Model Selection using Information Theory and the *MDL* Principle *

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Abstract

Information theory offers a coherent, intuitive view of model selection. This perspective arises from thinking of a statistical model as a code, an algorithm for compressing data into a sequence of bits. The description length is the length of this code for the data *plus* the length of a description of the model itself. The length of the code for the data measures the fit of the model to the data, whereas the length of the code for the model measures its complexity. The *minimum description length* (*MDL*) principle picks the model with smallest description length, balancing fit versus complexity. The conversion of a model into a code is flexible; one can represent a regression model, for example, with codes that reproduce the *AIC* and *BIC* as well as motivate other model selection criteria. Going further, information theory allows one to choose from among various types of non-nested models, such as tree-based models and regressions identified from different sets of predictors. A running example that compares several models for the well-known Boston housing data illustrates the ideas.

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1 Introduction

What's the best model? Certainly, the beauty of a model lies in the eyes of the beholder. Perhaps it's the "most natural" model, one that embodies our notions of cause and effect, with its form pre-ordained by our theory. Perhaps instead it's the "simplest" model, one that is easy to describe with few features determined from the data at hand. Alternatively, perhaps it's just the "most predictive" model, a model that predicts new observations more accurately than any other — a black box that churns out predictions with no obligation for interpretation.

More likely, the best model blends these attributes — theory, parsimony, and fit. If so, how should we balance these competing aims? How should we weigh the contribution of *a priori* theory versus the fit obtained by an automated search through a large database? Indeed, some criteria offer no reward for a strong theory. Naive use of the *AIC* and *BIC*, for example, implies that all regression models with the same R^2 and the same number of predictors are equivalent. Both measure the quality of a model from only its fit to the data and the count of its estimated parameters. The path that led to a model is irrelevant. To these, it does not matter whether we chose the predictors *a priori* or discovered them using stepwise regression; theory and explanation can come before or after estimation. It is little wonder that many view variable selection as mechanical optimization devoid of substantive content. The criteria described here *do* reward the investigator with a model chosen by theory, whether the theory indicate specific features of the model or opinions of what is expected.

And what of Occam's razor? Surely, if we have two regressions with the same R^2, one with two predictors and one with 20, common sense leads us to pick the model with just two predictors. But the catalog of models offered by modern statistics software is much richer than regressions with differing numbers of slopes. How, for example, can we compare a linear regression to a regression tree, especially when both obtain comparable fits to the data? We can't just count "parameters." The estimated parameters of these two types of models — estimated slopes in regression versus group averages and optimal cut-points in trees — are too different.

In what follows, I answer these questions by adopting an information theoretic view of model selection. Before delving into information theory, however, the next section describes three models for the well-known Boston housing data. These models illustrate key points throughout this paper.

2 Three Models for Housing Prices

This section describes three models for the median housing price reported in the Boston housing dataset which was created by Harrison and Rubinfeld (1978) to investigate the effects of pollution on housing values. This dataset has 14 characteristics of the 506 census tracts with housing units in the Boston SMSA in 1970. Table 1 lists the variables. The response for all three illustrative models is the median value of owner-occupied homes. Two of the models are standard OLS regressions. The third model is a regression tree. This dataset is on-line from Statlib at http://lib.stat.cmu.edu or with the software package *R* at http://cran.r-project.org/. I used the data packaged with *R*. Belsley, Kuh and Welsch (1980) popularized the use of this data in their study of regression diagnostics. Others (*e.g.* Breiman and Friedman, 1985) have used it to illustrate data mining. It has also been observed to contain censoring; the median value of homes is probably right-censored at $50,000. I will not explore these issues further.

I fit these models to a subset of 50 tracts selected randomly from the full collection.[1] The reason for restricting the estimation to a subset is to weaken the effects of the predictors and thereby make the problem of model selection more difficult. When fit to the full dataset, an OLS regression of *MEDV* on the 13 remaining variables has an R^2 of 74% with 11 predictors having absolute t-ratios larger than 3. When fit to the subset, the effects become subtle; only three predictors have a t-ratio larger than 3 in magnitude. Variable selection is more challenging when the effects are subtle; virtually any method works in the presence of a strong, obvious signal.

The two illustrative regression models are the same, but I want to make a distinction in how they were found. Suppose that my research concerns determinants of the value of housing. In particular, I have a theory that proposes that young families with several children drive up demand for larger houses, and that this group likes to have their big homes near good schools in safe communities. The model shown in Table 2 embodies these ideas; the interaction between the number of rooms and the pupil-teacher ratio *RM*PTRATIO* captures the notion that big houses lose value if they are near crowded schools. One can imagine that I could have proposed the form of this model (*i.e.*, picked the predictors) prior to looking at the data; its form originated in my theory rather than

[1] I used the `sample` function from *R* to pick these, avoiding documented outliers. To reduce the effects of outliers, I set aside 6 tracts (rows 366 and 369 – 373) from the full data set prior to sampling. The 50 sampled tracts are rows 18, 22, 25, 37, 43, 44, 46, 51, 58, 62, 69, 71, 74, 78, 90, 93, 100, 112, 126, 131, 135, 152, ,161, 170, 181, 190, 200, 203, 204, 212, 213, 221, 222, 235, 236, 268, 316 317, 321, 322, 391, 394, 397, 398, 417, 445, 462, 489, 495, 503 in the Boston data distributed with *R*.

Table 1: *The Boston housing dataset contains 14 variables that describe the 506 census tracts in the Boston SMSA in 1970, excluding tracts with no housing units. (Harrison and Rubinfeld, 1978; Belsley et al., 1980). Available on-line from Statlib (http://lib.stat.cmu.edu) or as part of the R software package (http://cran.r-project.org).*

MEDV	median value of owner-occupied homes in $1000's (response)
AGE	proportion of owner-occupied units built prior to 1940
BLACK	$1000(B - 0.63)^2$ where B is the proportion of blacks by town
CHAS	Charles River dummy variable (1 bounds river; 0 otherwise)
CRIM	per capita crime rate by town
DIS	weighted distances to five Boston employment centres
INDUS	proportion of non-retail business acres per town
LSTAT	percentage lower status of the population
NOX	nitric oxides concentration (parts per 10 million)
PTRATIO	pupil-teacher ratio by town
RAD	index of accessibility to radial highways
RM	average number of rooms per dwelling
TAX	full-value property-tax rate per $10,000
ZN	proportion of residential land zoned for lots over 25,000 sq.ft.

Table 2: *Regression model for a subset of 50 cases from the Boston housing data. The RMSE of the model for median house value MEDV is 2.69 with 45 d.f. and* $R^2 = 0.92$.

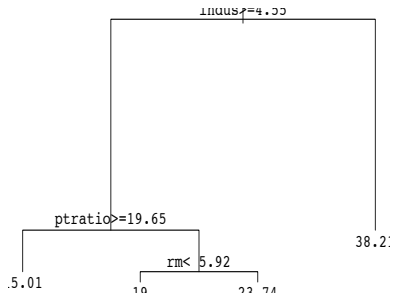
Variable	OLS Slope	SE	$\|t\|$	p-value
Intercept	-100.12	29.08	3.4	0.0013
RM	23.18	4.40	5.3	0.00000
RM*PTRATIO	-0.88	0.26	3.4	0.0015
CRIM	-1.01	0.14	7.4	0.00000
PTRATIO	4.33	1.69	2.6	0.014

from the data itself.

The second regression is identical to the first summarized in Table 2, but reaches this fit by a different means. Rather than being the product of theory, the second model is the result of an automatic search for structure, in this case, a stepwise regression. Indeed, not being an expert in housing values, I obtained the model in just this way. Using the `step` function in *R*, I ran a stepwise regression using the default parameters and let it choose 4 predictors. The stepwise selection was allowed to pick any of the possible interactions and quadratics among the predictors, and from these chose the single interaction between *RM* and *PTRATIO*. I limited the model to 4 predictors in order to be able to interpret "theoretically" the fitted model. Although stepwise was allowed to both add or delete variables, it proceeded by adding 4.

The third model is a regression tree. Recursive partitioning identifies groups of observations that share similar values of the response when compared to others. The result of applying recursive partitioning to a continuous response like *MEDV* is a so-called regression tree like that shown in Figure 1. Such models, along with similar models used for classification, were labeled CART models after the title of the book by Breiman, Friedman, Olshen and Stone (1984). The `rpart` function of *R* produced the regression tree shown in Figure 1, with the default rules stopping the recursive splitting (Venables and Ripley, 2002). The algorithm first divided the 50 tracts using the industrialization measure, separating those for which $INDUS \geq 4.55$ from the others. Among tracts with larger industrialization, it further split using *PTRATIO* at a value of 19.65. Finally, it split those with smaller *PTRATIO* into two groups, splitting at $RM = 5.92$. Taking the means of the resulting four "leaf nodes" at the bottom of the tree in Figure 1 as fitted values, the RMSE of this model is almost 4.0, larger than the RMSE for the stepwise regression (about 2.7).

