Information criteria for deciding between normal regression models

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Regression models fitted to data can be assessed on their goodness of fit, though models with many parameters should be disfavored to prevent over-fitting. Statisticians' tools for this are little known to physical scientists. These include the Akaike Information Criterion (AIC), a penalized goodness-of-fit statistic, and the AICc, a variant including a small-sample correction. They entered the physical sciences through being used by astrophysicists to compare cosmological models; e.g., predictions of the distance–redshift relation. The AICc is shown to have been mis-applied, being applicable only if error variances are unknown. If error bars accompany the data, the AIC should be used instead. Erroneous applications of the AICc are listed in an appendix. It is also shown how the variability of the AIC difference between models with a known error variance can be estimated. This yields a significance test that can potentially replace the use of ‘Akaike weights’ for deciding between such models. Additionally, the effects of model mis-specification are examined. For regression models fitted to data sets without (rather than with) error bars, they are major: the AICc may be shifted by an unknown amount. The extent of this in the fitting of physical models remains to be studied.

1. Introduction

(a) Background and overview

Physical scientists are familiar with the task of fitting a parametric model such as a regression model to a data set, by using maximum likelihood estimation (MLE) or other parameter estimation techniques. But they are less familiar with model selection: deciding among two or more models fitted to the same data in a way that for each model takes account of both its goodness of fit and its number of parameters. To what extent should one attempt to prevent over-fitting, i.e., ‘fitting the noise,’ by penalizing models with too many parameters? This question of parsimony can be viewed not only as a problem in data analysis, but as one in the philosophy of science [Keuzenkamp et al. 2001]. The case when the models being compared are incompatible, i.e., are non-nested in that they are not related by parametric restrictions, is especially vexing. So is the case when they are mis-specified, i.e., do not agree with the ‘truth’ (the unknown and perhaps infinite-dimensional data-generating process), regardless of what values for their parameters are chosen; so that fitting errors of non-zero mean are present.
Information criteria and normal regression

Techniques for model selection that penalize over-fitting have been applied in the life sciences, social sciences and econometrics, and several book-length expositions of these techniques by statisticians are available (Sakamoto et al. 1986; McQuarrie & Tsai 1998; Claeskens & Hjort 2008; Konishi & Kitagawa 2008). A fruitful concept is the AIC (Akaike Information Criterion), a certain penalized likelihood or goodness of fit statistic (Akaike 1973, reprinted as Akaike 1992). It is an estimate of the discrepancy, in a sense related to MLE and information theory, between a fitted statistical model and the unknown data-generating process; the latter being statistical also, if measurement uncertainties are incorporated. In simple cases the AIC is effectively a penalized sum of squared prediction errors. By comparing AIC’s one can compare models with different numbers of parameters, including incompatible models. But in the absence of a systematic theory of the variability of the AIC statistic, using AIC’s to decide between fitted versions of parametric models $M^1, M^2$ cannot be viewed as a procedure in classical statistical inference, i.e., as a significance test. No $p$-value, as in a frequentist assessment of the evidence against a null hypothesis, is actually calculated. Instead one simply says, e.g., that if $\Delta_{12} := AIC^2 - AIC^1$ is less than 2.0, the evidence that $M^1$ is to be preferred over $M^2$ is weak; and that if $\Delta_{12}$ is greater than 5.0, it is strong. The ‘Akaike weight’ $\exp(-AIC^i/2)$ is often viewed as an unnormalized probability (in some sense) that $M^i$ is to be preferred (Burnham & Anderson 2002), but this interpretation has not been universally accepted.

A few years ago, the AIC and related criteria (such as AICc, a variant including a small correction) entered the physical sciences by being introduced into astrophysics (Takeuchi 2000; Liddle 2007). They have been used to compare cosmological models, such as regression models of the distance–redshift relation that characterizes the expansion of the Universe. Unfortunately, in many papers a mistake in data analysis has been made. It can perhaps be attributed to a misreading of the expositions of Burnham & Anderson (2002) and Liddle (2007). The mistake is this. A data set may be accompanied by error bars (i.e., measurement uncertainties), or not. If the latter, regression model fitting will involve the estimation of a ‘nuisance parameter,’ namely the unknown variance $\sigma^2$ of the measurement errors. The AICc, which was designed to unbias completely the estimate of the Kullback–Leibler information-theoretic discrepancy provided by the AIC, is appropriate only if $\sigma^2$ is unknown. But data in the physical sciences are typically accompanied by error bars. When assessing statistical models that incorporate known error bars, the AIC and not the AICc should be used.

To show this, we first place the AIC in a general framework that can be used to derive many information-theoretic model-selection statistics. (See §2.) In §3a we restrict our focus to linear regression and MLE, and show that the applicability of the AICc is limited as claimed. In Appendix B, papers from the astrophysics literature that have erroneously applied the AICc are listed.

In §3b we obtain a further result: under reasonable conditions of misspecification, using the correct statistic (the AIC) to decide between normal regression models $M^1, M^2$ that incorporate error bars can indeed be viewed as a test of significance. That is, the decision can be made in a classical way. One can calculate a $p$-value associated to the null hypothesis that $M^1, M^2$ are equidistant in an information-theoretic sense from the true but unknown model $M^*$, as opposed to the alternative hypothesis that they are not. This is because the variability
of $\Delta^{12} = \text{AIC}^2 - \text{AIC}^1$ can be estimated. For data sets with error bars, this can potentially render Akaike weights obsolete. It is explained how the estimation can be carried out for mis-specified normal linear models, and a hypothesis test based on the estimate is proposed. The test can be extended to non-linear models.

In decisions between statistical models $M^1, M^2$ that incorporate known error bars, the validity of the uncorrected AIC is unaffected if the models are mis-specified, as is shown in §3. This result is unexpected, since the usual derivation of the AIC statistic (and indeed of the AICc) requires that there be nesting and no mis-specification; and its widespread application to non-nested, potentially mis-specified models has in fact been somewhat heuristic. In §4 we show that if the data set to which $M^1, M^2$ are fitted is not accompanied by error bars, problems with the AICc can indeed arise. For a normal linear model fitted to a data set without error bars, we discuss the behavior of the AICc under mis-specification, and obtain an asymptotically exact expression for the resulting shift. If the extent of the mis-specification is unknown, this shift may render the AICc of little value. This fact deserves to be better known.

Besides deriving the AIC and AIC corrections from first principles, we briefly discuss the applicability to normal linear models of such variants as $\text{AIC}^{\gamma}$, which suppresses over-fitting to a greater extent than does the AIC. Many additional variants have appeared in the literature, such as the KIC (Kullback Information Criterion) and KICc (Cavanaugh 1999, 2004), but they are beyond the scope of this paper. In the final section (§5), we summarize our results.

(b) AIC basics

A regression model fitted to data can be linear or non-linear, according to its parameter dependence. The linear case is familiar (Bevington & Robinson 2003; Draper & Smith 1998; Weisberg 2005). Suppose the data set comprises $y_1, \ldots, y_n \in \mathbb{R}$; which could be, e.g., the values of a response variable corresponding to $n$ distinct values of an explanatory variable $x$, chosen by an observer or an experimenter. Suppose that $y_1, \ldots, y_n$ would depend linearly on parameters $\beta_1, \ldots, \beta_k \in \mathbb{R}$ in the absence of measurement errors or other noise. That is, $y = X\beta$, where $y = (y_i)_{i=1}^n$, $\beta = (\beta_j)_{j=1}^k$ are column vectors and $X$ is an $n \times k$ design matrix. (It will be assumed throughout that $n > k$ and that $X$ is of full rank, i.e., of rank $k$.) A statistical model $M$ of the data would then be

$$y_i = \sum_{j=1}^k X_{ij}\beta_j + \epsilon_i,$$

where $\epsilon_1, \ldots, \epsilon_n$ are residuals, i.e., errors. In the simplest case the residuals would be taken to be independent. In a (homoscedastic) normal model one would also take $\epsilon_i \sim N(0, \sigma^2)$, i.e., take each $\epsilon_i$ to be normally distributed with mean zero and a common variance $\sigma^2$. The parameter $\sigma^2$ may be known, or it may be an unknown nuisance parameter that needs to be estimated (which is the case if error bars are supplied). Note that from a data set $\bar{y} = (\bar{y}_i)_{i=1}^n$ including error bars of differing lengths, i.e., known but differing variances $\sigma_1^2, \ldots, \sigma_n^2$, one can obtain a data set $y = (y_i)_{i=1}^n$ with a known common variance $\sigma^2$ by defining $y_i := (\sigma / \sigma_i)\bar{y}_i$.

Whether or not $\sigma^2$ is known, an estimate $\hat{\beta} = (\hat{\beta}_j)_{j=1}^k$ of $\beta$ can be computed by MLE, which reduces to ordinary least-squares for any normal linear model with
Information criteria and normal regression

4

independent, identically distributed (i.i.d.) errors. By a standard calculation, \( \hat{\beta} = (X'X)^{-1}X'y \). Accompanying the observed data vector \( y \) there is then a predicted data vector \( \hat{y} := X\hat{\beta} = Py \), where the ‘hat’ matrix \( P = X(X'X)^{-1}X' \) projects onto the column space of \( X \) (the estimation space \( L \subset \mathbb{R}^n \)). The residual sum of squares (RSS) for the fit is the sum of squared errors. That is,

\[
\text{RSS} = (y - \hat{y})' (y - \hat{y}) = (y - Py)' (y - Py) = y'Qy,
\]

where \( Q = I_n - P \) is complementary to \( P \) and projects onto the left null space of \( X \) (the error space \( L^\perp \subset \mathbb{R}^n \)). If \( \sigma^2 \) is known, so that the parameter vector \( \theta \) of \( M \) is simply \( \beta \), the standard definition of the AIC for the fitted model is

\[
\text{AIC} = \frac{\text{RSS}}{\sigma^2} + 2k.
\]

(1.3)

If alternatively \( \sigma^2 \) is unknown, so that \( \theta = (\beta; \sigma^2) \), it is

\[
\text{AIC} = n \ln(\hat{\sigma}^2) + 2(k + 1) = n \ln(\text{RSS}/n) + 2(k + 1),
\]

(1.4)

where \( \hat{\sigma}^2 = \text{RSS}/n \) is the maximum likelihood estimate of \( \sigma^2 \).

In both (1.3) and (1.4) the first term equals up to an unimportant constant the statistic \(-2\ln L(\hat{\theta}_N|y)\), where \( \ln L(\hat{\theta}_N|y) \) is the log-likelihood of the fitted model. So the first term is a measure of goodness of fit. In model selection a smaller AIC is preferred; hence the second term (which will be seen to originate as an unbiasing term) penalizes \( M \) according to its number of fitted parameters \( k \), resp. \( k + 1 \). It is usually differences of AIC’s that are important, so any term not involving \( k \) may be added to (1.3) and (1.4).

