | 29  |
| QBIC             | -  | 5  | 4  | 88 | -  | -  | -  | -  | -  | -  | -  | 84 | -  | 16  |
| Model (7): 6 components, n=1000 in 12 dimensions             |    |    |    |    |    |    |    |    |    |    | Model (7): 6 components, n=1000 in 12 dimensions             |    |    |    |    |    |
| AIC               | -  | -  | -  | -  | -  | 12 | 31 | 18 | 16 | 23 | -  | -  | 13 | 7  | 80  |
| QAIC             | -  | -  | -  | -  | -  | 49 | 34 | 9  | 5  | 3  | -  | -  | 75 | 21 | 4   |
| MRA              | -  | -  | -  | -  | 10 | 88 | 1  | 1  | -  | -  | -  | -  | -  | 10  |    |
| BIC              | -  | 27 | 4  | 63 | -  | -  | -  | -  | -  | -  | -  | 93 | 3  | 4   |
| QBIC             | -  | 7  | 3  | 81 | -  | -  | -  | -  | -  | -  | -  | 90 | 7  | 3   |

lie in the model class that we are considering.

#### 5.2.1. High dimensional simulation

We now examine the effect of increasing dimensions. Our 4D, 8D and 12D examples with 6 components were generated in the following way: The first two dimensions are the same as 2D Model (3) used in Section 5.1.1; the remaining dimensions are generated from standard normal variates. Like the 2D Model (3) the performance of the 5 criteria are judged under two scenarios (i) when the true model is in the model space (ii) and when the true model was not included in the search space. The results for both scenarios are given in Table 4, the
left panel corresponding to scenario (i), where we explore up to 10 components and the right panel corresponding to scenario (2) where we restrict ourselves to less than 6 components.

First we summarize the results from scenario (i). AIC grossly overestimates the number of components. QAIC overestimated the number of components but less so than the AIC, but more importantly its performance did not deteriorate much with the increase of dimensions. As dimension increases, BIC tends to underestimate the true number of components with higher percentage, and in many cases (20%, 23%, 25% for 4, 8 and 12 dimensions respectively) BIC even chose the 3 component model. QBIC and MRA erred on either side of the true model, but both of them chose the true model with higher percentage than BIC. Moreover, when QBIC and MRA underestimated they erred slightly selecting 5 components, while BIC selected 3 component model in many cases.

For scenario (ii) the results are consistent with the findings of the two dimensional case, i.e. the various information criterion overwhelmingly suggest that the 3 component model is the true model, whereas the MRA criterion combined with the quadratic measures clearly points out (in 96%, 92%, 90% for 4, 8 and 12 dimensions respectively) that we have not reached a global minimum and we should expand our search space.

These examples clearly show the usefulness of quadratic risk based methods in high dimensions, both for selecting the true model and providing a global infrastructure for model selection.

5.3. Application to real dataset

We apply our model selection criterion to a real dataset where the goal is to identify the number of gene groups displaying distinctive gene expression profile under a set of conditions. The details of the experiment is described in Chitikila et al. (2002) and our dataset was obtained through personal communication from Dr. F. Pugh of Pennsylvania State University. Here we present a very short description of the experimental design and preprocessing of the data.

The experiment was designed to answer an interesting questions in transcriptional genomics: Is the binding phenomenon of TATA binding proteins (TBP) affected by neighboring TAF1 proteins? The TBPs bind to the TATA box and play a crucial role in transcription
which finally results in protein synthesis. The TBP is intertwined to form a 3D structure in such a way that it forms a concave surface and a convex surface; the concave surface attaches to the TATA box, whereas the convex surface may attach to some other protein, for example the TAND region of TAF1 proteins. To understand this interplay of TBP and the TAND region of TAF1, a set of 19 experiments, were designed using 6226 yeast genes for each strain. The two main factors that were varied in these experiment are (i) whether the TAF1 proteins of the yeast cells had the TAND regions intact (wild types) or whether the TAND regions were removed (Δ-TAND’s), (ii) whether the concave region of the TBP proteins remained unmutated (wild type) or whether a yeast strain with mutation was used. Further 3 different types of mutations and a few controls were also used. Gene clusters displaying distinct gene expression profiles, one for each of the 4 combinations of the two levels of the two major factors would suggest a “interaction” model, whereas only two clusters would suggest that TBP’s are not influenced by neighboring proteins.

The analysis was done as follows. After leaving out genes which did not show significant change over different conditions, we analyzed n=2809 genes under d=19 conditions (dimensions), completely ignoring the information on the identity of the conditions. We used normal mixtures to fit the data and explored up to 8 components. The risk curves of each of the 4 model selection criteria is given in Figure 3. Based on the minimum risk, BIC chose three components whereas AIC chose nine components. For calculating the quadratic risk we first applied the sDOF analysis detailed in Section 4.2.2 and chose a range of \( h \). The risk curves given in Figure 4 are for \( h = 1.7 \) for which the sDOF was 226, but the minimum risk decision remained stable for a wide range of smoothing parameters. Based on the quadratic risk calculations QAIC chose six components and QBIC chose four components. Moreover using the MRA criterion it was clear that four components was adequate.