Figure 1: *Regression tree for the median house price, estimated using the* `rpart` *function of R. The collective standard deviation of the residuals about the averages of the 4 leaf nodes is 3.96.*



Which of these three models is the best? Methods that select a model while ignoring how it came into being cannot distinguish the two regressions. Methods that just count parameters run into problems when comparing either regression to the tree. How many parameters are in the regression tree in Figure 1? The fit at each leaf node is an average, but how should we treat the splitting points that define the groups? Can we treat them like other parameters (slopes and averages), or should we handle them differently? Research suggests that we need to assess such split points differently. For example, Hinkley's early study of inference for the break point in a segmented model (Hinkley, 1970) suggests that tests for such parameters require more than one degree of freedom.

The information theoretic view of model selection allows one to compare disparate models as well as account for the origin of the models. The process leading to the model is, in essence, part of the model itself, allowing *MDL* to reward a theoretical model for its *a priori* choice of predictors. The information theoretic view is also flexible. One can compare different types of models, such as the illustrative comparison of a regression equation to a regression tree.

3 A Brief Look at Coding

Good statistical models "fit well." Although the notion of fit varies from one model to another, likelihoods offer a consistent measure. By associating each model with a probability distribution, we can declare the best fitting model as the one that assigns the largest likelihood to the observed

data. If the model has parameters, we set their values at the maximum likelihood estimates.

Coding offers an analogous sense of fit. A good code is an algorithm that offers high rates of data compression while preserving all of the information in the data. The best code compresses data into the shortest sequence of bits. If we think of our response as occupying a file on a computer, then the best code for this response is the algorithm that compresses this file down to the smallest size — while retaining information that allows us to recover the original data. The trick in seeing how information theory addresses model selection is to grasp how we can associate a statistical model with a scheme for coding the response.

Suppose that I want to compress a data file, say prior to sending it as an attachment to an e-mail message. The heuristic of "sending a message to a receiver" is valuable in thinking about coding data; it is essential to identify what the receiver already knows about the data and what I have to tell her. If I can find a way to reduce the number of bits used to represent the most common patterns in the data, then I can reduce the overall size of the message. Obviously, I have to be able to do this unambiguously so as not to confuse the recipient of my e-mail; there must be only one way for her to decode the attachment. Such representations are said to be *lossless* since one can recover the *exact* source file, not just be close. Alternative "lossy" codes are frequently used to send sounds and images over the Internet. These offer higher rates of compression but do not allow one to recover the exact source image.

For the example in this section, the data to be compressed is a sequence of n characters drawn from the abbreviated 4-character alphabet *a*, *b*, *c*, and *d*. Since coding is done in the digital domain, I need to represent each character as a sequence of bits, 0s and 1s. The standard ASCII code for characters uses 8 or 9 bits per letter – quite a bit more than we need here since we have only 4 possibilities – but a simplified version works quite well. This fixed-length code (Code F) appears in the second column of Table 3. Code F uses two bits for each of the four possible values. For example, with $n = 5$, the attached sequence of 10 bits 0100000011 would be decoded by the recipient as

$$0100001100 = 01\ 00\ 00\ 11\ 00 \quad \stackrel{\text{decode}}{\longrightarrow} \quad b\,a\,a\,d\,a$$

where I use spaces to make the encoded data easier for us to read, but are not part of the code. With Code F, it takes $2n$ bits to send n of these letters, and the attached data is easy to recover.

More knowledge of the data allows higher compression with no loss in content. More knowledge in coding comes in the form of a probability distribution for the data. For example, suppose that

Table 3: *Sample codes for compressing a random variable that takes on four possible values a, b, c, and d with distribution p(y). Code F uses a fixed number of bits to represent each value, whereas Code V varies the number of bits as given by* $-\log_2 p(y)$.

Symbol y	Code F	Code V	$p(y)$
a	00	0	$1/2 = 1/2^1$
b	01	10	$1/4 = 1/2^2$
c	10	110	$1/8 = 1/2^3$
d	11	111	$1/8 = 1/2^3$

the data are a sample $Y_1, Y_2, \ldots, Y_n$ of grades that have the distribution

$$p(y) = \begin{cases} 1/2 & \text{if } y = a\,, \\ 1/4 & \text{if } y = b\,, \\ 1/8 & \text{if } y = c\,, \\ 1/8 & \text{if } y = d\,. \end{cases} \tag{1}$$

(Evidently, grade inflation is prevalent.) Code V in the third column of Table 3 conforms to these probabilities. Code V uses a varying number of bits to represent the 4 symbols, with the number of bits set to the negative of the base 2 log of the probability of each symbol. Thus, characters that occur with high probability get short codes. For example, Code V uses only 1 bit ($1 = -\log_2 1/2$) to represent the most likely symbol a, but uses three bits for the least likely symbols c and d.

Because of the varying length of the codes assigned by Code V, it may not be clear how to decode the compressed data. To see how this works, let's return to the previous example that encodes b, a, a, d, and a. First, we'll encode the data, then see how the receiver decodes it. Encoding is simply a matter of concatenating the bits given in the third column of Table 3:

$$b\,a\,a\,d\,a \quad \stackrel{\text{encode}}{\longrightarrow} \quad 10\ 0\ 0\ 111\ 0$$

Notice that the encoded message is shorter than the message obtained with Code F, requiring 8 bits rather than 10. The receiver of the message reverses this process. Basically, she parses the sequence of bits one at a time until she matches one of the codes in the third column of Table 3. The first character is a 1, which does not match any of the codes. The first two characters form the sequence 10 which is the code for b. The next character is a 0, which matches the code for a.

Continuing in this fashion, she can recover the original sequence. Keep in mind, however, that the receiver has to know Code V for this scheme to work.

Although Code V obtains higher compression for the sequence *baada*, it should also be apparent that Code F compresses some other sequences better. For example, to encode *dccab* requires 10 bits with Code F but consumes 12 bits for Code V. Code V is two bits better for one data series, but two bits worse for another. Why bother with Code V? The answer lies in the underlying probabilities. If the characters to be compressed are indeed a random sample with the distribution $p(y)$ given in (1), then the probability of the sequence for which Code V compresses better is

$$\begin{aligned} \mathrm{P}(baada) &= p(b)\,p(a)\,p(a)\,p(d)\,p(a) \\ &= \tfrac{1}{4}\,\tfrac{1}{2}\,\tfrac{1}{2}\,\tfrac{1}{8}\,\tfrac{1}{2} \\ &= \tfrac{1}{2^2}\,\tfrac{1}{2}\,\tfrac{1}{2}\,\tfrac{1}{2^3}\,\tfrac{1}{2} \\ &= 1/2^8\ . \end{aligned}$$

The probability of the sequence for which Code V does worse is 16 times smaller:

$$\begin{aligned} \mathrm{P}(dccab) &= p(d)\,p(c)\,p(c)\,p(a)\,p(b) \\ &= \tfrac{1}{2^3}\,\tfrac{1}{2^3}\,\tfrac{1}{2^3}\,\tfrac{1}{2}\,\tfrac{1}{2^2} \\ &= 1/2^{12}\ . \end{aligned}$$

Code V works well for sequences that are more likely according to the associated distribution $p(y)$. Higher probability means a shorter code. Code V represents *baada* using 8 bits, which is the negative of the log (base 2) of the likelihood of this sequence under the model $p(y)$,

$$\begin{aligned} \text{Length of Code V for } baada &= \ell(baada) \\ &= -\log_2 P(baada) = 8\ . \end{aligned}$$

Similarly, $\ell(dccab) = -\log_2 P(dccab) = 12$.

The Kraft inequality from information theory strengthens the connection between the length of a code for a sequence of symbols and the probability of those symbols. The Kraft inequality implies that however we decide to encode the characters in our message, we cannot have too many short codes because (Section 5.2, Cover and Thomas, 1991)

$$\sum_y 2^{-\ell(y)} \le 1\ , \tag{2}$$

where the sum runs over all possible values for y and $\ell(y)$ denotes the number of bits required to encode y. A code is said to be "Kraft-tight" if it attains this upper bound; both codes in Table 3

are Kraft-tight. We can thus interpret $2^{-\ell(y)}$ as a probability. That is, the Kraft inequality allows us to *define* a probability from the lengths of a code. If a code is not Kraft-tight, it essentially has reserved symbols for characters that cannot occur. Such codes can be improved by removing the unnecessary terms. For example, using the 8-bit ASCII code for our 4 character problem would not produce a Kraft-tight code.