The choice ‘2’ in (1.3) and (1.4) for the coefficient of \( k \) (resp. \( k + 1 \)) is motivated by information theory, as will be explained. But applied statisticians have long been interested in the effects on model selection of choosing a more general penalty term \( \gamma k \), where \( \gamma > 0 \) may differ from 2. The resulting modified AIC is denoted AIC\( \gamma \) (McQuarrie & Tsai 1998). Bhansali & Downham (1977) considered the effects of varying \( \gamma \) on order selection in autoregressive models, and showed empirically that it may be useful for \( \gamma \) to range, say, between 2 and 6. The abovementioned KIC like the AIC has an information-theoretic justification, and in the \( n \to \infty \) limit turns out to be equivalent to AIC\( \gamma \).

Mention should also be made of the AICu (McQuarrie et al. 1997), which is a heuristic modification of (1.4) in which the ML estimate \( \hat{\sigma}^2 \) is replaced by the unbiased estimator \( s^2 := \text{RSS}/(n - k) \) of \( \sigma^2 \). In the \( n \to \infty \) limit, AICu is also equivalent to AIC\( \gamma \). This can be seen by working to leading order in \( 1/n \) and using the asymptotic approximation \( n \ln[n/(n - k)] \sim k + O(1/n), n \to \infty \).

The most familiar modified or corrected AIC, AICc, is a less drastic modification of (1.4), the modification being a major one only for small \( n \). Under the assumption of i.i.d. normal residuals, and the traditional assumption of no mis-specification, it is given by

\[
\text{AICc} = n \ln(\hat{\sigma}^2) + \frac{2(k + 1)n}{n - k - 2}
\]

\sim \text{AIC} + \frac{2(k + 1)(k + 2)}{n} + O(1/n^2), \quad n \to \infty
\]

(1.5b)
(Sugiura 1978; Hurvich & Tsai 1989; Cavanaugh 1997). Why an $O(1/n)$ correction term should be added to (1.4), but not to the expression (1.3) that applies if $\sigma^2$ is known, will be explained.

2. Minimum discrepancy estimation

(a) A general framework

In this section the AIC, a penalized goodness-of-fit statistic, is placed in a model-selection framework that goes well beyond the use of MLE in regression. The AIC for a candidate model can be viewed as an unbiased estimator of its discrepancy, in a certain sense, from the true model. This will eventually lead to the introduction of a null hypothesis that two candidate models are equally discrepant, and to systematic results on AIC corrections. But the theme of this section is the existence of alternatives to the AIC, which have not yet been applied in the physical sciences. It is hoped that interest in this area will be stimulated. A framework resembling the one used here was first developed by Linhart & Zucchini (1986).

Suppose one has a parametric statistical model $M_\theta$ that will be used for approximation or fitting purposes, with $\theta \in \Theta$ (a parameter space); and a true, underlying statistical model $M^*$ of the data-generating process, which is not known explicitly. If each generated datum is an element of a set $S$, both $M_\theta$ and $M^*$ will be probability distributions on $S$. (The choice $S = \mathbb{R}^n$ is appropriate for regression, as in §1b.) Their respective probability density functions (PDF’s) will be denoted $f_\theta(y)$ and $g(y)$. In general it will not be assumed that $g = f_\theta^*$ for any $\theta \in \Theta$, i.e., mis-specification will be allowed. To any random sample $\eta_N$ of size $N$ from the true distribution $g$, comprising $y^{(1)}, \ldots, y^{(N)} \in S$, there corresponds an empirical distribution $g_N = g_{N,\eta_N}$ on $S$. It is defined by

$$g_{N,\eta_N}(\cdot) = N^{-1} \sum_{i=1}^{N} \delta(\cdot - y^{(i)}),$$

(2.1)

where $\delta(\cdot)$ is the Dirac delta function, if $S$ is a Euclidean space such as $\mathbb{R}^n$. If alternatively $S$ is a discrete space, then instead of a PDF there will be a probability mass function (PMF), defined using a Kronecker delta rather than a delta function. The restriction $N = 1$, meaning that there is only a single replication, i.e. only one observation of $y \in S$, was implicitly made in §1b where $y$ was a random vector in $\mathbb{R}^n$; but here it will be relaxed.

The definition of MLE, which is an almost universally applicable but hardly unique fitting scheme, is familiar. From the sample $\eta_N$ one constructs the likelihood function $\mathcal{L}(\theta|\eta_N) = \prod_{i=1}^{N} f_\theta(y^{(i)})$, and computes a parameter estimate $\hat{\theta}_N = \hat{\theta}_N(\eta_N)$ by maximizing the likelihood, or equivalently by minimizing the negative log-likelihood $-\ln \mathcal{L}(\theta|\eta_N)$. The best fit to the data is then the model $M_{\hat{\theta}_N}$, with PDF $f_{\hat{\theta}_N}$.

This scheme generalizes to minimum discrepancy estimation, which is itself a generalization of minimum distance estimation. In an abstract description one starts with $\eta_N$ or equivalently an $N$-point empirical distribution $g_N$ on $S$, and computes $\theta_N$ by minimizing $d(g_N; f_\theta)$ over $\theta \in \Theta$. That is, $\theta_N = \ldots$
Information criteria and normal regression

arg min_{\theta \in \Theta} d(g_N; f_{\theta}). Here d(g; f) signifies some real-valued measure of the discrepancy between the PDF’s g, f, which quantifies how difficult it is to discriminate between them. The case when d satisfies the axioms for a metric can be especially nice (Donoho & Liu [1988; Trosset & Sands [1995]), but this will not be assumed. Thus d may be asymmetric, i.e., directed, and may not satisfy the triangle inequality. Also, it may not satisfy d(g; f) \geq 0. But it is useful to require that d(g; f) \geq d(g; g), with equality holding only if g = f. Then the normalized discrepancy D(g; f) := d(g; f) − d(g; g) \geq 0 will satisfy D(g; f) = 0 only if g = f. As will be seen, it is sometimes possible for an unnormalized discrepancy d to be defined on a larger class of PDF’s than is the case for a normalized one.

In minimum discrepancy estimation one must distinguish between the model \( M_{\theta} \) fitted to an empirical distribution \( g_N \) generated by \( M^* \), which has PDF \( f_{\theta_N} \), and the best approximating model, the PDF of which is some \( f_{\theta_*} \).

Here \( \theta_* = \arg \min_{\theta \in \Theta} d(g; f_{\theta}) \) may differ from \( \hat{\theta}_N \). The value \( \theta_* \) is called the ‘pseudo-true’ value of \( \theta \). (If there is no mis-specification, i.e., \( g = f_{\theta_*} \) for some \( \theta_* \), it is the true value.) The discrepancy due to approximation (AD) is \( d(g; f_{\theta_*}) \). In the absence of mis-specification this would equal the constant \( d(g; g) \), and what would be more important would be the discrepancy due to estimation (ED), i.e. \( d(f_{\theta_*}; f_{\hat{\theta}_N}) \). The overall discrepancy (OD), of the fitted model from the truth, is the quantity \( d(g; f_{\hat{\theta}_N}) \). If there is no mis-specification, OD reduces to ED.

None of these three discrepancies can be calculated if the true model is unknown, though they can be estimated from the data \( \eta_N \), meaning from \( g_N \). (It is \( d(g_N; f_{\hat{\theta}_N}) \), the fitted discrepancy (FD) of the model from the data, that can be calculated from the data.) The following policy is an abstraction of Akaike’s.

Selection Policy. Given a discrepancy functional d, data \( \eta_N \) generated by an unknown true model \( M^* \) with PDF g, and candidate models \( M_{\theta_1}^1, M_{\theta_2}^2 \) with parametric PDF’s \( f_{\theta_1}^1, f_{\theta_2}^2 \) and parameter spaces \( \Theta^1, \Theta^2 \), one should ideally assess the goodness of fit of each model on the basis of its expected overall discrepancy from \( M^* \). That is, if when fitted to data \( \eta_N \) or equivalently to the empirical distribution \( g_N = g_{N, \eta_N} \), model \( M_{\theta_l}^l \) would have parameter \( \hat{\theta}_N^l = \hat{\theta}_N^l(\eta_N) \), one should select the model with the minimum value of

\[
d'(g, f_l^l) := E_{\eta_N} OD_d(g_N, \eta_N) = E_{\eta_N} d(g, f_{\theta_N^l(\eta_N)}^l).
\]

The expectation (i.e., averaging) is computed over data \( \eta_N \) generated by the true model, meaning over the PDF g. As an alternative, the double expectation

\[
d''(g, f_l^1) := E_{\eta_N^l} E_{\eta_N} d(g, f_{\theta_N^l(\eta_N)}^l),
\]

where data \( \eta_N, \eta_N^l \) are generated independently by g, may be employed.

The expected OD, \( d'(g, f_l^l) \), is a penalized version of the AD \( d(g; f_{\theta_*}) \), where \( \theta_* \) is the pseudo-true value of the parameter \( \theta^l \in \Theta^l \). It is at least as large as the AD, and because the number of ways in which the data-dependent fitted PDF \( f_{\theta_N^l(\eta_N)} \) can deviate from the pseudo-true PDF \( f_{\theta_*}^l \) is the dimensionality
of the parameter space $\Theta^l$, one expects that relying on the expected OD as a measure of closeness of $M^l_{\hat{\theta}^l_N}$ to $M^*$ will disfavor over-fitting in an AIC-like way.

It must be stressed that neither $d'(g, f^l)$ nor $d''(g, f^l)$ can be calculated directly, though they can be estimated (with bias) by the fitted discrepancy of the $l$’th model from the data, $FD^l_g(y_N) = d(g_{N, \hat{\theta}^l_N} ; f^l_{\hat{\theta}^l_N(y_N)})$. (This is an RSS-like quantity.)

The selection policy can therefore be implemented by choosing the model with the minimum value of a certain function MSC, defined as follows to be an unbiased estimator of the expected overall discrepancy. (It will specialize to the AIC.)

**Definition 2.1.** The model-selection criterion function based on a discrepancy functional $d$, denoted MSC$_d$ or simply MSC, is defined so that the value MSC$_d^l/2$ for the $l$’th model equals its fitted discrepancy $FD^l_d(\eta_N) = d(g_{N, \eta_N} ; f^l_{\theta^l_N(y_N)})$, plus an unbiasing term $B^l$ equal to $E_{\eta_N} OD^l_d(\eta_N)$ minus $E_{\eta_N} FD^l_d(\eta_N)$. That is,

$$B^l = d'(g; f^l) - E_{\eta_N} d(g_{N, \eta_N} ; f^l_{\hat{\theta}_N(y_N)})
= E_{\eta_N} d(g; f^l_{\hat{\theta}_N(y_N)}) - E_{\eta_N} d(g_{N, \eta_N} ; f^l_{\hat{\theta}_N(y_N)})$$

(2.4)

so that in expectation, MSC$_d^l/2$ equals the expected overall discrepancy, on which it is posited that model selection should be based.

**Remark.** Distinct discrepancies could be used for (i) performing the fitting and computing the FD, and (ii) computing the expected OD. This would generalize the selection policy (and turns out to be needed in the definition of the KIC, as will be discussed elsewhere). For practical reasons, one could also perform the fitting using MLE and compute the FD using a discrepancy not related to MLE (Linhart & Zucchini 1986, § 4.4). But this seems less theoretically justifiable.

