The exact form of the ‘Ockham factor’
in model selection

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Abstract

We explore the arguments for maximizing the ‘evidence’ as an algorithm for model selection. We show, using a new definition of model complexity which we term ‘flexibility’, that maximizing the evidence should appeal to both Bayesian and Frequentist statisticians. This is due to flexibility’s unique position in the exact decomposition of log-evidence into log-fit minus flexibility. In the Gaussian linear model, flexibility is asymptotically equal to the Bayesian Information Criterion (BIC) penalty, but we caution against using BIC in place of flexibility for model selection.

Keywords: Complexity, evidence, Ockham factor, flexibility, BIC penalty
1 Introduction

As Albert Einstein almost said, “Scientific models should be as simple as possible, but no simpler”. Ockham’s razor is a common term for this principle of simplicity. Sober (2015) contains a wide-ranging review, including what Einstein actually said, while Jefferys and Berger (1992) give an engaging and non-technical account of how Ockham’s razor emerges from a Bayesian treatment of model selection.

In philosophy, statistics, and machine learning, Ockham’s razor recommends that we favour less complex models where we can. But why this should be, and what we mean by ‘complex’, are subtle issues. In this paper, we describe one approach to implementing Ockham’s razor for model selection, based on a decomposition of the ‘evidence’ into a ‘fit’ term and a complexity term which we call ‘flexibility’. Our decomposition is exact for all models and all regularizers. We do not advocate one particular approach to model selection, but clarify the implications of and relations between various approaches, describing how one particular approach—maximizing the evidence—might be justified by both Bayesian and Frequentist statisticians.

Section 2 provides background, and section 3 provides and discusses various arguments for the use of the evidence in model selection. Section 4 presents our exact decomposition of evidence into ‘fit plus flexibility’, and we justify flexibility as a measure of model complexity. Section 5 illustrates using the Gaussian linear model, for which simple closed-form expressions are available. The Bayesian Information Criterion (BIC) penalty is shown to be an approximation to flexibility in this case, but we caution against its use in model selection in general, and even specifically in those cases where the BIC penalty and flexibility are asymptotically equivalent. Section 6 concludes with a summary.
2 Background

Our starting-point is a set of observations $y^{\text{obs}}$. A statistical model is proposed,

$$f(y; \theta), \quad \begin{cases} y \in \mathcal{Y} \subset \mathbb{R}^n \\ \theta \in \Theta \subset \mathbb{R}^d. \end{cases} \quad (1)$$

The defining features of such a model are

$$\forall \theta \in \Theta : \quad f(\cdot; \theta) \geq 0, \quad \int_{\mathbb{R}^n} f(y; \theta) \, dy = 1, \quad (2)$$

where the integral may be replaced by a sum if $\mathcal{Y}$ is countable. In addition, this model is augmented with a regularizer $R : \Theta \to \mathbb{R}$. The fitted value of the parameter is

$$\hat{\theta} := \arg\max_{\theta \in \Theta} \left\{ \log f(y^{\text{obs}}; \theta) - R(\theta) \right\}. \quad (3)$$

Thus the regularizer is functionally equivalent to a prior distribution

$$\pi(\theta) \propto e^{-R(\theta)}, \quad (4)$$

which we assume is proper, and in this case the fitted value $\hat{\theta}$ is identical to the Maximum A Posteriori (MAP) estimate of $\theta$.

As this outline makes clear, the estimated value $\hat{\theta}$ is a function of both the statistical model and the regularizer. To be precise, we would write ‘model and regularizer’ everywhere below, but this would be tedious; therefore we will write ‘model’, but in every case where we write ‘model’ we mean ‘model and regularizer’.

Define the ‘evidence’ of this model as

$$E := \int_{\Theta} f(y^{\text{obs}}; \theta) \, \pi(\theta) \, d\theta. \quad (5)$$
This value is also referred to as the ‘integrated likelihood’, or the ‘marginal
likelihood’ (Murphy, 2012, sec. 5.3). In a Bayesian approach it has the ad-
tional interpretation of the ‘predictive density’ of the observations (Box
1980, p. 385). The normalizing constant in the prior distribution (4) is not
required to compute \( \hat{\theta} \), but it is required to compute the evidence directly.