Codes derived from a probability distribution obtain the best compression of samples from this distribution. The entropy of a random variable determines the minimum expected code length. The entropy of a discrete random variable $Y \sim p(y)$ is

$$H(Y) = E \log_2 1/p(Y) = \sum_{y \in \mathcal{Y}} p(y) \log_2 \frac{1}{p(y)} . \tag{3}$$

It can be shown that if $\ell(y)$ is the length of *any* lossless code for the random variable Y, then (Sections 5.3-5.4, Cover and Thomas, 1991)

$$E\,\ell(Y) \geq H(Y) .$$

Thus the fixed-length Code F is optimal if the 4 values a, b, c and d are equally likely whereas Code V is optimal if the probabilities for these symbols are 1/2, 1/4, 1/8, and 1/8, respectively. What happens if one uses a code that does not conform to the underlying probabilities? The code is longer, on average, than it needs to be.

For the illustrations, both probabilities have the convenient form $p(y) = 2^{-j}$ with j an integer so that the code lengths are readily apparent and integers. In other cases, the method known as *arithmetic coding* allows one to compress data within one bit of the entropy bound even when the probabilities lack this convenient form. Given that one knows the true generating frequencies, arithmetic coding allows one to compress $Y_1, \ldots, Y_n$ into a code whose expected length is bounded by $1 + n\,H(Y_i)$ (Langdon, 1984). As we continue, I will also ignore the need for an actual code to have an integer length, using what is often called the *idealized* length (Barron, Rissanen and Yu, 1998).

To recap, the best code for a random variable $Y \sim p$ has idealized length

$$\ell(y) = -\log_2 p(y) , \tag{4}$$

and the length of this code for representing a sample of n independent responses $Y_1, Y_2, \ldots, Y_n \sim p$ is the negative log-likelihood,

$$\ell(y_1, \ldots, y_n) \;\; = \;\; -\log_2 L(y_1, \ldots, y_n)$$

$$= \quad -\log_2 p(y_1)\, p(y_2) \cdots p(y_n)\ . \tag{5}$$

The expected length of any other code for Y exceeds the resulting entropy bound (3). Analogous properties hold for continuous random variables like the Gaussian or Cauchy as well. Even though the likelihood $L(y_1, \ldots, y_n)$ for a continuous random variable no longer gives probabilities, the code length retains the convenient form seen in (4). To get a sense for how coding applies to continuous random variables, think of encoding a discrete approximation that rounds the continuous random variable to a certain precision. Cover and Thomas (1991) (Section 9.3) shows that the length of the code for the rounded values is the log-likelihood of the continuous data plus a constant that grows as one keeps more digits. One can handle dependent sequences by factoring the log-likelihood as

$$\ell(y_1, \ldots, y_n) = -\log_2 \left(p(y_1)\, p(y_2 \mid y_1)\, p(y_3 \mid y_1, y_2) \cdots p(y_n \mid y_1, \ldots, y_n)\right)\ .$$

Thus, we can associate a model with a code by finding a code matched to the likelihood implied by the model. The best code and the best model share a common heritage – both maximize the likelihood for the observed data. But this presents a problem for model selection. If coding just maximizes the likelihood, how does it avoid overfitting? The answer requires that we take a broader look at our original task.

4 The Minimum Description Length Principle

Just because we can compress data optimally by maximizing its likelihood does not mean that the recipient of our message can recover the original data. For this task, she needs to know how we encoded the data — she must know our model. The codes described here convey the model to her in a straightforward fashion. They include the parameter estimates as part of the message to the receiver, prefixing the compressed data. Hence, such messages are called *two-part codes*. The inclusion of the model as part of our message has a dramatic effect. A regression model with 10 estimated slopes might fit well and offer high compression of the data, but it also requires us to convey 10 estimated parameters to the receiver. A simpler regression with just two estimated slopes need only add 2. Unless the gain in compression (*i.e.*, the increase in the likelihood) is enough to compensate for the 8 additional estimates, the simpler model may in fact produce a shorter message.

Rissanen's *minimum description length* (*MDL*) principle (Rissanen, 1978) formalizes this idea. The description length of a fitted model is the sum of two parts.[2] The first part of the description

[2]Stochastic complexity, introduced in Rissanen (1986), enhances the *MDL* principle by removing redundancies

length represents the complexity of the model. This part encodes the parameters of the model itself; it grows as the model becomes more complex. The second part of the description length represents the fit of the model to the data; as the model fits better, this term shrinks. A precise definition requires a bit of notation. Let M_θ denote a parametric model indexed by a parameter vector θ, and let $L(\cdot \mid M_\theta)$ denote the likelihood implied by this model. Also, let Y denote n observations $y_1, y_2, \ldots, y_n$ of the response. Since we obtain the shortest code for the data by maximizing the likelihood, the MLE for θ, say $\hat{\theta}(Y)$, identifies the optimal model. The resulting description length of such a model is

$$\mathcal{D}(Y; M_{\hat{\theta}(Y)}) = \ell(M_{\hat{\theta}(Y)}) - \log_2 L(Y \mid M_{\hat{\theta}(Y)}) \; . \tag{6}$$

The *MDL* principle picks the model with the minimum description length. To compute the description length, though, we need to determine how many bits are required to encode the model $M_{\hat{\theta}(Y)}$ itself.

At this point, the flexibility and Bayesian flavor of coding emerge. Recall that every code embodies a probability distribution. Thus, any code for the model $M_{\hat{\theta}(Y)}$ also implies a probability distribution, one for the model itself. In the case of parametric models such as regression, the code must give the parameters that identify the specific model. The length of this code depends on which values we *expect* for $\hat{\theta}(Y)$. Choose poorly and one faces a rather large penalty for adding a parameter to the model.

Before describing how to encode the whole model, we need to consider first how to encode a single parameter. Since $\hat{\theta}(Y)$ is unlikely to be an integer, it is not obvious how to represent $\hat{\theta}(Y)$ with a discrete code. Fortunately, Rissanen (*e.g.* Rissanen, 1989, Section 3.1) shows that we can, in fact, round the MLE with little loss in data compression. The idea is to round $\hat{\theta}(Y)$ to the nearest coordinate of the form $\theta_0 + \tilde{z}\,\mathrm{SE}(\hat{\theta}(Y))$ for integer $\tilde{z}$ and define the estimator

$$\tilde{\theta}(Y) = \theta_0 + \mathrm{SE}(\hat{\theta}(Y)) \left\langle \frac{\hat{\theta}(Y) - \theta_0}{\mathrm{SE}(\hat{\theta}(Y))} \right\rangle = \theta_0 + \mathrm{SE}(\hat{\theta}(Y)) \, \langle \, z_{\hat{\theta}(Y)} \, \rangle \; , \tag{7}$$

where $\langle \, x \, \rangle$ denotes the integer closest to x. The rounded estimator lies within half of a standard error of the *MLE*, falling on the grid centered at a default value θ_0 (typically zero) plus a multiple $\langle \, z_{\hat{\theta}(Y)} \, \rangle$ of the standard error. Rounding a vector of estimates is considerably more complex but follows the this paradigm: approximate the MLE using a grid resolved to the nearest standard error (Rissanen, 1983).

inherent in a two-part code. While theoretically appealing, the results for model selection are essentially identical. The accompanying idea, known as parametric complexity, introduces other complications (Foster and Stine, 2003).

This rounding has negligible effect on the length of the second part of the code. If we encode the data using $\tilde{\theta}$ rather than the *MLE*, the length of the compressed data grows by less than a bit. (This result is perhaps one of the strongest arguments for showing rounded estimates in presenting statistical output. All of those superfluous digits offer no help in coding the data.) So, in practice, the description length is computed not as in (6) but rather using rounded estimates to denote the model,

$$\mathcal{D}(Y; M_{\hat{\theta}(Y)}) \;\approx\; \ell(M_{\tilde{\theta}(Y)}) - \log_2 L(Y \mid M_{\hat{\theta}(Y)}) \,. \tag{8}$$

All that is left is to encode the integer z-score. I will save that for the next section when we consider regression.