The alternative $d''$ to $d'$ was mentioned for two reasons. First, for MLE it is identical to $d'$, as will be seen. Second, using $d''$ makes selection in effect a procedure of cross validation, in which a fitted model is assessed according to its empirically expected prediction errors (Stone 1978). The definition (2.3) of $d''$ involves two hypothetical sets of data: one $(\eta_N)$ used to estimate the parameter $\theta^l$, and one $(\eta'_N)$ used to assess the fit of the resulting model. The equivalence between choosing models by cross-validation and Akaike’s technique of penalizing models by their number of parameters has long been recognized (Stone 1977; Kuha 2004).

(b) Discrepancies, information theory and MLE

The selection policy of §2 can be applied very generally, to both discrete and continuous models. Given a discrepancy functional $d$ and a sample $\eta_N$ comprising $y^{(1)}, \ldots, y^{(N)} \in S$, which yields an $N$-point empirical distribution $g_N = g_{N, \eta_N}$ on $S$, one would naively decide whether to select parametric model $M^l_{\theta^l}$ with PDF $f^l_{\theta^l}$ on $S$ on the basis of its fitted discrepancy $d(g_{N, \eta_N} ; f^l_{\theta^l(y_N)})$ from the sample. But the selection policy modifies this RSS-like quantity by adding an unbiasing term, giving an unbiased estimate MSC/2 of the expected overall discrepancy. Selection based on the latter disfavors over-fitting, as desired.
Information criteria and normal regression

This is the natural setting for the AIC and AICc statistics. But for regression models, in which $S = \mathbb{R}^n$ (and most often $N = 1$), the choice of a discrepancy functional closely tied to MLE and in fact to information theory must first be justified. Only for one special functional does the fitted discrepancy turn out to be the negative log-likelihood.

For discrete rather than continuous models, with $S$ a discrete set such as $\{1,\ldots,m\}$ or $\{1,2,3,\ldots\}$, a wide variety of discrepancy functionals $d(g; f)$ have been used in statistics and elsewhere. They include the Pearson $X^2$ statistic $\sum_{n \in S} [g(n) - f(n)]^2 / f(n)$, used when $S$ is the set of cells in a contingency table to compare an empirical and a theoretical distribution. The Neyman $X^2$ is similar. There are also many discrepancies rooted in information theory, such as the (discrete) Kullback–Leibler (KL) divergence, often called the informational divergence \cite{CsizarKorner2011}. Its normalized form is

\[
D_{\text{KL}}(g; f) := \sum_{n \in S} g(n) \ln \frac{g(n)}{f(n)} \geq 0
\]

and its denormalized form is

\[
d_{\text{KL}}(g; f) := - \sum_{n \in S} g(n) \ln f(n) \geq d_{\text{KL}}(g; g).
\]

They are related by $D_{\text{KL}}(g; f) = d_{\text{KL}}(g; f) - d_{\text{KL}}(g; g)$. The subtracted quantity $d_{\text{KL}}(g; g)$ is the (Shannon) entropy of the distribution $g$, and in statistical mechanics $D_{\text{KL}}(g; f)$ would therefore be called a relative entropy. The denormalized $d_{\text{KL}}(g; f)$ is sometimes called an ‘inaccuracy.’

Discrepancies in information theory are often of the ‘$\varphi$-divergence’ form $D_{\varphi}(g; f) := \sum_{n \in S} g(n) \varphi f(n)/g(n)$, for $\varphi$ some convex function \cite{Pardo2006}. For instance, if $\varphi(u) = -\ln u$ then $D_{\varphi} = D_{\text{KL}}$. If $\varphi(u) \propto 1 - u^{(1+\alpha)/2}$ then $D_{\varphi}$ becomes the so-called $\alpha$-divergence $D^{(\alpha)}$, which reduces to $D_{\text{KL}}$ in a scaled $\alpha \to -1$ limit. This generalized discrepancy arises in the geometry of statistical inference \cite{AmariNagaoka2000}, and there is a corresponding denormalized

\[
d^{(\alpha)}(g; f) \propto \sum_{n \in S} g(n)^{(1-\alpha)/2} \left[1 - f(n)^{(1+\alpha)/2}\right],
\]

a scaled $\alpha \to -1$ limit of which equals $D_{\text{KL}}(g; f)$. The self-divergence $d^{(\alpha)}(g; g)$ of $g$ is called in physics the Tsallis entropy of $g$ \cite{Tsallis1988}.

Many other discrepancies have been investigated. (See Kapur \citeyear{Kapur1989}, Chap. 7) and \cite{Basu2011}, Chap. 11.) But the KL divergence is perhaps the most important, because of its connection to MLE. From a sample $\eta_N$ comprising $y^{(1)},\ldots,y^{(N)} \in S$, where $S$ is a discrete set, obtaining a best-fit PMF $f_{\hat{\theta}_N}$ by maximizing over $\theta$ the likelihood $L_f(\theta|\eta_N) = f(\eta_N|\theta)$ of a candidate PMF $f_{\theta}$ on $S$ is equivalent to minimizing $D_{\text{KL}}(g_N; f_{\theta})$ or $d_{\text{KL}}(g_N; f_{\theta})$ over $\theta$, where $g_N = g_{N,\eta_N}$ is the $N$-point empirical distribution defined by the data. This is because $d_{\text{KL}}(g_N; f_{\theta})$ equals $-\ln L_f(\theta|\eta_N)$, the negative log-likelihood, as follows from (2.6). In particular, $d_{\text{KL}}(g_N; f_{\hat{\theta}_N})$ equals $-\ln L_f(\hat{\theta}_N|\eta_N)$. MLE can thus be interpreted as a minimum discrepancy estimation.

Now consider the continuous case, when the data lie in a space $S$ that is Euclidean, such as the choice $S = \mathbb{R}^n$ arising in regression. The selection policy of §2 requires the computation of (an unbiased version of) some
fitted discrepancy \( d(g_N; f_\theta_N) \). The empirical distribution \( g_N = g_{N, \eta_N} \) is a linear combination of \( N \) delta functions computed from the data \( \eta_N \), as in (2.1), and \( \theta_N = \theta_N(\eta_N) \) is computed by minimizing \( d(g_N; f_\theta) \) over \( \theta \), where \( f_\theta \) is a candidate PDF on \( S \). For the selection policy to be implemented as stated, the discrepancy functional \( d(g; f) \) being employed must allow its first argument to be a PDF \( g_N \) that is ‘atomic,’ in the sense that it is a combination of delta functions. This is a stringent requirement (Liese & Vajda 1987, §10.9).

When \( S = \mathbb{R} \), many statistical discrepancies \( d(g; f) \) have been employed; e.g., in the robust estimation of location and scale parameters of distributions on \( S \) (Sahler 1968; Parr & Schucany 1980). Most are computed from the cumulative distributions (CDF’s) \( G, F \) corresponding to \( g, f \), so they are well-defined even if one or the other is an empirical distribution. Also, most are metrics, or legitimate distances; in fact minimum discrepancy estimation grew out of minimum distance estimation, which has a long history (Parr 1981). Examples include the Kolmogorov–Smirnov and Cramér–von Mises discrepancies, which are widely used as goodness-of-fit statistics. But their generalizations to the multivariate case, when \( S = \mathbb{R}^n \) with \( n > 1 \), are not straightforward at all.

When \( S = \mathbb{R}^n \) with \( n \) arbitrary, the most widely used discrepancy is the (continuous) KL divergence, with its close ties to MLE. Its normalized form is

\[
D_{KL}(g; f) := \int_{\mathbb{R}^n} g(y) \ln \frac{g(y)}{f(y)} \, d^n y \geq 0 \tag{2.8}
\]

and its denormalized form is

\[
d_{KL}(g; f) := -\int_{\mathbb{R}^n} g(y) \ln f(y) \, d^n y \geq d_{KL}(g; g). \tag{2.9}
\]

They are related by \( D_{KL}(g; f) = d_{KL}(g; f) - d_{KL}(g; g) \), as in the discrete case. A key observation is that the integral in (2.9) is well-defined even if \( g \) is a purely atomic function of \( y \), such as an empirical PDF \( g_N \). But the integral in (2.8) is not, as one cannot take the logarithm of a sum of delta functions. The distinction can be viewed as arising from the entropy \( d_{KL}(g; g) \) not being defined when \( g = g_N \); any empirical distribution has undefined entropy. The good behavior of the integral in (2.9) justifies the use of \( d_{KL} \) in model selection, to the exclusion of \( D_{KL} \).

For any sample size \( N \geq 1 \), averaging over data \( \eta'_N \) sampled from the PDF \( g \) yields \( g \) itself; which is to say, \( E'_{\eta'_N} g_{N, \eta'_N} = g \). By the linearity in \( g \) of the integral in (2.9), it follows that \( E'_{\eta'_N} d_{KL}(g_{N, \eta'_N}; f) \) equals \( E d_{KL}(g; f) \). This confirms a claim made in §2.2 if \( d_{KL} \) is used as the discrepancy \( d \), the two expected overall discrepancies \( d', d'' \) defined in (2.2) (2.3) are equal, and give rise to identical model-selection polices. For non-KL discrepancies, this may not hold.

In the continuous case as in the discrete, the fitted discrepancy \( FD_{KL}(\eta_N) \), i.e., \( d_{KL}(g_{N, \eta_N}; f_\theta_N(\eta_N)) \), equals \(-\ln L_f(\theta_N|\eta_N) \), the negative of the fitted log-likelihood. Using \( d_{KL} \) as the discrepancy, as in the following definition, specializes the MSC of Definition 2.1 to what will be called a MSC of AIC type.

**Definition 2.2.** A \( d_{KL} \)-based model-selection criterion MSC, of AIC type, is defined thus: the value \( MSC^l/2 \) for the \( l \)th model, calculated after fitting, equals its negative log-likelihood \(-\ln L_f(\theta_N^l|\eta_N) \), plus an unbiasing correction \( B^l \) that
equals $E_{\eta_N}OD^I_{d_{KL}}(\eta_N)$ minus $E_{\eta_N}FD^I_{d_{KL}}(\eta_N)$. That is,

$$B^I = E_{\eta_N} d_{KL}(g; f^I_{\hat{\theta}_N(\eta_N)}) - E_{\eta_N} \left[ -\ln \mathcal{L}_f(\hat{\theta}_N|\eta_N) \right],$$

so that in expectation, $MSC^I/2$ equals the $d_{KL}$-based expected overall discrepancy, on which it is posited that model selection should be based.

In the following, only MSCs of AIC type will be employed. The choice of the KL divergence as the discrepancy used in model fitting has a clear justification: it allows the selection policy of §2 to be applied as stated.