Friel and Wyse (2012) provide a review of methods for estimating the evi-
dence, covering a literature which stretches back thirty years, while Gutmann
and Hyvärinen (2012) present a recent and promising approach using logistic
regression (see also Hastie et al., 2009, sec. 14.2.4).

Suppose that we would like to select a single model from a set of models
under consideration, indexed by \( i \in \mathcal{M} \). For example, \( \mathcal{M} \) might represent a
set of Gaussian linear models with different model matrices (see Section 5).
The claim we investigate in this paper is that maximizing the evidence is a
good way to select such a model. That is, if \( E_i \) is the evidence of model \( i \),
then

\[
i^* := \arg\max_{i \in \mathcal{M}} E_i
\]

is the best single model in \( \mathcal{M} \)—or one of the best.

The notion that there is a best single model in \( \mathcal{M} \) is a bold claim, because
it does not distinguish between the possibly different requirements of model-
selection for inference, and model-selection for prediction. In inference, the
intention would be to inspect the fitted components of the model in order to
make statements about the underlying system; for example, to see whether
a regression coefficient is negative, roughly zero, or positive. In this case,
it is helpful for interpretability to focus on a single model. In prediction,
the structure of the model is less important than its predictive performance
out-of-sample. In this case, the use of a single model would be a pragmatic
simplification, especially for operational systems. So in both cases there is
an apparent need for a single model, but there is no a priori reason to think
that one method will produce a best or nearly-best choice of model in both
cases.
3 Arguments for the evidence

For statisticians, the natural approach to choosing a single model from a set $\mathcal{M}$ is to use statistical decision theory, in which a loss function $L(i, j)$ quantifies the negative consequences of choosing model $i$ were model $j$ to be the true model. While there will be applications where a particular loss function suggests itself, in many cases the zero-one loss function is a pragmatic choice:

$$L(i, j) = \begin{cases} 0 & i = j \\ 1 & \text{otherwise.} \end{cases}$$

(7)

This loss function treats all wrong choices as equally-wrong. There is a useful generalization of this loss function, which includes ‘undecided’ among the actions, but we will not consider it further here (see Murphy, 2012, ch. 5).

In a Bayesian approach, the models in $\mathcal{M}$ are given prior probabilities, $w_i > 0$. The Bayes Rule for zero-one loss is to select the model with the largest posterior probability, where the posterior probabilities are proportional to $w_i E_i$. Thus if $\mathcal{M}$ is finite and the prior probabilities are uniform, then choosing $i^*$, the model with the largest evidence, is the Bayes Rule. More generally, if the evidence is concentrated relative to the prior probabilities, then choosing $i^*$ is ‘hopefully’ the Bayes Rule. A Bayesian statistician might reason: “I don’t want to spend too much effort thinking about my prior probabilities, but I believe that they are sufficiently uniform over $\mathcal{M}$ that that the model with the highest evidence will be the Bayes Rule, or a good approximation.” This reasoning goes back to the ‘Principle of Stable Estimation’ of L.J. Savage (see Edwards et al., 1963).

Clearly, this Bayesian argument is contingent on a willingness to contemplate and possibly provide prior probabilities for the models in $\mathcal{M}$. This may be anathema to some Frequentist statisticians, who might otherwise accept the need for a loss function, and tentatively accept the choice of the zero-one loss function. But these statisticians will recognize the validity of
the Complete Class theorems, which in this context state that choosing the model with the largest evidence cannot be inadmissible under zero-one loss, because it is the Bayes Rule for a prior which assigns positive probability to all models; see, e.g., DeGroot (1970, ch. 8), Schervish (1995, ch. 3), or Berger (1985, ch. 8). Avoiding inadmissible decision rules is a low bar but an important one. So statisticians of all persuasions should at least contemplate choosing the model with the highest evidence, on the basis of zero-one loss, but this argument is suggestive, rather than compelling; and more suggestive in the Bayesian approach than in the Frequentist approach.