Before moving on to regression, it is worthwhile to step back and note the similarity of *MDL* to other methods of model selection. In particular, many criteria, such as *AIC* and *BIC*, select the model that minimizes a penalized likelihood. For example, if $\dim(\theta)$ denotes the dimension of a parameter, then *AIC* picks the model that minimizes

$$AIC(\hat{\theta}) = \dim(\hat{\theta}) - \log L(Y \mid M_{\hat{\theta}}) \,. \tag{9}$$

Comparing (9) to the description length in (8), we see that the code length required to represent the model, $\ell(M_{\tilde{\theta}(Y)})$, plays the role of a penalty factor. In this sense, one can think of information theory as a means to generating a richer class of penalties.

5 Encoding a Regression Model

Two choices determine the penalty $\ell(M_{\tilde{\theta}(Y)})$ for model complexity in the *MDL* criterion. First, we have to decide how to encode the rounded z-scores that locate the rounded parameter estimate $\tilde{\theta}(Y)$. Second, we have to associate the estimates with predictors. This section addresses coding a parameter, and the next deals with identifying the predictors.

The choice of a code for the rounded estimates is equivalent to the dilemma faced by a Bayesian who must choose a prior distribution. A large-sample approach leads to the association between *MDL* and *BIC*. Rissanen (Section 3.1, Rissanen, 1989) proposes the following code. If $\tilde{\theta} = \theta_0$, then encode $\tilde{\theta}$ using 1 bit, say 0. Alternatively, start the code with a 1 and then identify $\tilde{\theta}$ by giving its position in a large, albeit finite, grid that has on the order of $\sqrt{n}$ positions. To encode $\tilde{\theta} \neq 0$ thus requires about $1 + \frac{1}{2}\log_2 n$ bits, 1 to say that the estimate is not θ_0 and $\frac{1}{2}\log_2 n$ for the grid position. This coding for $\tilde{\theta}$ implies that we have a "spike-and-slab" prior distribution for

the parameter. The code devotes half of its probability (a one-bit code) to the null value θ_0 (the spike) and distributes the other half of the probability uniformly over a large range (the slab). The resulting *MDL* criterion for the best model minimizes

$$\mathcal{D}_s(Y; M_{\tilde{\theta}(Y)}) = \dim(\theta) \left(1 + \tfrac{1}{2} \log_2 n\right) - \log_2 L(Y \mid M_{\hat{\theta}(Y)}) \; . \tag{10}$$

Since the leading complexity term shares the form of the *BIC* penalty, it may appear that *MDL* and *BIC* are equivalent. They are indeed equivalent under the spike-and-slab prior for $\tilde{\theta}$, but other priors give different results.

An important theme in the development of coding has been the gradual shift from the use of optimal priors tailored to specific problems to so-called *universal priors* that work well over a wide range of distributions. Analogous to robust estimates in statistics, universal priors encode about as well as the best prior, but do not require that one know the "true" model. This sense of robustness makes universal priors well-suited to model selection since we would prefer to make as few assumptions as possible, but retain whatever efficiencies are possible. Building on the work of Elias (1975), Rissanen (1983) proposed a universal prior for representing the rounded MLE $\tilde{\theta}$. Like the spike-and-slab prior, Rissanen's universal prior also invests half of its probability at the null value θ_0. Rather than evenly dividing the remaining probability over a wide slab, the universal prior drops off ever so slowly. The idealized length of the universal code for an integer $j \neq 0$ is approximately (Elias, 1975; Rissanen, 1983)

$$\ell_u(j) = 2 + \log_2^+ |j| + 2 \log_2^+ \log_2^+ |j| \; , \tag{11}$$

where $\log_2^+(x)$ is the positive part of the log function, so that $\log_2^+(x) = 0$ for $|x| \leq 1$. For example, $\ell_u(\pm 1) = 2$, $\ell_u(\pm 2) = 3$, and $\ell_u(3) \approx 4.91$. Though it decays slowly (its tail decays like that of a code designed for representing the log of a Cauchy random variable), $\ell_u(j)$ concentrates more probability near θ_0 than the spike-and-slab prior. If we let

$$\tilde{z}_j = \langle\, (\hat{\theta}_j - \theta_{0,j})/\mathrm{SE}(\hat{\theta}_j) \,\rangle, \quad j = 1, \ldots, \dim(\theta) \tag{12}$$

denote the rounded z-scores that locate $\tilde{\theta}$, then we can write this description length as

$$\mathcal{D}_u(Y; M_{\tilde{\theta}(Y)}) = \sum_{j=1}^{\dim(\theta)} \ell_u(\tilde{z}_j) - \log_2 L(Y \mid M_{\hat{\theta}(Y)}) \; , \tag{13}$$

The analysis in Foster and Stine (1999) shows that this description length leads to a version of *MDL* that resembles *AIC*, in effect penalizing the likelihood by a multiple of the dimension of the parameter vector, *without* the $\log_2 n$ term appearing in (10).

The universal prior seems more suited to regression than the spike-and-slab prior. With θ denoting the slopes in a regression, it is natural to set the null value $\theta_0 = 0$. The spike-and-slab prior offers an "all or nothing" representation of the parameter space: either θ is exactly zero or it could be anywhere. In comparison, the universal prior holds 0 as the most likely coefficient, but expects non-zero slopes to be relatively close to the null value.

Returning to the original problem of picking the best from among 3 models for the median housing value, we can now compute description length for the first regression model. Since the structure of this theoretically-motivated model (*i.e.*, the choice of its predictors) is known in advance, I can assume that both sender and receiver (in the coding sense) know which variables are in the model. Thus, the sender need only send the encoded estimates $\tilde{\theta}$ in the first part of the code for Y. Assuming a normal distribution for the errors,[3] the length of the second part of the code (the part that represents the encoded data) is the log-likelihood (omitting constants that do not affect selection)

$$\begin{aligned} -\log_2 L(Y \mid M_{\hat{\theta}(Y)}) &= \tfrac{n}{2}\log_2(RSS(\hat{\theta})/n) \\ &= \tfrac{50}{2}\log_2(326.9/50) \\ &= 67.7 \text{ bits} , \end{aligned}$$

where $RSS(\hat{\theta})$ is the residual sum-of-squares for the fitted model. To this we have to add the number of bits required for the model, here a list of the estimated slopes. For this example, I use universal codes. Including the intercept, this length is the sum of the universal code lengths for the rounded t-statistics in Table 2,

$$\begin{aligned} \ell(M_{\tilde{\theta}(Y)}) &= \ell_u(-3) + \ell_u(5) + \cdots + \ell_u(3) \\ &= 4.91 + 6.75 + \cdots + 4.91 \\ &= 29.3 \text{ bits} . \end{aligned}$$

The description length for the theoretical regression is then

$$\mathcal{D}(\text{theoretical regression}) = 67.7 + 29.3 = 97.0 \text{ bits} .$$

The second regression, which results from stepwise selection, introduces a new aspect to the calculation of the description length, and so I will handle it in the next section.

[3]Coding requires that a model offer a probability distribution for the data. I will use the normal distribution here, but one can substitute any other likelihood as suits the problem.

6 Allowing for Variable Selection in Regression

The description length obtained in the prior section *presumes* that the receiver of the encoded data *knows* which predictors to associate with the encoded estimates. Otherwise, the first part of the code is useless. If the choice of regressors is unknown in advance and determined by a search of the data itself, as in stepwise regression, then we have to identify which predictors have been chosen.

An obvious way to identify the predictors is to include in the message a boolean vector of 0s and 1s. Suppose that we and the receiver share an ordered list of the p possible variables that we might choose as predictors. Then, we can further prefix our message to the receiver with p bits, say $\gamma = \{\gamma_1, \gamma_2, \ldots, \gamma_p\}$, that identify the $q = \sum \gamma_j$ predictors in the model. If $\gamma_j = 1$, then the jth predictor is in the model; otherwise, $\gamma_j = 0$.

The addition of this prefix rewards models whose predictors have been identified from an *a priori* theory rather than a data-driven search. The illustrative stepwise regression picks from $p = 103 = 13 + 12 + \binom{13}{2}$ possible regressors (13 linear terms, 12 quadratics after removing *CHAS* which is a dummy variable, plus the interactions). Taking the direct approach, we have to add 103 bits (consisting of 99 0s and four 1s) to the description length of the theoretical model to identify the four predictors, and so

$$\begin{aligned} \mathcal{D}(\text{stepwise, with interactions}) &= p + \mathcal{D}(\text{theoretical regression}) \\ &= 103 + 97.0 = 200.0 \text{ bits} . \end{aligned}$$

The larger the collection one searches, the longer γ becomes and the greater the penalty. *MDL* rewards theory by avoiding the need to include γ as part of the model. A stepwise model must fit far better than the theoretical model to overcome this penalty.