But it should be noted that there are alternatives that merit examination. By adapting the selection policy it may be possible to employ quite different discrepancies, such as the abovementioned $\alpha$-divergence. This requires a brief explanation. The continuous, denormalized version of the $\alpha$-divergence is

$$d^{(\alpha)}(g; f) \propto \int_{\mathbb{R}^n} g(y)^{(1-\alpha)/2} \left[ 1 - f(y)^{(1+\alpha)/2} \right] \, q^n \, y,$$  \hspace{1cm} (2.10)

which is undefined if $g$ is an empirical distribution. But the $\alpha = 0$ case of this, $d^{(0)}(g; f)$, is equivalent to the Hellinger distance, which has long been used in parametric estimation [Beran 1977]. From data $\eta_N$, or an empirical distribution $g_N = g_{N,0_N}$ defined from it as in (2.1), a fitted parametric model $f_{\hat{\theta}}$ can indeed be found by minimizing the Hellinger distance. The fitting, though, involves a preliminary step: replacing the delta functions of (2.1) by approximate deltas. That is, one first engages in kernel density estimation, by convolving $g_N$ with some integral kernel. The integral in (2.10) will be well-defined if the resulting ‘smoothed’ $g$ is used. Alternatively, the model PDF $f$ as well as the data PDF $g_N$ can be smoothed [Basu et al. 1997, §3.3]. However, the smoothing of $g_N$ can apparently be justified only in the large-sample ($N \to \infty$) limit. In what follows $N = 1$, and the limit taken (if any) will be $n \to \infty$. The usefulness in this setting of a preliminary smoothing of the empirical distribution remains to be explored.

3. Selection with error bars

In this section we specialize to the case when the true model $M^*$ and the candidate models fitted to a set of $n$ data points are normal regression models, incorporating known error bars as explained in §1b. We investigate the model-selection criterion function given in Definition 2.2 (a $d_{KL}$-based MSC of AIC type).

In §3a it is shown that irrespective of $n$ and the extent of mis-specification, the MSC for a candidate linear model reduces to the standard AIC of (1.3): a sum of squared residuals penalized by $2k$, i.e., by twice the number of parameters. Interestingly, it is possible to derive the modified AIC known as the AICc, in which the penalty $\gamma k$ replaces $2k$, by slightly modifying the selection policy of §2. But even when $n$ is small, the standard AIC is never extended by an $O(1/n)$ correction term; thus the use of the AICc is not appropriate here. This realization is new. In Appendix B, papers from the astrophysics literature that have erroneously applied the AICc are listed.

In §3b the variability of $\Delta^{12} := AIC^2 - AIC^1$ is determined, and an asymptotically valid hypothesis test for model selection that is based on $\Delta^{12}$
is proposed. At any specified significance level $\alpha$, the test either rejects or accepts the null hypothesis that the fitted models $M_1, M_2$ are equally close to $M^*$ in the ‘expected overall discrepancy’ sense of § 2. For mis-specified linear models incorporating error bars, this approach to model selection can potentially replace the rule-of-thumb use of Akaike weights. The variability estimation and the test of significance can be extended to the case of non-linear models, as is sketched.

(a) Expected discrepancies

Consider a true model $M^*$ and a candidate linear model $M$ that are both normal, as in § 1. They are $y = y_0 + \epsilon_0$ and $y = X\beta + \epsilon$, where $\beta = (\beta_j)_{j=1}^k$ is a column vector of parameters, and the error vectors $\epsilon_0, \epsilon$ have mean zero and covariance matrices $\sigma_0^2 I_n, \sigma^2 I_n$. Thus $\epsilon_0 = \sigma_0 z_0$ and $\epsilon = \sigma z$, where $z_0$ and $z$ are vectors of independent standard normal variables. It is not assumed that $y_0$ is in the column space of the $n \times k$ design matrix $X$, i.e., mis-specification is allowed.

In this section the variance $\sigma^2$ is specified and not estimated, so the full parameter vector $\theta$ of $M$ is simply $\beta$. If the true variance $\sigma^2_0$ is known, as is the case when the data are accompanied by error bars, then it is natural to choose $\sigma^2 = \sigma^2_0$. But for the moment this will not be assumed: statistical as well as deterministic mis-specification will be allowed.

There is assumed to be only one observation ($N = 1$), so only one instance of the random vector $y \in S = \mathbb{R}^n$ is available as a datum. Thus $y$ will be written for $\eta$, and the subscript $N$ dropped. MLE is equivalent to choosing $\beta \in \mathbb{R}^k$ so as to minimize the discrepancy (in the $d_{KL}$ sense) of the 1-point atomic PDF $g_y(\cdot) = \delta(\cdot - y)$ on $\mathbb{R}^n$ from $M_\beta$. Equivalently, MLE minimizes the negative log-likelihood $-\ln L(\beta | y)$ of $M_\beta$. It yields a fitted model $M_\hat{\beta}$, where the estimated parameter vector $\hat{\beta} = \hat{\beta}(y) \in \mathbb{R}^k$ is given by $\hat{\beta} = (X'X)^{-1}X'y$. The $n \times n$ hat matrix $P$ and its complement $Q = I_n - P$, which project onto the estimation and error subspaces of $\mathbb{R}^n$, i.e., the column and left null spaces of $X$, are defined as usual by $P = X(X'X)^{-1}X'$. The predicted data vector $\hat{y}$ is defined by $\hat{y} = Py$. The RSS (sum of squared residuals) is $(y - \hat{y})' (y - \hat{y}) = y'Qy$.

The policy of §2 requires that to the extent that it can be estimated, the expected overall discrepancy $E_Y OD(y)$ should be used for model selection. The AIC-type selection criterion MSC (see Definition 2.2) has the property that MSC/2 for $M$ is an unbiased estimator of $E_Y OD(y)$. It is defined by

$$\text{MSC}/2 = FD(y) + E_Y [OD(y) - FD(y)],$$

where the fitted discrepancy $FD(y)$, i.e., $d_{KL}(g_Y; f_{\hat{\beta}(y)})$, is simply the negative log-likelihood $-\ln L(\hat{\beta} | y)$ of the fitted model $M_\hat{\beta}$. Since $OD(y)$ is $d_{KL}(g; f_{\beta(y)})$, the second, unbiasing term in (3.1), which was denoted $B$ in the previous section, can be calculated from the Gaussian PDF’s $g, f_\beta$ of $M^*, M_\beta$. They are

$$g(y) = (2\pi \sigma^2_0)^{-n/2} \exp \left[-(y - y_0)'(y - y_0)/2\sigma^2_0\right],$$

$$f_\beta(y) = (2\pi \sigma^2)^{-n/2} \exp \left[-(y - X\beta)'(y - X\beta)/2\sigma^2\right].$$

where

$$\hat{\beta}(y) = \frac{\sum_{i=1}^n y_i x_{i1} \cdot \ldots \cdot x_{ik}}{\sum_{i=1}^n x_{i1}^2 \cdot \ldots \cdot x_{ik}^2}.$$
For convenience we shall write
\[
d_{KL}(f; f) := d_{KL}(f_\beta, f_\beta) = \frac{n}{2} \left[ 1 + \ln(2\pi) \right] + \frac{n}{2} \ln \left( \sigma^2 \right),
\]
(3.4)
since \( d_{KL}(f_\beta, f_\beta) \) does not depend on \( \beta \). By examination,
\[
FD(y) = -\ln \mathcal{L}_f(\hat{\beta}|y) = d_{KL}(f; f) - \frac{n}{2} + \frac{\text{RSS}}{2\sigma^2}
\]
(3.5)
expresses the fitted discrepancy in terms of the RSS, which is \( y^tQy \).

In the following theorem, \( \lambda := y_0^tQy_0/\sigma_0^2 \) is an \( M \)-specific mis-specification parameter, \( \chi^2_r \) is a chi-squared random variable with \( r \) degrees of freedom and \( \chi^2_{r}(\lambda) \) is a similar but non-central variable, with non-centrality parameter \( \lambda \). (For central and non-central chi-squared distributions, see Appendix A.)

**Theorem 3.1.** Under the model \( M^* \), the overall and fitted discrepancies of the fitted model \( \hat{M}_{\hat{\beta}}(y) \), \( OD = OD(y) \) and \( FD = FD(y) \), are distributed according to
\[
OD = d_{KL}(g; f_{\hat{\beta}(y)}) \sim d_{KL}(f; f) + \frac{n}{2} \left( \frac{\sigma_0^2}{\sigma^2} - 1 \right) + \frac{\sigma_0^2}{2\sigma^2} \chi^2_k(\lambda),
\]
\[
FD = d_{KL}(g_y; f_{\hat{\beta}(y)}) \sim d_{KL}(f; f) - \frac{n}{2} + \frac{\sigma_0^2}{2\sigma^2} \chi^2_{n-k}(\lambda),
\]
where \( \hat{\beta}(y) = (X^tX)^{-1}X^ty \in \mathbb{R}^k \) is the fitted value of the parameter \( \beta \). For the discrepancies due to approximation and estimation, \( AD \) and \( ED = ED(y) \), the corresponding statements are
\[
AD = d_{KL}(g; f_{\beta_\star}) = d_{KL}(f; f) + \frac{n}{2} \left( \frac{\sigma_0^2}{\sigma^2} - 1 \right) + \frac{\sigma_0^2}{2\sigma^2} \lambda,
\]
\[
ED = d_{KL}(f_\beta; f_{\hat{\beta}(y)}) \sim d_{KL}(f; f) + \frac{\sigma_0^2}{2\sigma^2} \chi^2_k,
\]
where \( \beta_\star = (X^tX)^{-1}X^ty_0 \in \mathbb{R}^k \) is the pseudo-true value of the parameter \( \beta \).

**Proof.** Use the definition (2.9) of \( d_{KL} \) and the definitions (3.2), (3.3) of \( g, f_\beta \). Each integral over \( \mathbb{R}^n \) in the computation of a \( d_{KL} \) is a normal expectation that can be evaluated in closed form. In the expressions for \( OD, FD, ED \) the distributions \( \chi^2_k(\lambda), \chi^2_{n-k}(\lambda), \chi^2_k \) arise respectively as the distributions of
\[
(Py - y_0)^t(Py - y_0)/\sigma_0^2 = (Pz_0 - Qy_0/\sigma_0)^t(Pz_0 - Qy_0/\sigma_0),
\]
(3.6a)
\[
(Py - y)^t(Py - y)/\sigma_0^2 = (z_0 + y_0/\sigma_0)^tQ(z_0 + y_0/\sigma_0),
\]
(3.6b)
\[
(Py - Py_0)^t(Py - Py_0)/\sigma_0^2 = z_0^tPz_0,
\]
(3.6c)
if one uses the fact that \( P, Q \) are \( n \times n \) projection matrices of ranks \( k, n-k \). (For distributions of quadratic forms, see Appendix A.) Similarly, the ‘\( \lambda \)’ in the expression for \( AD \) is the non-random value of \( (Py_0 - y_0)^t(Py_0 - y_0)/\sigma_0^2 \).
Information criteria and normal regression

Theorem 3.2. The corresponding expectations over $\mathcal{M}^*$-generated data are

$$
E_y \text{OD}(y) = d_{KL}(f; f) + \frac{n}{2} \left( \frac{\sigma_0^2}{\sigma^2} - 1 \right) + \frac{\sigma_0^2}{2\sigma^2} (k + \lambda),
$$

$$
E_y \text{FD}(y) = d_{KL}(f; f) + \frac{n}{2} \left( \frac{\sigma_0^2}{\sigma^2} - 1 \right) + \frac{\sigma_0^2}{2\sigma^2} (-k + \lambda),
$$

$$
\text{AD} = d_{KL}(f; f) + \frac{n}{2} \left( \frac{\sigma_0^2}{\sigma^2} - 1 \right) + \frac{\sigma_0^2}{2\sigma^2} \lambda,
$$

$$
E_y \text{ED}(y) = d_{KL}(f; f) + \frac{\sigma_0^2}{2\sigma^2} k.
$$

Thus in expectation only, the variable $\text{OD} - d_{KL}(f; f)$ is the sum of $\text{AD} - d_{KL}(f; f)$ and the variable $\text{ED} - d_{KL}(f; f)$.