The second argument is more Frequentist, because it claims that \( \hat{i}^* \) is a model-selection algorithm with attractive properties. Making this case for inference tends to be model-dependent and often requires asymptotic arguments; we concur with Le Cam (1990, p. 165), whose Principle 7 states “If you need to use asymptotic arguments, do not forget to let your number of observations tend to infinity”; we touch on this principle at the end of section 5. Instead, we focus on the argument for choosing \( \hat{i}^* \) for prediction, using a canonical example which also has much practical relevance: polynomial regression.

In the regression

\[
y_i = \beta_0 + \beta_1 x_i + \beta_2 x_i^2 + \cdots + \beta_p x_i^p + \text{error}_i
\]

there is a simple index of models in terms of the degree \( p \). Under standard fitting procedures such as Ordinary Least Squares, and its Bayesian treatment with a vague prior on \( \beta \), models with higher degree will never fit worse, in terms of root mean squared error, and will usually fit better. Nevertheless, the wiggliness of high-degree polynomials compromises their predictive accuracy, particularly outside the convex hull of the observations. This property
is captured by the following schematic:

![Diagram showing the relationship between degree, fit, and prediction.](image)

...in which there is a ‘sweet spot’ between low and high degree which is optimal for prediction. Most textbooks contain a detailed discussion of this property; see, e.g., Bishop (2006, ch. 1) or Murphy (2012, ch. 1). Jefferys and Berger (1992) provides a wide-ranging and non-technical discussion with historical examples.

The logic of polynomial regression would seem to apply much more generally: models with the equivalent of high degree will fit better but predict worse than models of medium degree. This can be represented as ‘overfitting’: models of high degree fit into the noise, and thereby carry the noise into the prediction, which decreases accuracy. Or, to put it another way, models need some ‘stiffness’ in order to resist noise. The ‘degree’ of polynomial regression is replaced by the more ambiguous term ‘complexity’, and the schematic becomes

![Diagram showing the relationship between complexity, fit, and prediction.](image)

...see, e.g., Hastie et al. (2009, Fig. 2.11). It is only a short step from this...
schematic to an outline model-selection criterion for prediction: to reward fit but to penalize complexity, hoping to settle at or near the sweet-spot between low and high complexity.

While there are many forms that such a criterion might take, one form has emerged as nearly ubiquitous, which is to maximize the scalar quantity

$$\log f(y_{\text{obs}}; \hat{\theta}) - \text{penalty}$$

where \text{penalty} is a measure of complexity that can depend on the model and on the observations. The first author to derive a criterion of this form was Akaike (1973), whose penalty did not depend on the data, and there have been many proposals since: this is still an active field of research in statistics (see, e.g., Gelman et al., 2014, ch. 7).

Now to return to our main topic, evidence. David MacKay (MacKay, 1992, 2003) argued that the log-evidence itself has the form of (8), at least approximately. MacKay’s argument had two strands. First, there was ‘proof by picture’, a compelling illustration that the evidence will sometimes select less complex models over more complex models, shown here as Figure 1. This picture embodies Jefferys and Berger (1992)’s informal definition of complexity: “the more complex hypothesis tends to spread the probability more evenly among all the outcomes” (p. 68).

But the second strand is less compelling. MacKay applied a first-order Laplace approximation to compute the evidence, and showed that, under this approximation,

$$\log E \approx \log f(y_{\text{obs}}; \hat{\theta}) - \text{penalty}$$

where \text{penalty} has an explicit form in terms of the model and the observations, but its form is not important to our argument. We know, as a matter of logic, that \text{penalty} in (9) must behave something like a model complexity penalty. This follows because the first term on the righthand side will tend to be larger for more complex models, and hence if the evidence can sometimes
Figure 1: Similar to MacKay (2003), Figure 28.3 (p. 344). For visualization, the observation $y$ is assumed to be a scalar. The more complex Model 1 spreads its predictive density over a wider set of values in the data-space $\mathcal{Y}$, and hence the evidence will favour the less complex Model 2 in some regions of $\mathcal{Y}$. In this case the evidence favours the more complex model at $y^{\text{obs}} = y'$, and the less complex model at $y^{\text{obs}} = y''$. 