The size of the penalty in this example suggests that perhaps we'd have done better by searching a smaller subset of predictors. For example, perhaps the description length would have been smaller had we searched only linear predictors rather than considering second-order effects. If we restrict the stepwise search to the 13 candidates in the Boston data, the four-predictor model identified by the `step` procedure (with predictors *RM*, *CRIM*, *PTRATIO*, and *BLACK*) has residual sum-of-squares 371.5 (compared to 326.9 with interactions). Because this search is more restrictive, the description length for this model is less than that of the previous stepwise regression, even though the fit deteriorates. This model requires only 13 bits to indicate which predictors appear in the model,

$$\mathcal{D}(\text{stepwise, no interactions}) = 13 + 27.0 + 25 \log_2(371.5/50)$$

$$= \quad 13 + 27.0 + 87.3 = 127.3 \text{ bits.}$$

The description length is so much smaller because, although it does not compress the data so well (it has a larger *RSS*), the model is easier to describe. We need identify which of the 13 predictors we used rather than which of the 103 second-order predictors. Notice also how easily we have just compared two non-nested regression models.

To this point, I have used a simple scheme to indicate which predictors appear in the model: add the p indicators in γ. While straightforward, this approach implies that we expect fully half of the p predictors to be in the model. The intuition for this claim again lies in the relationship between a code and a probability. We can think of each γ_j as boolean random variable. Our use of 1 bit for $\gamma_j = 0$ and 1 bit for $\gamma_j = 1$ implies that we think the choices are equally likely, occuring with probability 1/2. From this perspective, the use of the 103 bit prefix for the quadratic stepwise model seems silly; no one would anticipate 50 of these variables to be in the model.

When we expect few of the possible predictors to join the model (as seems appropriate when casting a large net), we can identify those chosen in a rather different fashion, one that offers a shorter code if indeed the predictors are sparse. The scheme is most obvious if we think of encoding a model that picks just 1 out of a large collection of p possible predictors. Rather than identify this variable using a long vector of p bits, we can simply encode its index, say j, using about $\log_2 p$ bits. That's a lot shorter code, $\log_2 p$ versus p, one that reflects our expectation of a model with few predictors.

Applied to the second-order stepwise model, this approach leads to a smaller description length. Since $p = 103$, we can identify each predictor using 7 bits (6 for the index plus 1 to tell if this is the last predictor in the model). The length of the prefix thus drops from 103 down to 28, and the description length for the second-order stepwise model becomes less than that of stepwise linear model and much closer to that obtained by the theoretical model. It would appear that of we use a better code that recognizes sparseness, we can "afford" to search through second-order features after all. An asymptotically equivalent criterion for model selection is the risk inflation criterion *RIC* (Foster and George, 1994). The motivation for *RIC* is rather different (a minimax argument); however, the development of *RIC* also emphasizes the problem of picking one or two predictors from a large collection of variables. *RIC* works particularly well in data-mining applications, allowing stepwise regression to compete with classification engines such as C4.5 (Foster and Stine, 2002).

Although the search of second-order effects can conceivably pick any of 103 predictors, R adheres to the so-called principle of marginality. This condition requires that a regression with an

interaction, say, $X_1 * X_2$, must also include both main effects X_1 and X_2. For example, the illustrative regression in Section 2 has the interaction *RM*PTRATIO* as well as both *RM* and *PTRATIO*. Fox (1984) (Section 2.1.3 and elsewhere) discusses the rationale for the principle of marginality. Because *R* restricts its search in this way, the 103 bit prefix allows for many models that will never be identified, such as one that consists only of interactions. The use of a 103-bit prefix is rather like using the ASCII character code to represent the four symbols *a*, *b*, *c* and *d* in the example of Section 3; the prefix has reserved symbols for representing models that cannot occur. Adherence to the principle of marginality has no effect on the use of *AIC* or *BIC* because both count only the number of parameters, ignoring the number of predictors that have been considered.

As introduced above, *RIC* shares this flaw. Coding, however, suggests a remedy for this problem and leads to a yet shorter description length for the model. As we'll see in Section 8, a shorter prefix allows us to pick a model with more predictors since the shorter prefix amounts to a smaller penalty for complexity. *RIC* identifies the predictors using a sequence of indices, with a continuation bit indicating if more indices follow. Let p_1 denote the number of original predictors; $p_1 = 13$ for the Boston dataset. To identify one of these requires about $\log_2 p_1$ bits. For the illustrative model, we can identify each main effect using 5 bits (4 for the index, one for the continuation bit) rather than 7. We can then identify the interactions by indicating which, if any, of the prior main effects form interactions. Since we have only three main effects, we can also identify an interaction using $2(2) + 1 = 5$ bits. (We need two bits to identify each of the main effects, plus a continuation bit to say if more interactions follow.) For the illustrative second-order stepwise model, this code reduces the length of the *RIC* prefix from 28 down to $3(5) + 5 = 20$ bits. I will denote this variation on *RIC* as RIC^*

Table 4 summarizes the description lengths of these regression models (as well as the regression tree described in the next section). For each model, the table shows the number of bits required to

1. identify *which* predictors appear in the model,
2. encode the estimated *slopes* of these predictors, and
3. compress the *data* for the response itself.

Though none of the models attain the description length of the theoretical model, a stepwise search can come quite close when the model is represented by a code well matched to the sparseness of the context and the structure of the fitted model.

Table 4: *Components of the description length for 5 models of the value of housing in a sample of 50 tracts from the Boston housing data. For each model, p denotes the number of possible predictors. The components of description length identify which of the p predictors appear in the model, give the estimated slopes of these, and finally the length of the compressed data.*

Regression Models

Model	*RSS*	p	$\mathcal{D}$	which	slopes	data
Stepwise, linear	371.5	13	127.3 =	13	+ 27.0	+ 87.3
Theoretical	240.5	4	97.0 =	0	+ 29.3	+ 67.7
Stepwise, quadratic, γ	240.5	103	200.0 =	103	+ 29.3	+ 67.7
Stepwise, quadratic, *RIC*	240.5	103	125.0 =	28	+ 29.3	+ 67.7
Stepwise, quadratic, *RIC**	240.5	103	117.0 =	20	+ 29.3	+ 67.7

Regression Tree

RSS	p	$\mathcal{D}$	nodes	splits	means	data
768.4	13	136.7 =	7	+ 24	+ 7.1	+ 98.5

7 *MDL* for a Regression Tree

The code for a regression tree resembles those we have seen for regression. We have to identify the variables, represent the estimated parameters (here, averages of subsets of the response), and finally add the length for the compressed data. Trees also require that we locate the split-point for any groups that are divided. To guide the coding, here is the summary produced by `rpart` for the regression tree shown in Figure 1:

```
1) root 50 3950.0 23.0
  2) indus>=4.55 41  951.0 19.6
    4) ptratio>=19.6 15  209.0 15.0 *
    5) ptratio< 19.6 26  239.0 22.3
      6) rm< 5.92 8   24.9 19.0 *
      7) rm>=5.92 18   90.1 23.7 *
  3) indus< 4.55 9  445.0 38.2 *
```

The data shown for each node identifies how that node was formed from its parent node and gives the number of tracts, sum-of-squares, and average of the values in the node. For example, prior

to splitting, the data at the "root node" (Node 1) consists of 50 observations with a total sum of squares 3950 around a mean value 23.0. Indentation conveys the shape of the tree. The following description length has many of the features that are used in coding a classification tree (Manish, Rissanen and Agrawal, 1995), but is adapted to coding a continuous response. A version of *MDL* for building classification trees has even been patented (Rissanen and Wax, 1988).

To encode this tree, we begin at the top. The root node splits into two nodes defined by whether $INDUS \leq 4.55$. In the same way that we identified the predictors in regression, we can identify that the variable being split is *INDUS* using 3 bits, plus one more bit to indicate whether this is a splitting node or a terminal node. We can locate the split itself by indicating how many observations fall, say, into the "left" node; that requires 5 bits since $\log_2 64 = 6$. Node 3 is terminal, so we can encode it immediately. We need only indicate that it is a terminal node, identify its mean to the available accuracy, and compute the number of bits needed for the data. Lacking a sense for the location of this average (*i.e.*, how would we choose θ_0), I use a uniform prior like that described for the spike-and-slab prior. With only $n_3 = 9$ observations in Node 3, we require on the order of $\frac{1}{2}\log_2 9$ bits to identify the mean to adequate precision. The data for this node require (again, dropping constants that do not affect the comparison of models and assuming normality) $(9/2)\log_2(RSS/50) = 4.5 \log_2 15.4 = 17.8$ bits. Since Node 2 is not a terminal node, we move down to the next level.