Proof. Use $E[\chi_r^2(\lambda)] = r + \lambda$, with $\chi_r^2$ equalling $\chi_r^2(0)$. ■

Corollary 3.3. In the definition of the AIC-type model-selection criterion MSC for model $\mathcal{M}$, according to which MSC/2 equals FD($y$) plus an unbiasing term $B$, the term $B$ (i.e. $E_y [\text{OD}(y) - \text{FD}(y)]$) equals $\frac{\sigma_0^2}{2\sigma^2}$ times 2$k$. Hence

$$
\text{MSC} = 2d_{KL}(f; f) + \text{RSS}/\sigma^2 + \frac{\sigma_0^2}{2\sigma^2} 2k.
$$

Proof. Compute $E_y [\text{OD}(y) - \text{FD}(y)]$ from the theorem, and then use the formula (3.5) for FD($y$). ■

Thus with the exception of a constant term equal to $2d_{KL}(f; f)$, which does not affect the relative ranking of models, for any normal linear model $\mathcal{M}_\beta$ fitted to data the AIC-type selection criterion reduces to the standard AIC given in (1.3): the usual RSS/\sigma^2, penalized by twice the number of parameters. Provided, that is, the model incorporates a $\sigma^2$ equal to the variance parameter $\sigma_0^2$ of the true model $\mathcal{M}^*$. There must be no statistical mis-specification: $\mathcal{M}$ must incorporate error bars of the correct length. If so, the formula (1.3) is exact for all $n$. There is no sign of any small-$n$ correction term, such as appears in the AICc.

It must be stressed that deterministic mis-specification is allowed here. There may be a non-zero value for the mis-specification parameter $\lambda = y_0^T Q y_0/\sigma_0^2$, indicating that the constant vector $y_0$ in the definition of the true model $\mathcal{M}^*$ does not lie in the estimation space, i.e., the column space of the design matrix $X$; so the model $\mathcal{M}_\beta$ does not agree with the true model $\mathcal{M}^*$ for any value of $\beta$. Because the parameter $\lambda$ appears in both $E_y \text{OD}(y)$ and $E_y \text{FD}(y)$, it cancels.

The preceding analysis was based entirely on the model-selection policy of (2) according to which the expected overall discrepancy $E_y \text{OD}(y)$ of the true model $\mathcal{M}^*$ from a candidate model $\mathcal{M}$ should be used for selection purposes. This policy gives rise to the AIC, but it is interesting to consider the effects of generalizing it slightly. By the formulas of Theorem 3.2, this policy is equivalent to choosing the model with the smallest value of the sum AD + $E_y \text{ED}(y)$, the discrepancy due to approximation plus the expected discrepancy due to
estimation. Suppose that instead, one assessed the goodness of fit of $M$ to $M^*$ by employing (any multiple of) the convex combination
\[
(\frac{1}{\gamma})AD + (1 - \frac{1}{\gamma}) E_y ED(y),
\]
where $\gamma \geq 1$ is free. By increasing $\gamma$ one emphasizes the discrepancy due to estimation, rather than the discrepancy of $M^*$ from $M$ due to approximation (which if there were no mis-specification would be a constant, i.e., would effectively be zero). If there is no statistical mis-specification ($\sigma^2 = \sigma_0^2$), it follows from the formulas in the theorem that an unbiased estimator of this convex combination, obtained by unbiasing $FD$, is $MSC_\gamma = 0$, where
\[
MSC_\gamma = 2 d_{KL}(f; f) + RSS/\sigma^2 + \gamma k.
\]
With its constant first term dropped, the model-selection criterion $MSC_\gamma$ becomes what is widely known as the AIC$\gamma$, which penalizes any model by $\gamma$ times its number of parameters. As $\gamma$ increases, over-fitting is increasingly disfavored.

The conceptual difference between the two sorts of error in statistical model fitting was pointed out by Inagaki (1977), and an AIC$\gamma$-like criterion resembling (3.7) was defined for autoregressive models by Bhamansali (1986, Eq. (2.12)). But it seems not have been noticed that for normal linear models, AIC$\gamma$ arises rather naturally. Of course in applications, domain-specific considerations that are less axiomatic than practical may affect the choice of $\gamma$.

(b) AIC variability and a significance test

The procedure of deciding among candidate normal linear models will now be placed in the classical hypothesis testing framework. A test of significance for the evidence that $M_1$, $M_2$ are not equally close to the true data-generating process $M^*$ will be proposed. The test is valid in the $n \to \infty$ limit, when applied to models that in a certain precise sense, are separately mis-specified. It is assumed that the data points are accompanied by error bars, i.e., that the residual variance $\sigma^2$ is known and is incorporated in $M_1$, $M_2$.

The proposed test is based on the statistic $\Delta_{12} := AIC^2 - AIC^1$ and an expression for its variance, and can potentially replace the traditional use of Aikake weights. Focusing on the variability and hence the significance of an AIC difference has much in common with the approaches of Efron (1984) and Fraser & Gebotys (1985). But unlike Efron we do not use a bootstrap procedure, and unlike Fraser & Gebotys we allow arbitrary mis-specification. The general approach is distinguished from the likelihood ratio testing approach originating with Cox (1962), in that it decides between $M_1$, $M_2$ on the basis of which is closer to the truth, not on the basis of which is more likely to be correct.

For regression applications, consider the case when the models are fitted to a random vector $y \in \mathbb{R}^n$ that is generated by an unknown true model $y = y_0 + \epsilon_0$, and $N = 1$: only one observation of the random vector $y$ is available as a datum. The candidates $M^l$, $l = 1, 2$, are defined by $y^{(l)} = X^{(l)} \beta^{(l)} + \epsilon^{(l)}$, where $X^{(l)}$ is an $n \times k_l$ design matrix of full rank (with $k_l < n$) and $\beta^{(l)} \in \mathbb{R}^{k_l}$ is a column vector of parameters. The estimation space $L^l \subset \mathbb{R}^n$ (i.e., the column space of $X^{(l)}$) is a linear subspace of dimension $k_l$. Since the models are given, the subspaces $L_1, L_2$ are specified in advance; thus the analysis below is in a sense conditional. The
error vectors $\epsilon, \epsilon(1), \epsilon(2)$ are taken to be $\sigma_0 z_0, \sigma_0 z(1), \sigma_0 z(2)$, where $z_0, z(1), z(2)$ are vectors of $n$ independent standard normal variables.

In this setting the $d_{KL}$-based MSC of AIC type reduces to the standard AIC, by Corollary 3.3. Dropping the additive constant $d(f; f)$, we write

$$\text{AIC}^d = \text{RSS}^d / \sigma_0^2 + 2k_l,$$

$$\text{RSS}^d / \sigma_0^2 = \left[ y - \hat{y}(l) \right]^t \left[ y - \hat{y}(l) \right] / \sigma_0^2$$

(3.8a)

(3.8b)

since $\hat{y} := P(l)y$. (Cf. (3.6b).) The $n \times n$ matrices $P(l), Q(l)$ project onto $L_l, L_l^\perp \subset \mathbb{R}^n$, with $Q(l) = I_n - P(l)$; note that $\text{tr} P(l) = k_l$ and $\text{tr} Q(l) = n - k_l$.

Being an inhomogeneous quadratic form in $z_0$, $\text{RSS}^d / \sigma_0^2$ has a non-central chi-squared distribution, which is $\chi_{n-k_l}^2 (\lambda(l))$, where $\lambda(l) := y(l)Q(l)y_0 / \sigma_0^2$ characterizes the mis-specification of model $M^l$ against $M^*$. $\text{AIC}^d$ is therefore distributed by

$$\text{AIC}^d \sim \chi_{n-k_l}^2 (\lambda(l)) + 2k_l.$$  

It should be noted that as $r \to \infty$, the distribution of $\chi_\lambda^2 (\lambda)$ is increasingly normal, whether or not $\lambda$ grows with $r$; thus as $n \to \infty$, the distribution of $\text{AIC}^d$ is increasingly normal. But it is the distribution of $\Delta^{12} := \text{AIC}^2 - \text{AIC}^1$ that is of interest in model selection, and this is determined by the joint distribution of $\text{AIC}^1, \text{AIC}^2$, and hence by the joint distribution of the quadratic forms $y^tQ(1)y$ and $y^tQ(2)y$. As will be seen, obtaining an $n \to \infty$ limit theorem requires that the relationship between $Q(1), Q(2)$ be somewhat restricted.

**Theorem 3.4.** The expectation and variance of $\text{AIC}^1, \text{AIC}^2$ and the difference $\Delta^{12} := \text{AIC}^2 - \text{AIC}^1$ are given by

$$E\text{AIC}^d = \text{tr} Q(l) + y(l)Q(l)y_0 / \sigma_0^2 + 2k_l$$

$$\text{Var} \text{AIC}^d = 2 \text{tr} Q(l) + 4 y(l)Q(l)y_0 / \sigma_0^2$$

$$E \Delta^{12} = \text{tr}(Q(2) - Q(1)) + y(l)Q(l)y_0 / \sigma_0^2$$

$$\text{Var} \Delta^{12} = 2 \text{tr} [(Q(2) - Q(1))^2] + 4 y(l)Q(l)y_0 / \sigma_0^2.$$  

Proof. The first three of these follow immediately from (3.9) by using $E \left[ \chi_\lambda^2 (\lambda) \right] = r + \lambda$ and $\text{Var} \left[ \chi_\lambda^2 (\lambda) \right] = 2r + 4 \lambda$. All four follow from (3.8) by using the known expressions for normal moments (i.e., the moments of the components of the normal random vector $y \in \mathbb{R}^n$).

The joint distribution of a pair of quadratic forms in a normal vector such as $y \in \mathbb{R}^n$ is complicated, and in general can only be expressed in terms of special functions (Mathai & Provost 1992). But some cases can be treated in closed form. For instance, $y^tQ(1)y$ and $y^tQ(2)y$ are independent if (and only if) $Q(1)Q(2) = 0$, by the Craig–Sakamoto theorem (Ogawa & Olkin 2008). A case more important in applications is the following. Suppose that normal linear regression models $M^1, M^2$, such as the pair considered here, satisfy $M^2 \subset M^1$. That is, $M^2$ is a reduced version of the fuller model $M^1$, obtained by parametric
Information criteria and normal regression

restriciton. Then they are nested: their estimation subspaces \(L_1, L_2\) are related by \(L_2 \subseteq L_1\), and \(L_2 \perp \supseteq L_1\), so that \(Q^{(1)}Q^{(2)} = Q^{(1)}\). If the vector \(y_0\) in the true model \(M^*\) satisfies \(y_0 \in L_2 \subset L_1\), so that neither of \(M^1, M^2\) is mis-specified and \(\lambda^{(1)} = \lambda^{(2)} = 0\), then in addition to the distributional statement \(\text{RSS}^2/\sigma_0^2 \sim \chi^2_{N-K_1}\), one has \((\text{RSS}^2 - \text{RSS}^1)/\sigma_0^2 \sim \chi^2_{K_1-K_2}\). If alternatively \(y_0 \in L_1 \setminus L_2\), so that \(M^2\) is mis-specified but the fuller model \(M^1\) is not, then

\[
\Delta^{12} + 2(K_1 - K_2) = (\text{RSS}^2 - \text{RSS}^1)/\sigma_0^2 \sim \chi^2_{K_1-K_2}(\lambda^{(2)}). \tag{3.10}
\]

Such situations are familiar from multivariate regression, and lead to (partial) F-tests of the significance of linear regressors (Mardia et al. 1979). However, we wish also to handle \(Q^{(1)}, Q^{(2)}\) or equivalently \(L_1, L_2\) that are less closely related: non-nestedness and more general mis-specifications should be allowed.