Figure 1: Similar to MacKay (2003), Figure 28.3 (p. 344). For visualization, the observation $y$ is assumed to be a scalar. The more complex Model 1 spreads its predictive density over a wider set of values in the data-space $\mathcal{Y}$, and hence the evidence will favour the less complex Model 2 in some regions of $\mathcal{Y}$. In this case the evidence favours the more complex model at $y^{\text{obs}} = y'$, and the less complex model at $y^{\text{obs}} = y''$. 

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be smaller for more complex models, as Figure 1 demonstrates, then penalty must sometimes be larger for more complex models.

However, Laplace approximations, of first or higher order (see, e.g., Robert and Casella, 1999, sec. 3.5) can perform poorly in practice, which is why there has been such sustained interest in developing MCMC methods for computing posterior expectations over the last three decades (see, e.g., Andrieu et al., 2003, for some history). Their performance today is likely to be worse than ever, in our current era of massively over-parameterized models and exotic regularizers (e.g. to promote sparsity). Therefore MacKay’s decomposition is suggestive, but does not provide a strong reason to believe that the evidence on its own represents a fit term minus a complexity term suitable for all applications.

This long discussion of the Frequentist argument for using evidence to choose a single predictive model indicates once again that the argument is suggestive but not compelling. There have been a number of conjectural steps: the generalization from polynomial degree to model complexity, the idea that the ‘sweet spot’ of optimal complexity can be found by penalizing the maximized log-likelihood, and then MacKay’s construction which suggests that log-evidence has the approximate form of penalized log-likelihood. Therefore it is gratifying that in the next section we can show that there is an exact equality between log-evidence, fit, and a complexity penalty, which holds in complete generality, and where the penalty has a simple and intuitive form.

4 ‘Flexibility’

Our approach uses a simple result that is a reformulation of Bayes’s Theorem:

$$E = \frac{f(y_{obs}; \theta_0) \pi(\theta_0)}{\pi^*(\theta_0)}$$  (10)
which holds for all $\theta_0 \in \Theta$ for which $\pi^*(\theta_0) > 0$, where $\pi^*$ is the posterior distribution. Chib (1995, p. 1314) refers to this equality as the basic marginal likelihood identity (BMI); it also goes by the name Candidate’s formula, after Besag (1989).

If we set $\theta_0 = \hat{\theta}$ from (3), then we immediately deduce

$$
\log E = \log f(y^{\text{obs}}, \hat{\theta}) - \log \frac{\pi^*(\hat{\theta})}{\pi(\hat{\theta})}
$$

from (10). By our argument at the end of the previous section, the second term on the righthand side must behave something like a model complexity penalty. To identify it explicitly, we give it the name

$$
\text{flexibility} := \log \frac{\pi^*(\hat{\theta})}{\pi(\hat{\theta})},
$$

which will be positive, except possibly in pathological situations where there is a conflict between the prior distribution and the likelihood. We have, under this definition,

$$
\log E = \log f(y^{\text{obs}}, \hat{\theta}) - \text{flexibility}
$$

an exact decomposition of the evidence, which holds for all models. This is the unique decomposition for which the ‘fit’ term is $\log f(y^{\text{obs}}, \hat{\theta})$. A different estimate for $\theta$, such as the Generalized Method of Moments (GMM) estimate, would give a different penalty term in the decomposition of the evidence. However, given that the regularizer is operationally equivalent to a prior distribution, the penalized likelihood (or MAP) estimate $\hat{\theta}$ seems the most natural value to use for $\theta_0$.

We contend that flexibility is a reasonable way to measure model complexity. A model will be ‘flexible’ if it contains a large number of degrees of freedom, in the engineering sense (e.g. represented by $\dim \Theta$, which might be
the number of basis functions), and if its parameters are unconstrained in the prior distribution (or regularizer). A model will be ‘inflexible’ (or ‘stiff’) either if it contains few degrees of freedom, or if its parameters are constrained in the prior distribution, or both. A flexible model will often be able to concentrate its posterior probability into a small data-determined region of its parameter space, relative to its prior probability, and hence its flexibility will be high. An inflexible model in the same situation will be prevented from concentrating, lacking either the capacity to shape itself to the data, or else having the capacity but being prevented from doing so by the prior probability. Thus its flexibility will be low. Complex models will typically be flexible, in this sense, and simple models will be inflexible.