We repeat the initial procedure as we work our way down the tree. We identify the next split again using $8 = 3 + 5$ bits (3 to pick the variable, 5 to locate the split). Node 4 is terminal, and it takes $\frac{1}{2}\log_2 n_4$ for its average and $(15/2)\log_2 15.4 = 29.6$ bits for the data. Node 5 leads to yet another split, costing 9 more bits. The final terminal nodes require $\frac{1}{2}\log_2(n_6\, n_7)$ bits for the two means and $(26/2)\log_2 15.4 = 51.3$ bits for the data in both. If we accumulate the steps, we arrive at the following description length:

$$\begin{aligned}
\mathcal{D}(\text{tree}) &= 7 + 3(8) + \tfrac{1}{2}\textstyle\sum \log_2 n_t + (n/2)\log_2(RSS/n) \\
&= 7 + 24 + \tfrac{1}{2}\log_2(9)(15)(8)(18) + (50/2)\log_2(768.4/50) \\
&= 136.7 \text{ bits.}
\end{aligned}$$

The first summand counts the bits used to indicate if nodes are terminal. The second summand counts the bits required for the 3 splits. The third summand denotes the cost of coding the means of the 4 terminal nodes (with n_t observations in the tth terminal node), and the last summand is for coding the data itself.

Though the differences are not large, the *MDL* principle prefers a regression over this tree, unless we use the rather crude prefix to identify the predictors. The illustration in the next section offers further comparison of the methods for selecting regressors.

8 Comparing Nested Regressions

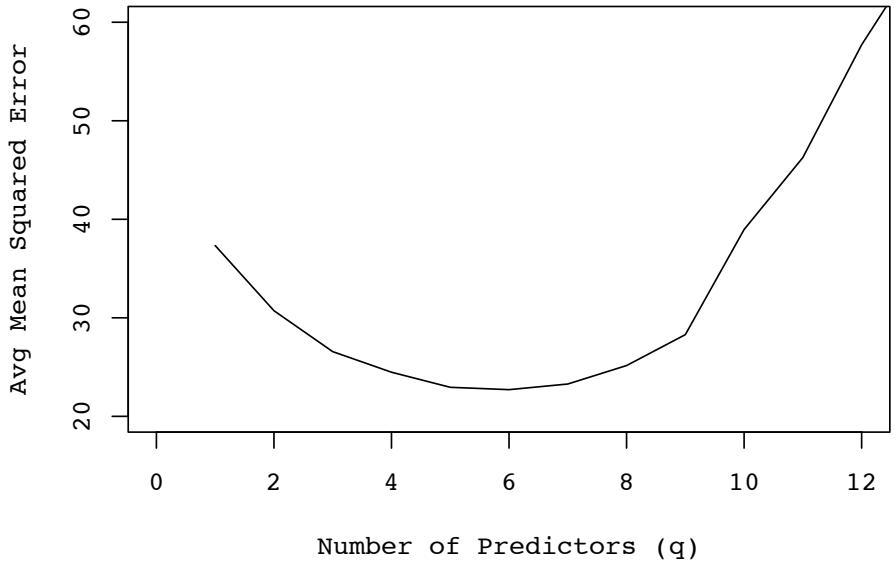
This section focuses on the common problem of picking the best model from a sequence of nested regressions found by stepwise regression. My aims for this section are two-fold. First, this familiar setting allows me to contrast several model selection criteria in a context where all of them apply. The second aim is more subtle and returns to the role of theory in model selection. Surprisingly, perhaps, theory still plays a role even though we are using an automatic search. The theory, though, is less specific than the one that motivates the first regression in Section 2. Rather than indicate a particular model, having a "weak" theory that indicates only whether we expect many predictors can improve our ability to pick models. Such theories can be hard to come by, and recent developments in model selection may soon fill this gap.

I use cross validation to show how such weak theory influences the success of model selection. To gauge "success" here, I will simply measure the out-of-sample mean squared error. Obviously, other issues, such as interpretation and structure, are relevant in model selection, but I would like to focus for the moment on prediction. For this cross validation, I divided the Boston data randomly into 10 samples, each with 50 observations. (Recall that I set aside 6 outlying tracts, leaving 500.) For each subset, I ran a forward stepwise regression that allows second-order effects. I computed the associated mean squared error of each model in this sequence when used to predict the 450 observations in the other 9 samples. A "good" model selection criterion ought to identify the most predictive model in this sequence, allowing the stepwise search to find good predictors but stopping before overfitting.

Notice that the sample sizes in this cross validation are reversed from the usual partitioning. This 10-fold cross-validation validates using 9 of the 10 groups, estimating the fit using the single remaining group. Given 450 observations and a strong signal, most selection procedures would pick similar models and the validation estimates would be too noisy to discriminate among them. With samples of 50, the differences among the chosen models are more apparent.

How well can a stepwise regression predict? I do not have a "true model" for this data, but we can get a sense of what is possible from the cross-validation itself. Figure 2 shows the mean squared

Figure 2: *The mean squared error of forward stepwise regressions attains its minimum near 23 for the models with 6 predictors.*



error for sequences of models found by stepwise regression. To obtain this plot, I repeated the cross-validation randomization 15 times. For each of these randomizations, I performed a 10-fold cross validation. Thus, I fit 150 sequences of stepwise regressions. Alternatively, one can think of this as a "balanced" simulation with each of the 500 observations appearing in 15 samples. Figure 2 shows the mean squared error as a function of the model size. Though the averaged models of given size need not have the same predictors, the out-of-sample error increases once the model includes more than 6 or 7 predictors. A good model selection procedure should thus pick about this many predictors. Adding more only increases the variation of the fit; using fewer misses an opportunity.

This comparison uses the 4 criteria introduced in Section 6, the *AIC*, *BIC*, *RIC* and RIC^*. I implemented these as follows. Let $L(Y, \hat{\beta}_q)$ denote the normal likelihood obtained by a regression with an intercept and q slopes, estimated using OLS. In keeping with the usual implementations for a regression model with q predictors, I computed

$$AIC(q) = q - \ln L(Y, \hat{\beta}_q)$$

and

$$BIC(q) = \tfrac{q}{2} \ln n - \ln L(Y, \hat{\beta}_q) \ ,$$

where the log-likelihood is

$$\ln L(Y, \hat{\beta}_q) = (n/2)\left[1 + \ln(2\pi RSS(q)/(n-1-q))\right] \ . \tag{14}$$

The appendix explains the use of the unbiased variable estimator in the likelihood. I defined *RIC* as (Foster and George, 1994; Miller, 2002),

$$RIC(q) = q\,(1 + \ln p) - \ln L(Y, \hat{\beta}_q) \ .$$

The penalty $q \ln p$ suggests a code that requires on the order of $\log_2 p$ bits to identify each predictor. Similarly, with p_1 denoting the number of searched main effects and q_1 the number of these in the model, I defined

$$RIC^*(q) = q_1(1 + \ln p) + (q - q_1)(1 + 2\ln q_1) - \ln L(Y, \hat{\beta}_q) \ .$$

Figure 3 illustrates *AIC*, *BIC*, and *RIC* for one of the 150 samples in the cross validation. In the figure, the solid line shows the negative log-likelihoods; sequences of letters show the three penalized log-likelihoods. For example, the "a" sequence (for *AIC*) is just the baseline log-likelihood offset by 1 for $q = 1$, 2 for $q = 2$, and so forth. Whereas the negative log-likelihood (being a monotone function of the residual sum-of-squares) monotonically decreases, each penalized series has a well-defined minimum. In this case, *AIC* picks the model with $q = 14$ predictors whereas *RIC*, because of its larger penalty (q versus $q + q \log p$) chooses a parsimonious model with $q = 3$ predictors and *BIC* picks a model with 8.

Figure 4 and Table 5 summarize the the out-of-sample accuracy of the models chosen by these criteria. Referring back to the plot of the out-of-sample *MSE* in Figure 2, good models (*i.e.*, models that predict well out-of-sample) should have about 6 predictors. With the smallest penalty, *AIC* chooses excessively large models with about 15 predictors (on average); *AIC* often overfits and so has rather large *MSE* (98 versus a lower bound of about 23). In contrast, *BIC* picks about 8 and both versions of *RIC* pick fewer still. Though its models obtain smaller *MSE* than those chosen by *BIC*, the boxplots in Figure 4 suggest that much of this difference arises from the few samples when *BIC* overfits. The boxplots suggest that most of the time, models identified by *BIC* do well. The modified criterion RIC^* lies between these two, with more predictors than *RIC* but fewer than *BIC*. It matches the *MSE* of models picked by *BIC* but with fewer predictors.