To motivate the proposed hypothesis test a simple limit theorem will now be proved, on the distribution of \(\Delta^{12}\) in a case often encountered in the physical sciences. This is when the models \(M^1, M^2\) are at least slightly mis-specified relative to the (unknown, presumably infinite-dimensional) true model \(M^*\), in the rather consequential sense that each has a non-zero mean fitting error per data point. Hence one expects that in the \(n \to \infty\) limit, the mis-specification parameters \(\lambda^{(i)} := y_0^iQ^{(i)}y_0/\sigma_0^2\) will grow proportionately to \(n\) (generically, at different rates). For further discussion of mis-specification regimes, see §4.

In the theorem a certain trace condition will appear as a hypothesis. It is motivated by the following consideration. From \(\text{tr} Q^{(i)} = n - K_i\) it follows that \(\text{tr}(Q^{(2)} - Q^{(1)}) = K_1 - K_2\). If there is nestedness and \(L_2 \subset L_1\), then \(Q^{(2)} - Q^{(1)}\) is also a projection, and idempotent; thus for any specified \(m \geq 1\), \(\text{tr}[(Q^{(2)} - Q^{(1)})^m] = O(1)\), i.e. it does not grow with \(n\). It is reasonable to suppose that this condition will hold if \(M^1, M^2\), even if non-nested, are sufficiently similar to justify their being used as competing models of the same data. (Note that if the condition holds for \(m = 2\) then it holds for all \(m \geq 2\), by a standard trace norm inequality.) The condition does not hold in the maximally dissimilar case \(Q^{(1)}Q^{(2)} = 0\), as \(\text{tr}[(Q^{(2)} - Q^{(1)})^2]\) then equals \(\text{tr}Q^{(1)} + \text{tr}Q^{(2)}\).

**Definition 3.5.** Consider a sequence of triples \((M^1, M^2, M^*)\) indexed by \(n\) (including sequences of vectors \(y_0 \in \mathbb{R}^n\) and design matrices), with a common error variance \(\sigma_0^2\). The \(n \times n\) projections \(Q^{(1)}, Q^{(2)}\) are defined as usual. If as \(n \to \infty\), \(y_0^i[(Q^{(2)} - Q^{(1)})^2]y_0\) is bounded below by a positive multiple of \(n\), while (much more routinely) the mis-specification parameters \(\lambda^{(i)} = y_0^iQ^{(i)}y_0/\sigma_0^2\) of the two models are bounded above by a positive multiple of \(n\), the models are said to be **asymptotically separately mis-specified**.

**Remark.** Nested models \(M^1, M^2\) will be asymptotically separately mis-specified if \(\lambda^{(1)}, \lambda^{(2)}, |\lambda^{(1)} - \lambda^{(2)}|\) all grow proportionately to \(n\).

**Theorem 3.6.** In this setting of a sequence of triples \((M^1, M^2, M^*)\) indexed by \(n\), if the candidate models are asymptotically separately mis-specified, and also satisfy the trace condition that \(\text{tr}[(Q^{(2)} - Q^{(1)})^2] = O(1)\), then the distribution of \(\Delta^{12} := AIC^2 - AIC^1\), the expectation and variance of which are given in Theorem 3.4, is asymptotically normal as \(n \to \infty\).
Remark. Under the conditions of this theorem, \( \text{Var} \Delta^{12} \) will be bounded below by a positive multiple of \( n \). This is because according to Theorem 3.3, \( \text{Var} \Delta^{12} \) equals a combination of \( \text{tr}[(Q^{(2)} - Q^{(1)})^2] \) and \( y_0^t[(Q^{(2)} - Q^{(1)})^2]y_0 \).

Proof. The second cumulant \( c_2[\Delta^{12}] = \text{Var} \Delta^{12} \) is bounded below by a positive multiple of \( n \), as just remarked. It is easily seen that each higher cumulant \( c_m[\Delta^{12}] \), \( m \geq 3 \), is \( O(n) \). For instance, \( c_3[\Delta^{12}] \) equals a combination of \( \text{tr}[(Q^{(2)} - Q^{(1)})^3] \) and \( y_0^t[(Q^{(2)} - Q^{(1)})^3]y_0 \), and these are respectively \( O(1) \) and \( O(n) \). Therefore the moments of \( (\Delta^{12} - E \Delta^{12}) / \left[ \text{Var} \Delta^{12} \right]^{1/2} \) tend to those of \( N(0, 1) \), because its higher cumulants tend to zero.

The hypothesis test is suggested by the following. Recall that up to an unimportant additive constant, AIC/2 is an unbiased estimator of the expected overall discrepancy \( E_y \text{OD}^i(y) \), i.e. the negative of the expected log-likelihood after fitting, the expectation being over data generated by \( M^* \).

**Corollary 3.7.** In the above setting, under the null hypothesis that \( E_y \text{OD}^1(y) = E_y \text{OD}^2(y) \) for all \( n \), i.e., that \( M^1, M^2 \) are equally discrepant from \( M^* \) for all \( n \), the distribution of

\[
\Delta^{12} / \left\{ 2 \text{tr}[(Q^{(2)} - Q^{(1)})^2] + 4 y_0^t[(Q^{(2)} - Q^{(1)})^2]y_0/\sigma_0^2 \right\}^{1/2}
\]

tends to \( N(0, 1) \) as \( n \to \infty \).

Proof. The denominator is \( \left[ \text{Var} \Delta^{12} \right]^{1/2} \), as given in Theorem 3.4.

An unbiased estimator of \( \text{Var} \Delta^{12} \) is the quantity

\[
-2 \text{tr}[(Q^{(2)} - Q^{(1)})^2] + 4 y_0^t[(Q^{(2)} - Q^{(1)})^2]y_0/\sigma_0^2
\]

as follows by evaluating its expectation over \( y \). It is not guaranteed to be positive, but the probability of its being so tends to unity as \( n \to \infty \), since the second term increasingly dominates the first. (A maximum likelihood estimator could perhaps be used instead, but even when \( M^1, M^2 \) are nested and \( \Delta^{12} \) has essentially a non-central chi-squared distribution as in (3.10), MLE is difficult to perform (Anderson 1981).) The expression (3.11) is the key to the following test, which can be applied at any fixed \( n \).

**Hypothesis Test.** To test the null hypothesis \( H_0 \) that \( M^1, M^2 \) are equally discrepant from the true model \( M^* \), against the alternative that they are not, calculate what is asymptotically an \( N(0, 1) \) test statistic,

\[
z^{(12)} := \Delta^{12} / \left\{ -2 \text{tr}[(Q^{(2)} - Q^{(1)})^2] + 4 y_0^t[(Q^{(2)} - Q^{(1)})^2]y_0/\sigma_0^2 \right\}^{1/2}.
\]

If \( |z^{(12)}| > z_0 \), where \( P(|Z| > z_0) = \alpha \) for a standard normal variable \( Z \), the evidence against \( H_0 \) is significant at level \( \alpha \). Equivalently, the \( p \)-value associated to \( H_0 \) is given by the formula \( p = P(|Z| > |z^{(12)}|) \). To test against a one-sided alternative that one model is less divergent than the other, proceed similarly.
Estimating the variance of the AIC difference by (3.11) is what makes this \( z \)-test possible. (The small probability that the estimated variance may be non-positive should be noted.) It should be stressed that the normality of the test statistic is a good approximation only for large-\( n \) models \( M^1, M^2 \) that differ appreciably in their mis-specification. In general one would need to exploit the joint distribution of the forms \( \mathbf{y} Q^{(1)} \mathbf{y} \) and \( \mathbf{y} Q^{(2)} \mathbf{y} \), which is complicated.

This test of the significance of an AIC difference is modelled after a \( z \)-test proposed by Linhart (1988). His test is based on the large-sample (\( N \to \infty \)) properties of minimum discrepancy estimators, and is not restricted to normal regression. Our test applies when \( N = 1 \), and is valid in the rather different \( n \to \infty \) limit. However, the need for an asymptotic mis-specification occurs in his analysis, as in ours. In its absence, the test statistic could have a limiting non-central chi-squared distribution, rather than a normal one (cf. Steiger et al. 1985).

Throughout this section we have dealt with linear regression models. But it is not difficult to extend the estimation of \( \text{Var} \Delta_{12} \), and hence the proposed hypothesis test, to models \( M^1, M^2 \) that are non-linear. The following is a sketch. Suppose that model \( M^l, l = 1, 2 \), is defined by \( \mathbf{y} = \mathbf{y}_0^{(l)} + \mathbf{e}^{(l)} \), where \( \mathbf{y}_0^{(l)} = \mathbf{y}_0^{(l)}(\beta^{(l)}) \) is a sufficiently smooth function, not necessarily linear, of the parameter vector \( \beta^{(l)} \in \mathbb{R}^{k_l} \). In the non-linear case the estimation subspace \( L_l \subset \mathbb{R}^n \) is replaced by an estimation submanifold of dimension \( k_l \), but \( M^l \) can be fitted to any datum \( \mathbf{y} \in \mathbb{R}^n \) by non-linear regression (Bates & Watts 1988). There will be a best-fit choice \( \hat{\beta}^{(l)} \in \mathbb{R}^{k_l} \) for the parameter vector, and a predicted vector \( \hat{\mathbf{y}}^{(l)} = \mathbf{y}_0^{(l)}(\hat{\beta}^{(l)}) \).

As usual, the residual sum of squares \( \text{RSS}^l \) equals \( [\mathbf{y} - \hat{\mathbf{y}}^{(l)}]^t [\mathbf{y} - \hat{\mathbf{y}}^{(l)}] \).

The difference from the linear case is this: \( \text{RSS}^l \) is no longer quadratic in \( \mathbf{y}_0 \), as in Eq. (3.8b). But it is straightforward to derive a power series in \( \mathbf{y}_0 \) for \( \text{RSS}^l \) from a Taylor expansion of \( \mathbf{y}_0(\beta^{(l)}) \) about the point \( \beta^{(l)} = \hat{\beta}^{(l)} \). In much the same way, one can obtain an expansion of \( \text{Var} \Delta_{12} \) in powers of \( \mathbf{y}_0 \). From this one can readily construct an unbiased estimator of \( \text{Var} \Delta_{12} \) as a power series in \( \mathbf{y} \), by requiring unbiasedness to each order. By employing a truncation of this series, which is a generalization of the quadratic estimator (3.11), one can extend the proposed test to candidate normal regression models that are non-linear. Thus for non-linear models as for linear ones, it may be possible to employ a decision procedure that relies on the variability of the \( \Delta_{12} \) statistic, rather than on Akaike weights.