Our exact decomposition of the log-evidence has changed neither the Bayesian nor the Frequentist arguments for using the evidence for model selection, although it has sharpened MacKay’s construction. So does it have any practical value? We think it does. Eq. (12) shows that

\[ \log f(y^{\text{obs}}, \hat{\theta}) - \text{penalty} = \log E - (\text{penalty} - \text{flexibility}) \]  

Therefore any method which penalizes the maximum of the log-likelihood with \text{penalty} is equivalent to a method which penalizes the log-evidence with \text{penalty}'. A decision \textit{not} to set \text{penalty} = \text{flexibility} is equivalent to a decision to penalize the log-evidence, with a penalty of an explicit but perhaps unanticipated form.

Our decomposition presents this type of decision in a new light. Suppose you choose to penalize log-likelihood with something other than \text{flexibility}. Your client, or your client’s auditor, might well ask “What deficiency of the evidence as a criterion for model selection are you addressing with your choice of \text{penalty}’?” You might answer, “The evidence has no epistemic value to me: I regard \text{(12)} as a purely mathematical result, and can provide a rationale for my \text{penalty} in terms of log-likelihood.” The difficulty with this position
is that log-evidence clearly does have epistemic value, as demonstrated by the Bayesian and admissibility arguments. Thus any rationale for penalizing log-likelihood is more compelling if it can be cross-referenced to log-evidence.

This viewpoint also operates in the other direction: a decision to penalize log-evidence is equivalent to a decision to penalize log-likelihood with something other than flexibility.

There will always be applications in model selection where a strong case can be made for a penalty which is not flexibility. But we propose that flexibility is a reasonable default choice, which has some cross-party appeal. Thus a Bayesian might say,

We selected the model which maximized the evidence, which is similar and sometimes the same as selecting the model which has the largest posterior probability, which itself is the Bayes Rule for zero-one loss. But we note that the same model would have been selected using a penalized log-likelihood approach in which the model complexity penalty is ‘flexibility’.

And a Frequentist might say

We selected the model which maximized the log-likelihood penalized by the ‘flexibility’ penalty for model complexity; in other words, we maximized the evidence. But we note that the same model would have been selected under a Bayesian approach which maximized posterior probability with a uniform prior distribution, which is an admissible decision rule for zero-one loss.

In situations where the choice of complexity penalty is not clear-cut, choosing flexibility seems to be a simple and defensible way forward. The next section considers the case where the flexibility has a closed-form expression, and a simple asymptotic approximation.
5 Illustration: Gaussian linear model

Consider the Gaussian linear model with model-matrix $G \in \mathbb{R}^{n \times d}$ and observation error variance $\sigma^2$. We use a quadratic regularizer parameterized by $\lambda$:

$$R(\theta) = \frac{1}{2} \lambda^2 \| \theta \|^2$$

or, equivalently in terms of the prior distribution,

$$\pi(\theta) = \mathcal{N}(0_d, P^{-1})$$

where $P := \lambda^2 I_d$ is the prior precision. This implies that the posterior distribution has the form

$$\pi^*(\theta) = \mathcal{N}(\hat{\theta}, (P^*)^{-1})$$

where $\hat{\theta}$ is the posterior expectation, as well as the MAP estimate, and $P^*$ is the posterior precision,

$$P^* = \frac{1}{\sigma^2} G^T G + P$$

$$\hat{\theta} = \frac{1}{\sigma^2} (P^*)^{-1} G^T y_{\text{obs}};$$

these are both functions of $(\sigma, \lambda)$, which we treat as known. Hence

$$\text{flexibility} = \frac{1}{2} \log \left( \frac{\det P^*}{\det P} \right) + \frac{\lambda^2}{2} \| \hat{\theta} \|^2.$$  

This is the exact result. In the limit as $\lambda \to \infty$, $P^* P^{-1} = I$ and $\hat{\theta} = O(1/\lambda^2)$; thus flexibility = $O(1/\lambda^2)$, confirming that, asymptotically, flexibility decreases to zero as the penalty on the quadratic regularizer increases, although $\lambda$ might
have to be huge to overwhelm the $G^TG$ term in $P^*$.