What happens, though, if the data are simpler than these, with fewer relationships between predictors and response? To convey what happens in this case, I altered the cross validation. Rather

Figure 3: *Negative log-likelihood (solid curve) and penalized likelihoods as used by AIC (a), BIC (b), and RIC (r) to choose the best model from a sequence of 25 models given by forward stepwise regression for a random subset of the Boston housing data.*

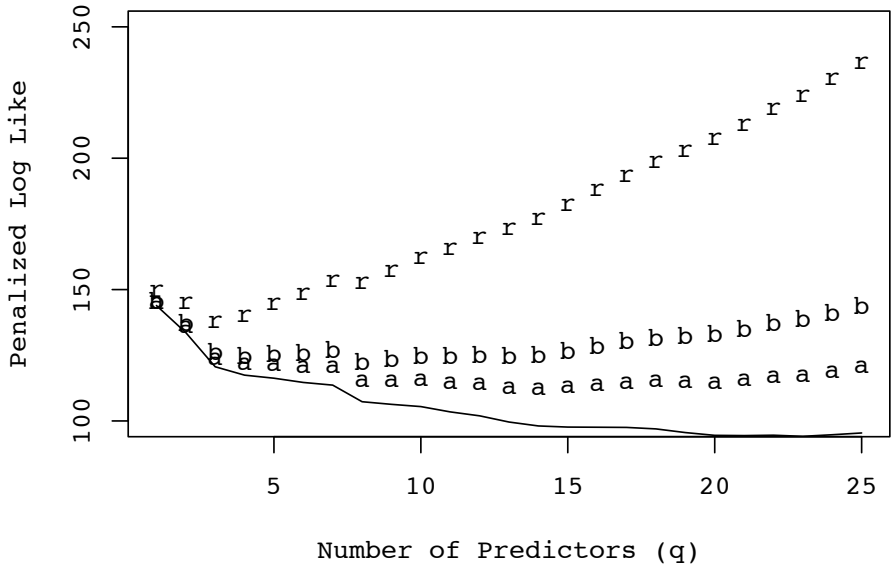
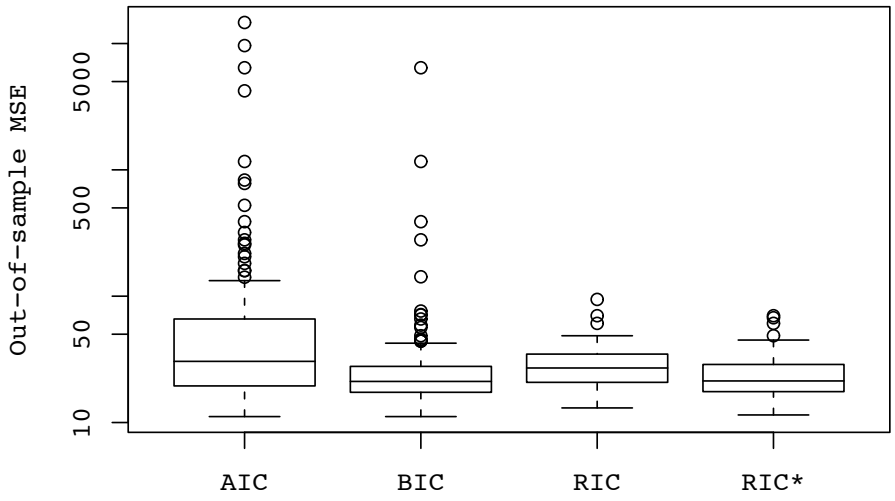


Table 5: *Average number of predictors q and out-of-sample mean squared error for the selected regression models chosen by AIC, BIC, RIC, and RIC*.*

	Boston data		Scrambled Boston data	
Criterion	q	*MSE*	q	*MSE*
AIC	15.0	98.0	4.6	89.2
BIC	7.9	43.1	1.6	39.4
RIC	2.7	28.3	1.0	36.6
*RIC**	4.2	24.1	1.1	36.3

Figure 4: *Mean squared errors of models selected by the AIC, RIC, and RIC* in a cross-validation using the Boston housing data.*

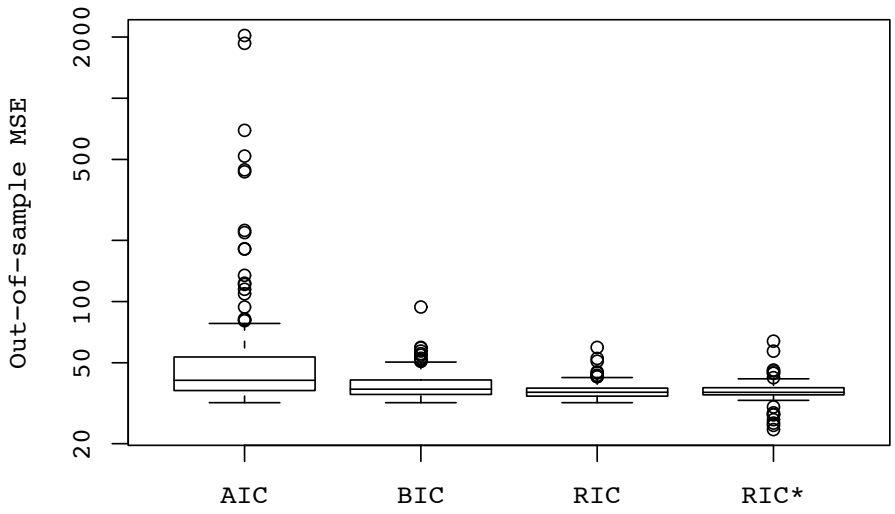


than use the actual Boston data, I "scrambled" the values in all of the columns but for *MEDV* and *RM*. I randomly permuted the values in the other columns, leaving these two alone. Consequently, the other columns have the same marginal distributions, but are no longer associated with either *MEDV* or *RM*. We now *know* that only one predictor is related to the response. By relating it to a coding procedure, we noted in Section 6 that *RIC* was designed for selecting predictors when few are related to the response. So, it should come as no surprise to see in Figure 5 that *RIC* produces models with the smallest *MSE* when validation analysis is repeated with the scrambled data. *AIC* overfits, as does *BIC* to some extent.

Comparing the results in Figures 4 and 5 suggests a lurking problem: the best criterion depends upon how many predictors are "useful." Both *BIC* and, to a lesser extent, *AIC* work well in problems in which many predictors are related to the response, such as the original Boston data. Because *RIC* is "tuned" to pick models from data with few useful predictors, it may miss some signal (Figure 4). When there is just one predictor, though, *RIC* does quite well. So, it would seem we are stuck: we have to know how many predictors are useful in order to decide which criterion will work best for us.

Recent research has attempted to remove this "need to know" by offering adaptive criteria

Figure 5: *Mean squared errors of models selected by the AIC, RIC, and RIC* in a cross-validation using the scrambled Boston housing data for which only one predictor is associated with the response.*



that work almost as well as criteria that have been tuned to the problem at hand. One can motivate an adaptive criterion from information theory (Foster and Stine, 1996), multiple comparisons (Abramovich, Benjamini, Donoho and Johnstone, 2000), and empirical Bayes (George and Foster, 2000). From the point of view of information theory, adaptive criteria encode the Boolean selection vector γ indirectly using an efficient, adaptive code that works well regardless of the size of the model. Compared to *AIC* or *BIC* (which assume about half of the considered variable should belong in the model) and *RIC* (which assumes only one), an adaptive criterion represents γ about as well as is possible, regardless of q.

9 Discussion

Information theory and the *MDL* principle allow one to construct a wide range of model selection criteria. *MDL* both rewards theory and allows searches of large collections of models. The task for the modeler is to choose the right combination. Coding — thinking of a model as a code for the data — offers an important heuristic to guide the development of customized criteria suited to the problem at hand.

Returning to the question "Which model is best?," we see that the answer depends on how we approach the analysis. *MDL* rewards a theory that generates a model that a less-informed analyst might need an exhaustive search to discover. The four-predictor regression in Table 2, when identified *a priori*, is certainly the best of the illustrative models. Without such a clairvoyant theory, *MDL* rates this model highly *only if* we have chosen to encode the identify of the regression slopes in a manner suited to searching many possible effects. Again, *MDL* exploits our knowledge of the problem at hand, this time in the form of our expectation for how many predictors should appear in the final model. Codes like those related to the *RIC* incorporate the notion that the analyst expects only a few of the searched factors to affect the response. Coding just the index rather than the long string of bits reflects our expectation of a model with few predictors. Though the regression tree fairs poorly in this illustration, *MDL* does allow us to compare it to regression models.