There is a sense in which selecting four components is the right answer for this problem. Biologists conjecture that if the interaction model is true there should be 4 groups of genes each displaying a separate profile under the 4 conditions. Among the 3 clusters given by BIC, one profile matched with the distinct expression profile for Δ-TAND with no mutation, but the other two gene clusters were mixed. On the other hand the four clusters given by QBIC clearly identifies four distinct patterns under the major combinations, thereby providing
Fig. 3. Risk Calculation for the yeast gene expression dataset

a meaningful summary and cluster analysis of this high dimensional data. Additionally QAIC and more prominently QBIC shows a local minima for a two components mixture. This suggested there might be two big groups. Further exploration shows that the two top clusters differentiated the mutated and unmutated TBP yeast strains.

6. Conclusion and Future Direction

In this paper we have developed a comprehensive tool for high dimensional model selection, using quadratic risk. Key to the calculation of quadratic risk is its representation and decomposition using appropriate projection operators, and the estimation of these operators using empirical versions. Decomposing the quadratic risk into the model lack of fit and the parameter estimation cost enabled us to build a method, QBIC, that mimics BIC.

One feature of the derivation of our methodology, one that separates it from the AIC and BIC, is that the asymptotic expansions are based on nonparametric goodness of fit tests, not likelihood ratio asymptotics. We believe that our unified approach for building and estimating quadratic risk could pave the way for designing appropriate model selection
criterion for a host of previously unsolved problems, especially where the irregularity of parameter space eliminates the asymptotic theory underlying the use of AIC, BIC and similar other criteria. In addition, the risk of the empirical estimate, which is a natural outcome of our risk analysis, provides a threshold that enables us to assess whether the model that was selected was itself a good fit. Unlike AIC and BIC where only the optimum model is chosen, model adequacy provides us with the extra information of whether any of the models are adequate, or if there is a range of models that are adequate.

In addition, we also showed that the use of an appropriate kernel could enable one to minimize the computational burden associated with a high-dimensional problem. Moreover, there is certainly more to learn about the structure of a dataset than can be revealed by analyzing a data with a single model selection criterion. This is an area of future research.

References

Akaike, H. (1973). Information theory and an extension of the maximum likelihood principle. In *Second International Symposium on Information Theory (Tsahkadsor, 1971)*, pp. 267–281. Budapest: Akadémiai Kiadó.

Blom, G. (1976). Some properties of incomplete U-statistics. *Biometrika* 63(3), 573.

Bollen, K., S. Ray, and J. Zavisca (2006). A scaled unit information prior approximation to the bayes factor. Technical report, University of North Carolina and SAMSI.

Chitikila, C., K. L. Huisinga, J. D. Irvin, A. D. Basehoar, and B. F. Pugh (2002). Interplay of tbp inhibitors in global transcriptional control. *Molecular Cell* 10, 871–882.

Fraley, C. and A. Raftery (1999). Mclust: Software for modelbased cluster analysis.

Haughton, D. M. A. (1988). On the choice of a model to fit data from an exponential family. *The Annals of Statistics* 16, 342–355.

Lindsay, B., M. Markatou, S. Ray, K. Yang, and S. Chen (2007). Quadratic distances on probabilities: A unified foundation. Technical report, To Appear in the *Annals of Statistics*.

McLachlan, G. and D. Peel (2000). *Finite Mixture Models*. John Wiley and Sons Inc.
Appendix: Proof of Proposition 2.1

We start with an asymptotic approximation to Parameter Estimation Error \( = \left[ d_K(F_\tau, M_\hat{\theta}) - d_K(F_\tau, M_{\theta_\tau}) \right] \).

Now we define a function in the \( \theta \)-space, by \( L(\theta_\tau, \hat{\theta}) = d_K(M_\hat{\theta}, M_{\theta_\tau}) \), which has the form

\[
L(\theta_\tau, \hat{\theta}) = \int \int K(x, y) \ d(M_\hat{\theta} - M_{\theta_\tau})(x)d(M_\hat{\theta} - M_{\theta_\tau})(y).
\]

For density function \( m_\hat{\theta} \) we assume that we can create a Taylor expansion in \( \theta_\tau \) such that

\[
(m_\hat{\theta} - m_{\theta_\tau})(x) = (\hat{\theta} - \theta_\tau)^T u_{\theta_\tau}(x) \ dM_{\theta_\tau}(x) + o \left( |\hat{\theta} - \theta_\tau| \right).
\]

Thus we get the following quadratic approximation for the loss

\[
mL(\theta_\tau, \hat{\theta}) = m(\hat{\theta} - \theta_\tau)^T \left[ \int \int u_{\theta_\tau}(x)K(x, y)u_{\theta_\tau}(y)^T M_{\theta_\tau}(x)M_{\theta_\tau}(y) \right] (\hat{\theta} - \theta_\tau) + o(m|\hat{\theta} - \theta_\tau|^2)
\]

Next, under standard regularity assumptions, it is a well known result for maximum likelihood that

\[
m^{1/2}(\hat{\theta} - \theta_\tau) = m^{1/2} \bar{J}^{-1} \left( \frac{1}{m} \sum_i u_{\theta_\tau}(x_i) \right) + o_p(1).
\]

This shows that the error term in (36) is \( o_p(1) \). In addition, substituting this expression into the first term gives the relationship:

\[
mL(\theta_\tau, \hat{\theta}) = m \int \int V(x, y) \hat{F}(x)\hat{F}(y) + o_p(1)
\]

(37)
as needed for the proposition. Note that $\int V(x, y) M_{\theta_\tau} (y) = 0$, so the asymptotic mean for $mL(\theta_\tau, \hat{\theta})$ is

$$E \left[ \iint V(x, y) \hat{F}(x) \hat{F}(y) \right] = \text{trace}_{M_{\theta_\tau}} (V).$$