Now consider the effect of $n \to \infty$ when $d$ is fixed. Under IID sampling,

$$n^{-1}G^TG \xrightarrow{P} H \quad (16a)$$

$$\hat{\theta} \xrightarrow{P} m \quad (16b)$$

where $H$ and $m$ are both non-random limits. Substituting into (15) and rearranging,

$$\text{flexibility} - \frac{d \log n}{2} \xrightarrow{P} \frac{1}{2} \left\{ -d(\log \sigma^2 + \log \lambda^2) + \log \det H + \lambda^2 \|m\|^2 \right\}. \quad (17)$$

The second term on the lefthand side is the Bayesian Information Criterion (BIC) penalty. Thus, for the Gaussian linear model and IID sampling,

$$\text{flexibility} = \text{BIC penalty} + O_p(1), \quad d \text{ fixed, } n \to \infty. \quad (18)$$

This large-$n$ calculation is also applicable for non-Gaussian models which satisfy the conditions for asymptotic posterior Normality (see, e.g., Schervish, 1995, sec. 7.4).

However, we advise caution. First, as already noted, we cannot presume an approximately Gaussian posterior distribution in modern practice, and therefore

$$\text{flexibility} \approx \text{BIC penalty}$$

is a poor generic approximation. Second, it is not safe to drop $O_p(1)$ terms in model comparison (Gelfand and Dey, 1994). In the Gaussian linear model, (17) shows that flexibility is approximately the sum of a term in $\log n$ and a term tending to a constant. But $\log n$ grows very slowly: as memorably expressed by Gowers (2002, p. 117), $\log n$ is about 2.3 times the number of digits in the decimal expression of $n$. It could take a truly massive $n$ for the $\log n$ term to dominate the flexibility in every one of the models in $\mathcal{M}$, as
required to be reasonably sure that flexibility and the BIC penalty would give the same outcome. In practice, choosing to approximate flexibility with the BIC penalty is effectively a choice to use a different penalty. In the terms of section 4, this is equivalent to penalizing the log-evidence. Unless the application provides a specific justification for penalizing the log-evidence, it is more defensible to estimate the evidence directly.

6 Summary

There are many issues to consider in model selection, starting with whether it is even sensible to select a single model from a set of candidates. Pragmatically, though, operating with a single data-selected model is a powerful simplification in both inference and prediction. Accepting this, the next issue is what loss function is appropriate for selecting a single model. While it is not obligatory to formulate model selection as a decision problem, it is hardly defensible to make a choice without contemplating the consequences of an error. The zero-one loss function used in this paper is a reasonable default choice, but if the candidate models live in a metric space there would be alternatives which could use the distances between models more effectively.

After these two steps, selecting the single model which maximizes the evidence is ‘hopefully’ the Bayes Rule and definitely admissible, under zero-one loss. This is the basis of the Bayesian argument for maximizing the evidence, and a reassuring feature for all statisticians.

But we have also described maximizing the evidence from a Frequentist perspective, that of penalizing fit using a measure of model complexity. The general justification of this penalization approach is heuristic—avoiding the dangers of overfitting—and therefore there cannot be a ‘right’ complexity penalty. Our contribution in this paper is to clarify that there is a unique measure of complexity, which we term ‘flexibility’, under which the log-evidence decomposes exactly into ‘fit minus flexibility’. Thus there is a
second argument for maximizing the evidence, if ‘flexibility’ is accepted as a reasonable way to quantify and penalize model complexity.

These are two arguments to the conclusion that maximizing the evidence is a sensible way to allow the data to select a single model, one Bayesian and one Frequentist. Neither argument on its own is compelling, but there must be some appeal in a criterion which has ‘cross-party’ support. As we describe in Section [1], the decision not to use flexibility as the complexity penalty should raise questions in the mind of an auditor which might be better unasked—unless the statistician has a good answer. This is a weak justification, to be sure, but model selection and model complexity are subtle and ambiguous topics, and in many applications we might welcome even a weak justification.

Finally, if flexibility is accepted as a reasonable way to quantify and penalize model complexity, then we strongly recommend estimating the evidence directly, rather than using ‘evidence equals fit minus flexibility’ and then replacing flexibility with a simpler term such as the BIC penalty.

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