This discussion of model selection begs the question "What is a model anyway?" Although a careful answer requires details outside the scope of this paper (*e.g.* McCullagh, 2002), the essential properties needed are a likelihood for the data and a "likelihood" for the model as well. This requirement rules out some popular approaches based on various method-of-moments estimators, such as *GMM*. If, however, our theory allows us to express our beliefs asf a probability distribution, then *MDL* offers a framework in which we can judge the value of its merits.

One thing that *MDL* does not ask of us, however, is the existence of a true model. Although the spike-and-slab formulation leads to a so-called "consistent model selection criterion" (*i.e.*, one that identifies the true model with probability 1 as the sample size increases), *MDL* only requires a probability model for the data. As we have seen, some versions of the *MDL* behave like *AIC* and are thus, like 5% hypothesis tests, not consistent. The better the model that we can write down, the shorter the code for the data. None have to be the "true model" that generated the data. And, because the code for the data must describe the model itself, one cannot simply tune the model ever more closely to a specific sample.

Several reviews of information theory for model selection will be of interest to readers who would like to learn more about the use of information theory in model selection and statistics. In order of increasing mathematical sophistication, these are Lee (2001) (which uses polynomial regression as the motivating example), Bryant and Cordero-Braña (2000) (testing, especially for contingency tables), Hansen and Yu (2001) (regression and priors), Lanterman (2001) (relationship to Bayesian methods) and Barron et al. (1998) (coding methods). Rissanen (1989) (Section 3.2) describes the

differences between coding and *MDL* and the Bayesian approach. As suggested by the number of citations, the book of Cover and Thomas (1991) gives an excellent introduction to information theory in general.

Appendix: Estimating σ^2

This appendix considers the effects of using an estimate of σ^2 when computing description lengths. The codes described in this paper ignore the fact that σ^2 is unknown and must be added to the code. Since all of the models require such as estimate, adding it as part of the code does not affect the comparisons. A reduction in the estimated error variance does, however, increase the z-scores of predictors in the model, and we need to account for this effect. The adjustment essentially replaces the *MLE* for σ^2 in the likelihood by the familiar unbiased estimator.

Recall that the second part of the two-part code for a regression represents the encoded data. For a model with q predictors, the *MLE* for σ^2 is

$$\hat{\sigma}_q^2 = \frac{\sum_i (Y_i - \hat{\beta}_0 - \hat{\beta}_1 X_1 - \cdots - \hat{\beta}_q X_q)^2}{n} = \frac{RSS(q)}{n} \ . \tag{15}$$

The description length for the data is then the negative log-likelihood

$$\begin{aligned} -\log_2 L(q) &= \frac{n}{2\ln 2}\left(1 + \ln(2\pi\hat{\sigma}^2)\right) \\ &= \frac{n}{2\ln 2}\ \ln\frac{RSS(q)}{RSS(q+1)} \ . \end{aligned}$$

Only the leading term affects the comparison of models. The gain in data compression by expanding a model with q predictors to one with $q+1$ is thus

$$\log_2 L(q+1) - \log_2 L(q) = \frac{n}{2\ln 2}\left(\ln RSS(q) - \ln RSS(q+1)\right) \ . \tag{16}$$

To measure the impact of estimating σ^2 on the first part of the code, treat the sequence of predictors as defining a sequence of orthogonal expansions of the model. The ordered predictors chosen by forward selection can be converted into an uncorrelated set of predictors, using a method such as Gram-Schmidt. Further, assume that the resulting orthogonal predictors – which I will continue to call $X_1, \ldots, X_q$ – are normalized to have unit length, $X_j' X_j = 1$. Denote the test statistics for these in a model with q predictors as $\hat{z}_{0,q}, \ldots, \hat{z}_{q,q}$ for

$$\hat{z}_{j,q} = \hat{\beta}_j / \hat{\sigma}_q \ ,$$

and denote those from the model with $q+1$ parameters as $\hat{z}_{0,q+1}, \ldots, \hat{z}_{q,q+1}, \hat{z}_{q+1,q+1}$. Because of orthogonality, only the estimate of the error variance changes in the first q z-scores when X_{q+1} joins the model, so

$$\hat{z}_{j,q+1} = \hat{z}_{j,q} \, \frac{\hat{\sigma}_q}{\hat{\sigma}_{q+1}} \, . \tag{17}$$

The addition of a predictor then increases the length of the code for the model parameters from $\ell_u(\hat{z}_{0,q}) + \cdots + \ell_u(\hat{z}_{q,q})$ to $\ell_u(\hat{z}_{0,q+1}) + \cdots + \ell_u(\hat{z}_{q+1,q+1})$. If the estimated error variance *decreases*, then the test statistics for the first q predictors *increase* and potentially require longer parameter codes. We need to capture this effect.

An approximation simplifies the comparison of the description lengths. First, the definition of the universal length $\ell_u(j)$ given in (11) implies that (ignoring the need for $\log_2^+$)

$$\begin{aligned}
\ell_u(z\,c) &= 2 + \log_2 z + \log_2 c + 2\log_2(\log_2 z + \log_2 c) \\
&= 2 + \log_2 z + \log_2 c + 2\log_2\left(\log_2(z)\left(1 + \frac{\log_2 c}{\log_2 z}\right)\right) \\
&= \log_2 z + 2\log_2\log_2 z + \log_2 c + 2\log_2\left(1 + \frac{\log_2 c}{\log_2 z}\right) \, .
\end{aligned}$$

If $c \approx 1$ and z is of moderate size, we can drop the last summand and obtain

$$\ell_u(z\,c) \approx \ell_u(z) + \log_2 c \, . \tag{18}$$

The approximation is justified since we only need it when $c = RSS(q)/RSS(q+1)$ and z is the z-score of a predictor in the model (and so is at least 3 to 4).

The approximation (18) leads to an expression for the length of the code for the model parameters. Going from a model with q predictors to one with $q+1$ increases the length of the model prefix by about

$$\begin{aligned}
\ell_u(\hat{z}_{q+1,q+1}) + \sum_{j=0}^{q} \ell_u(\hat{z}_{j,q+1}) - \ell_u(\hat{z}_{j,q}) &= \ell_u(\hat{z}_{q+1,q+1}) + \sum_{j=0}^{q} \ell_u(\hat{z}_{j,q}\ \hat{\sigma}_q/\hat{\sigma}_{q+1}) - \ell_u(\hat{z}_{j,q}) \\
&\approx \ell_u(\hat{z}_{q+1,q+1}) + (q+1)\log_2 \frac{\hat{\sigma}_q}{\hat{\sigma}_{q+1}} \\
&= \ell_u(\hat{z}_{q+1,q+1}) + \frac{q+1}{2\ln 2} \ln \frac{RSS(q)}{RSS(q+1)} \, .
\end{aligned} \tag{19}$$

The *MDL* principle indicates that one chooses the model with the shorter description length. In this case, we choose the model with $q+1$ predictors if the gain in data compression given in equation (16) is larger than the increase in the length for the parameters given by (19). That is, we add X_{q+1} to the model if

$$\frac{n}{2\ln 2} \, \ln \frac{RSS(q)}{RSS(q+1)} \geq \ell_u(\hat{z}_{q+1,q+1}) + \frac{q+1}{2\ln 2} \ln \frac{RSS(q)}{RSS(q+1)} \, ,$$

or equivalently if

$$\frac{n-q-1}{2\ln 2}\,\ln\frac{RSS(q)}{RSS(q+1)} \geq \ell_u(\hat{z}_{q+1,q+1})\ .$$

If we assume that the change in fit $\delta^2 = RSS(q) - RSS(q+1)$ is small relative to $RSS(q+1)$, then

$$\begin{aligned}
\frac{n-q-1}{2\ln 2}\,\ln\frac{RSS(q)}{RSS(q+1)} &= \frac{n-q-1}{2\ln 2}\,\ln\frac{RSS(q+1)+\delta^2}{RSS(q+1)} \\
&= \frac{n-q-1}{2\ln 2}\,\ln(1+\delta^2/RSS(q+1)) \\
&\approx \frac{n-q-2}{2\ln 2}\,\frac{\delta^2}{RSS(q+1)} \\
&= \frac{1}{2\ln 2}\,\frac{\delta^2}{s^2_{q+1}} \\
&= \frac{1}{2\ln 2}\,t^2_{q+1}\ ,
\end{aligned}$$

where $s^2_{q+1} = RSS(q+1)/(n-q-2)$ is the usual unbiased estimate of σ^2 and $t^2_{q+1} = \delta^2/s^2_{q+1}$ is the square of the standard t-statistic for the added variable. As a result, the use of the unbiased estimator s^2_q allows us to judge the benefit to a model of adding X_j in the same fashion we would take were we to know σ^2.

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