### 4. Selection without error bars

The applicability in model selection of the AIC and AICc statistics will now be considered, in the case when the linear regression models being assessed are fitted to a data set without error bars. This is quite different from the case when error (i.e. residual) variances are known and have been incorporated in each model. The calculations below reveal the need for the AICc correction, but also reveal a serious difficulty when a candidate model is mis-specified by an unknown amount. It has long been known that applying the AIC(c) to a mis-specified model is problematic (Sawa 1978; Reschenhofer 1999), but we obtain precise expressions...
Information criteria and normal regression

for the asymptotic \((n \to \infty)\) shift in the AICc, coming from the mis-specification. Our results are similar to those of Noda et al. (1996), but are more explicit.

As in §3.4, take each candidate regression model \(M^l\) to be normal linear, of the form \(y = X(l)\beta(l) + \epsilon(l)\) where \(\epsilon(l) = \sigma z(l)\), with \(z(l)\) a column vector of independent standard normals. The parameter \(\theta(l) = (\beta(l); \sigma^2)\) now includes besides \(\beta(l) \in \mathbb{R}^k\) the residual variance \(\sigma^2\), which must also be fitted. By MLE, if a single datum \(y \in \mathbb{R}^n\) is available, then \(\hat{\sigma}^2 = \hat{\sigma}^2 = y^tQ(l)y/n\), where \(Q(l)\) projects onto the left null space of \(X(l)\) (the error space). The true model \(M^*\) is \(y = y_0 + \epsilon_0\) with \(\epsilon_0 = \sigma_0 z_0\), in which both \(y_0 \in \mathbb{R}^n\) and \(\sigma_0^2\) are unknown.

The deterministic mis-specification of \(M^l\), if any, is quantified by the parameter \(\lambda(l) = y_0^tQ(l)y_0/\sigma_0^2\), which is a measure of the distance in \(\mathbb{R}^n\) between \(y_0\) and the column space of \(X(l)\) (the estimation space). In many reasonable data gathering and regression procedures, \(n\) can be taken arbitrarily large; so the large-\(n\) behavior of \(\lambda(l)\) merits discussion.

One possibility is that \(\lambda(l)/n\) will tend to a limit as \(n \to \infty\), like \(\hat{\sigma}^2 = y^tQ(l)y/n\). That is, in the limit some fraction of the RSS may be attributable to fitting errors of non-zero mean, coming from mis-specification, rather than to the random errors of mean zero and typical size \(\sigma_0\) that come from stochasticity in the data-generating process \(M^*\). (This possibility was discussed in §3.4) Another possibility is that \(\lambda(l)\) will grow sublinearly in \(n\) or even tend to a finite value, for a subtle reason: as \(n\) increases, it may be possible to enhance the regression by improving or expanding the model \(M^l\), giving an even better fit to \(M^*\). But it must be stressed that in the present framework, which does not make explicit the possibility of taking \(n\) to infinity or even of varying \(n\), there is no way of distinguishing the fractional contribution made to RSS by a non-zero mis-specification \(\lambda(l)\), or of estimating its magnitude. Of course, in applications where \(\lambda(l)/n\) is available, then \(\lambda(l)/n\) is an unbiased estimator of the expected overall discrepancy \(E_y OD(y)\) under \(M^*\). This is because according to the policy of §2, it is the latter that should be used in model selection. For the discrepancy \(d_{KL}: OD(y)\) equals \(d_{KL}(g; f_{\hat{\theta}(y)})\), in which \(\hat{\theta} = (\hat{\beta}, \hat{\sigma}^2)\) is the fitted parameter obtained by MLE. Here \(\hat{\beta}(y) = (X^tX)^{-1}X^t y \in \mathbb{R}^k\) as usual; and now \(\hat{\sigma}^2 = y^tQy/n\), where \(Q = I_n - P\) and \(P\) projects onto the column space of \(X\). The PDF’s \(g, f_{\hat{\theta}}\) of \(M^*, \hat{\theta}\) are

\[
g(y) = (2\pi \sigma_0^2)^{-n/2} \exp \left[ -\frac{(y - y_0)^t(y - y_0)}{2 \sigma_0^2} \right], \quad (4.1)
\]

\[
f_{\hat{\theta}}(y) = (2\pi \sigma^2)^{-n/2} \exp \left[ -\frac{(y - X\beta)^t(y - X\beta)}{2 \sigma^2} \right], \quad (4.2)
\]

and by direct computation,

\[
d_{KL}(f_{\hat{\theta}}, f_{\hat{\theta}}) = C_n + \frac{n}{2} \ln (\sigma^2) \quad (4.3)
\]

as in (3.3), where we now write \(C_n := (n/2) [1 + \ln(2\pi)]\).
What can be calculated from the datum \( y \in \mathbb{R}^n \) is not OD(\( y \)) but the fitted discrepancy FD(\( y \)), i.e., \( d_{KL}(g_y; f_{\hat{\theta}(y)}) \), where \( g_y \) is a 1-point atomic PDF. This is simply the negative log-likelihood \(- \ln \mathcal{L}_f(\hat{\theta}|y)\) of the fitted model \( M_{\hat{\theta}} \). As in §3a, the MSC is given by

\[
MSC/2 = FD(y) + B := FD(y) + E_y [OD(y) - FD(y)],
\]

where the ‘\( B \)’ term performs the unbiasing. Also much as before (see (3.3)),

\[
FD(y) = - \ln \mathcal{L}_f(\hat{\theta}|y) = d_{KL}(f_{\hat{\theta}}; f_{\theta}) - \frac{n}{2} \frac{\mathrm{RSS}}{\hat{\sigma}^2}
\]

expresses the fitted discrepancy in terms of the RSS, which is \( y^t \mathbf{Q} y \). But now, under the true model \( M^* \) the fitted variance \( \hat{\sigma}^2 \) as well as the RSS is a random variable. Since \( \hat{\sigma}^2 \) equals \( \mathrm{RSS}/n \), (4.5) simplifies to

\[
FD(y) = - \ln \mathcal{L}_f(\hat{\theta}|y) = d_{KL}(f_{\hat{\theta}}; f_{\theta}) = C_n + \frac{n}{2} \ln (\hat{\sigma}^2) .
\]

The following is the counterpart of Theorem 3.1. In the statement, \( \lambda := y_0^t \mathbf{Q} y_0/\sigma_0^2 \) is the (presumably unknown) \( M \)-specific mis-specification parameter.

**Theorem 4.1.** Under the model \( M^* \), the overall and fitted discrepancies of the fitted model \( M_{\hat{\theta}(y)} \), OD = OD(\( y \)) and FD = FD(\( y \)), are distributed according to

\[
\text{OD} = d_{KL}(g; f_{\hat{\theta}(y)}) \sim C_n + \frac{n}{2} \ln (\hat{\sigma}^2) + \frac{n}{2} \left( \frac{\sigma_0^2}{\hat{\sigma}^2} - 1 \right) + \frac{\sigma_0^2}{2 \hat{\sigma}^2} \chi^2_{n-k}(\lambda),
\]

\[
\text{FD} = d_{KL}(g_y; f_{\hat{\theta}(y)}) \sim C_n + \frac{n}{2} \ln (\hat{\sigma}^2) ,
\]

where \( \hat{\sigma}^2 \) equals \( (\sigma_0^2/n) \) times a random variable with distribution \( \chi^2_{n-k}(\lambda) \), and \( \chi^2_{k}(\lambda) \) signifies a random variable that is independent of \( \hat{\sigma}^2 \).

**Proof.** That \( \hat{\sigma}^2 \) equals \( (\sigma_0^2/n) \) times a random variable with non-central chi-squared distribution \( \chi^2_{n-k}(\lambda) \) follows from the representation

\[
\hat{\sigma}^2/(\sigma_0^2/n) = y^t \mathbf{Q} y/\sigma_0^2 = (z_0 + y_0/\sigma_0)^t \mathbf{Q}(z_0 + y_0/\sigma_0) .
\]

(Cf. (3.6a).) As in the proof of Theorem 3.1, OD(\( y \)) is calculated by using the definition (2.3) of \( d_{KL} \) and the definitions (4.1), (4.2) of \( g, f_{\theta} \). The definite integral in the definition of \( d_{KL} \) can be evaluated in closed form, and the resulting quadratic form \((\mathbf{P} y - y_0)^t(\mathbf{P} y - y_0)/\sigma_0^2 \) has distribution \( \chi^2_{k}(\lambda) \). (Cf. (3.6a).) That this and the quadratic form \( \hat{\sigma}^2 = y^t \mathbf{Q} y/n \) are independent follows from the ‘if’ part of the Craig–Sakamoto theorem, mentioned above, since the projection matrices \( \mathbf{P}, \mathbf{Q} \) are complementary: they satisfy \( \mathbf{P} \mathbf{Q} = 0 \).

**Theorem 4.2.** The unbiasing term ‘\( 2B \)’ in the definition (4.4) of the AIC-type selection criterion MSC is expressed in terms of the moments of non-central
chi-squared random variables by

\[ 2 B = 2 E_y [\text{OD}(y) - \text{FD}(y)] \]

\[ = n \left\{ n E \left[ \left( \chi^2_{n-k}(\lambda) \right)^{-1} \right] - 1 + [E (\chi^2_k(\lambda)) E \left( \chi^2_{n-k}(\lambda) \right)^{-1}] \right\} \]

\[ = n \left\{ -1 + (n + k + \lambda) \left[ \frac{1}{n-k-2} - \frac{1}{(n-k)(n-k-2)} \lambda + \cdots \right] \right\}. \]

**Proof.** This comes from the formulas of Theorem 4.1 by exploiting \( \hat{\sigma}^2 \sim (\sigma_0^2/n) \chi^2_{n-k}(\lambda) \) and independence. The first moment \( E (\chi^2_k(\lambda)) \) equals \( k + \lambda \), and the series in \( \lambda \) for the negative first moment \( E \left[ (\chi^2_r(\lambda))^{-1} \right] \) (where \( r = n - k \)), appearing in square brackets, is taken from Appendix A.

The preceding calculation reduces when \( \lambda = 0 \) and \( \mathcal{M} \) is not mis-specified to a derivation of the AICc that has been given by several authors (Sugiura 1978; Hurvich & Tsai 1989; Cavanaugh 1997). But it is the generalization to non-zero \( \lambda \), which is similar to one of Hurvich & Tsai (1991), which is of interest. The chi-squared variables in the formula for the unbiasing term, which if \( \lambda \) were zero would be central, become non-central with non-centrality parameter \( \lambda \).

As was explained above, in some applications it is reasonable for the mis-specification \( \lambda \) of a candidate model to be large in the sense that it grows linearly in \( n \); that is, if the regression procedure is such that \( n \) can be taken arbitrarily large. But it is also useful to consider the case of ‘medium mis-specification,’ when to leading order \( \lambda \) grows proportionately to \( n^{1/2} \), and that of ‘small mis-specification,’ when \( \lambda \) is bounded in \( n \) as \( n \to \infty \). Hence \( \lambda \) will now be allowed to grow according to \( \lambda \sim \lambda_1 n + \lambda_{1/2} n^{1/2} + \lambda_0 + o(1), n \to \infty \).

**Theorem 4.3.** Let the additive constant \( 2C_n \) be dropped from the definition of the AIC-type selection criterion MSC. Then if the mis-specification \( \lambda \) of a model \( \mathcal{M} \) equals zero, its MSC reduces to the standard AICc given in (1.5),

\[ \text{AICc} = n \ln \left( \hat{\sigma}^2 \right) + \frac{2(k + 1)n}{n - k - 2} \]

\[ \sim \text{AIC} + \frac{2(k + 1)(k + 2)}{n} + O(1/n^2), \quad n \to \infty, \]

where \( \text{AIC} = n \ln \left( \hat{\sigma}^2 \right) + 2(k + 1) \).

In the regime of small mis-specification, when \( \lambda \sim \lambda_0 + o(1) \) as \( n \to \infty \) with \( \lambda_0 > 0 \),

\[ \text{MSC} \sim \text{AICc} - \frac{\lambda_0(2k + \lambda_0)}{n} + O(1/n^2), \quad n \to \infty. \]

In the regime of medium mis-specification, when \( \lambda \sim \lambda_{1/2} n^{1/2} + o(n^{1/2}) \) as \( n \to \infty \) with \( \lambda_{1/2} > 0 \),

\[ \text{MSC} \sim \text{AIC} - \lambda_{1/2}^2 + o(1/n^{1/2}), \quad n \to \infty. \]

In the regime of large mis-specification, when \( \lambda \sim \lambda_1 n + o(n) \) as \( n \to \infty \) with \( \lambda_1 > 0 \), the MSC equals AIC plus a \( \lambda_1 \)-dependent quantity growing with \( n \).
Proof. Substitute the leading-order behavior of $\lambda$ into the formula given in Theorem 4.2. It should be noted that if $\lambda \sim \lambda_1 n$, all terms of the power series in $\lambda$ for $E \left[ (\chi^2_{n-k} - 1)^{-1} \right]$ will contribute, as each will be of order $1/n$. $\blacksquare$

This theorem has disconcerting implications for the usefulness of the AIC and AICc in model selection. It reveals how different the case of an unknown error variance $\sigma^2$ is, from the case of a known $\sigma^2$ (treated in §3a).

If $\lambda = 0$ and the model is not mis-specified, the theorem confirms that including the standard AICc correction term of magnitude $O(1/n)$ is justified. This term may affect the selection procedure if $n$ is small. But if $\lambda = \lambda_0 + O(1/n)$ as $n \to \infty$ with $\lambda_0$ non-zero, the coefficient of $1/n$ in the correction term will deviate from the AICc form. Since $\lambda_0$ is typically not known, this renders difficult any small-$n$ correcting of the AIC. In the regime of medium mis-specification the problem is worse: the $O(1)$ unbiasing term $2(k + 1)$ in the AIC itself is shifted by an amount depending on $\lambda_1/2$. And in the regime of large mis-specification, in which applications of model selection may well lie, the AIC is shifted by a potentially large amount, growing with $n$. This shift may swamp the term $2(k + 1)$.

Theorem 4.3 indicates that when deciding between candidate models that have been fitted to a data set without error bars, it may be unwise to use the AICc or even the AIC, if there is any possibility that the models are mis-specified relative to the true data-generating process $M^*$, and if the amount of mis-specification is unknown but is expected to be substantial. Since in the physical sciences $M^*$ is typically infinite-dimensional, candidate models that are mis-specified, at least to some extent, are expected to occur quite widely.

5. Summary and discussion

In this paper the AIC and AICc were developed from first principles, to clarify their ability to assess competing regression models of the sort common in the physical sciences: ones with normal errors and known error variances, coming from the error bars of a size-$n$ data set. The data set was viewed as providing a single observation $(N = 1)$ of an $S$-valued random quantity, the space $S$ being $\mathbb{R}^n$.

In §2 a model selection policy was formulated, applying to arbitrary $S$ and arbitrary $N$. The Kullback–Leibler divergence $d_{KL}$ was then chosen as the discrepancy functional, which the policy left unspecified. The choice of $d_{KL}$ ensures that fitted models are compared on the basis of their fitted log-likelihoods, suitably unbiased (i.e., penalized). It was noted that other measures of the discrepancy between a parametric model and a data set could be used, such as the popular Hellinger distance. This option is worth exploring, since MLE is not robust and may not be the best choice if, say, the regression is non-linear or non-normal errors are present. But as was explained, this will require that the selection policy be modified to include a form of kernel density estimation.

It was shown in §3a that when fitting a linear regression model to data with error bars, the AIC and not the AICc should be used. (For comments on the recent astrophysics literature, see Appendix B.) If the model incorporates a known error variance $\sigma^2$, its mis-specification if any does not affect the validity of the AIC, though it causes certain discrepancy statistics to have non-central rather than central chi-squared distributions. That no additional unbiasing of the AIC
is needed when $\sigma^2$ is known has in fact been noticed (Kuha 2004, p. 209), but seems to have attracted little attention. In applications of the AIC in the physical sciences, it is of considerable importance.

In §3 it was shown that in the same setting as that of §3, the variability of an AIC difference can be estimated. A test of significance was proposed, which exploits what under reasonable conditions of mis-specification is the asymptotic ($n \to \infty$) normality of this statistic. The significance test is a test for selection, which can potentially replace the use of Akaike weights in deciding between regression models with known error variances.

The approach of §3 to model selection resembles the approach of Commenges et al. (2008). In a general large-sample ($N \to \infty$) context, not focused on the comparison of regression models, they proposed a test for selection based on a difference of two AIC’s. They were able to work out the asymptotic distribution of a normalized version of this difference by exploiting large-sample theory for the likelihood ratio statistic. This included the classical result of Wald (1943) on the comparison of nested models, involving a non-central chi-squared distribution, and an asymptotic normality result of Vuong (1989), who dealt with non-nested models. The test proposed in §3 is similar in spirit, but in the formulation used here the $n \to \infty$ limit of a regression model is rather different from an $N \to \infty$ large-sample limit, and requires its own analysis.

In §4 the usual derivation of the AICc statistic, applying to linear regression models fitted to data sets without error bars, was extended to models with non-zero mis-specification $\lambda$. The appearance of a non-central chi-squared in the distribution of the overall Kullback–Leibler discrepancy is not unexpected. But the behavior of the unbiasing term in the large-$n$ limit is cause for concern. The case when the model mis-specification $\lambda$ is $o(1)$ as $n \to \infty$ is the nicest. (It has a close analogue in the large-sample theory of the likelihood ratio: the case of ‘local alternatives,’ when the true value of a model parameter is taken to approach the pseudo-true value as $N \to \infty$.) Except in this case, the shift in the AICc due to the mis-specification may swamp in the large-$n$ limit the AICc correction term, and even the usual $2(k+1)$ unbiasing term. For mis-specified regression models fitted to data without error bars, this may well affect the usefulness of the AICc as a tool in model selection. The extent to which this problem occurs in the physical sciences remains to be studied.

Appendix A. Non-central chi-squared distributions and quadratic forms

A (central) $\chi^2$ distribution with $r$ degrees of freedom, denoted $\chi^2_r$, is the distribution of the sum of the squares of $r$ independent standard normal random variables. That is, if $z$ is a column vector of $r$ standard normals, then $z^t z \sim \chi^2_r$.

There is a generalization: if $P$ is an $n \times n$ projection matrix of rank $s$ with $0 \leq s \leq r$, the quadratic form $(Pz)^t (Pz) = z^t Pz$ has distribution $\chi^2_s$.

A $\chi^2$ distribution with $r$ degrees of freedom and non-centrality parameter $\lambda$, denoted $\chi^2_r(\lambda)$, is the distribution of $(z + u)^t (z + u)$, where $u$ is a fixed column vector. That is, it is the distribution of the squares of $r$ independent unit-variance normal variables, not necessarily of mean zero. The parameter $\lambda$ equals $u^t u$.

There is a generalization: the quadratic form $[Pz + u]^t [Pz + u]$ has distribution...
\( \chi^2(\lambda) \) with \( \lambda = u^T u \). A second generalization is that \( [P(z + u)]^T [P(z + u)] = (z + u)^T P(z + u) \) has distribution \( \chi^2(\lambda) \) with \( \lambda = u^T P u \).

When \( r > 1 \), the PDF of \( \chi^2(\lambda) \) cannot be expressed in terms of elementary functions, though it can in terms of the confluent hypergeometric function \(_0F_1\), or alternatively a modified Bessel function of the first kind. If \( X \sim \chi^2(\lambda) \) then \( X \) has mean and variance

\[
EX = r + \lambda, \quad \text{Var} X = 2r + 4\lambda, \tag{A.1}
\]
and negative first moment

\[
E[X^{-1}] = e^{-\lambda/2} \sum_{m=0}^{\infty} \frac{(\lambda/2)^m}{m!} \frac{1}{r - 2 + 2m}. \tag{A.2}
\]

For details, see Mathai & Provost (1992) and Bock et al. (1984).

Appendix B. The AICc in recent papers

The AIC and AICc have recently entered the physical sciences and in particular astrophysics by being used to compare cosmological models. Such models have a relatively small number of parameters, and competing models are usually not nested. Models have been compared, e.g., on the basis of their predictions of the distance–redshift relation, which characterizes the expansion of the Universe. After a model is fitted by non-linear regression to observational data, its goodness of fit is assessed by calculating its AIC or AICc. One recent comparison of models, employing the AIC and the Bayesian criterion BIC, is that of Shi et al. (2012).

A search reveals that many though not all publications in this area use the AIC and AICc in a fashion that on the basis of the present work, can be considered correct. If the observational data are accompanied by error bars, or a common error variance \( \sigma^2 \) is known or assumed, the AIC should be used; and if the variance is treated as a nuisance parameter to be fitted, the AICc should be used. Davis et al. (2007), Li et al. (2010) and Tan & Biswas (2012) employ the AICc, despite their data sets being accompanied by error bars, which strictly speaking is incorrect; but they observe in their analyses that the AICc correction is of negligible size and does not affect model comparisons. The paper of Tan & Biswas is especially valuable from a statistician’s point of view, because they investigate AIC(c) variability empirically rather than theoretically, using a bootstrap procedure.

Unfortunately, a number of papers in the literature are based on data with explicit error bars, but use the AICc without commenting on whether its \( O(1/n) \) correction term affects their results. This includes the papers of Biesiada & Piórkowska (2009), February et al. (2010), Kelly et al. (2010), Dantas et al. (2011), Basilakos & Pourz (2012), Papageorgiou et al. (2012) and Wang & Zhang (2012). A re-examination of the model comparisons in these papers is surely desirable.
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Information criteria and normal regression 27

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