

# bestglm: Best Subset GLM

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## Abstract

The function `bestglm` selects the best subset of inputs for the GLM family. The selection methods available include a variety of information criteria as well as cross-validation. Several examples are provided to show that this approach is sometimes more accurate than using the built-in R function `step`. In the Gaussian case the leaps-and-bounds algorithm in `leaps` is used provided that there are no factor variables with more than two levels. In the non-Gaussian GLM case or when there are factor variables present with three or more levels, a simple exhaustive enumeration approach is used. This vignette also explains how the applications given in our article [Xu and McLeod \(2009\)](#) may easily be reproduced. A separate vignette is available to provide more details about the simulation results reported in [Xu and McLeod \(2009, Table 2\)](#) and to explain how the results may be reproduced.

*Keywords:* best subset GLM, AIC, BIC, extended BIC, cross-validation.

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## 1. Introduction

We consider the GLM of  $Y$  on  $p$  inputs,  $X_1, \dots, X_p$ . In many cases,  $Y$  can be more parsimoniously modelled and predicted using just a subset of  $m < p$  inputs,  $X_{i_1}, \dots, X_{i_m}$ . The best subset problem is to find out of all the  $2^p$  subsets, the best subset according to some goodness-of-fit criterion. The built-in R function `step` may be used to find a best subset using a stepwise search. This method is expedient and often works well. When  $p$  is not too large, `step`, may be used for a backward search and this typically yields a better result than a forward search. But if  $p$  is large, then it may be that only a forward search is feasible due to singularity or multicollinearity. In many everyday regression problems we have  $p \leq 50$  and in this case an optimization method known as leaps-and-bounds may be utilized to find the best subset. More generally when  $p \leq 15$  a simple direct lexicographic algorithm ([Knuth 2005, Algorithm L](#)) may be used to enumerate all possible models. Some authors have criticized the *all subsets* approach on the grounds that it is too computationally intensive. The term data dredging has been used. This criticism is not without merit since it must be recognized that the significance level for the  $p$ -values of the coefficients in the model will be overstated – perhaps even extremely so. Furthermore for prediction purposes, the LASSO or regularization method may outperform the subset model's prediction. Nevertheless there are several important applications for subset selection methods. In many problems, it is of interest to determine which are the most influential variables. For many data mining methods such as neural nets or support vector machines, feature selection plays an important role and here too subset selection can help. The idea of data-dredging is somewhat similar to the concern about over-training with artificial neural nets. In both cases, there does not seem to be any

rigorous justification of choosing a suboptimal solution. In the case of GLM and linear models our package provides a variety of criterion for choosing a parsimonious subset or collection of possible subsets.

In the case of linear regression, [Miller \(2002\)](#) provides a monograph length treatment of this problem while [Hastie, Tibshirani, and Friedman \(2009, Ch. 3\)](#) discuss the subset approach along with other recently developed methods such as LARS and LASSO. Consider the case of linear regression with  $n$  observations,  $(x_{i,1}, \dots, x_{i,p}, y_i), i = 1, \dots, n$  we may write the regression,

$$y_i = \beta_0 + \beta_1 x_{i,1} + \dots + \beta_p x_{i,p} + e_i. \quad (1)$$

When  $n > p$  all possible  $2^p$  regressions could be fit and the best fit according to some criterion could be found. When  $p \leq 25$  or thereabouts, an efficient combinatorial algorithm, known as branch-and-bound can be applied to determine the model with the lowest residual sum of squares of size  $m$  for  $m = 1, \dots, p$  and more generally the  $k$  lowest subsets for each  $m$  may also be found.

The **leaps** package ([Lumley and Miller 2004](#)) implements the branch-and-bound algorithm as well as other subset selection algorithms. Using the **leaps** function, **regsubsets**, the best model of size  $k, k = 1, \dots, p$  may be determined in a few seconds when  $p \leq 25$  on a modern personal computer. Even larger models are feasible but since, in the general case, the computer time grows exponentially with  $p$ , problems with large enough  $p$  such as  $p > 100$ , can not be solved by this method. An improved branch-and-bound algorithm is given by [Gatu \(2006\)](#) but the problem with exponential time remains.

One well-known and widely used alternative to the best subset approach is the family of stepwise and stagewise algorithms [Hastie et al. \(2009, Section 3.3\)](#). This is often feasible for larger  $p$  although it may select a sub-optimal model as noted by [Miller \(2002\)](#). For very large  $p$  [Chen and Chen \(2008\)](#) suggest a tournament algorithm while **subselect** ([Cadima, Cerdeira, Orestes, and Minhoto 2004; Cerdeira, Silva, Cadima, and Minhoto 2009](#)) uses high dimensional optimization algorithms such as genetic search and simulated annealing for such problems.

Using subset selection algorithm necessarily involves a high degree of selection bias in the fitted regression. This means that the  $p$ -values for the regression coefficients are overstated, that is, coefficients may appear to be statistically significant when they are not. ([Wilkinson and Gerard 1981](#)) and the  $R^2$  are also inflated [Renchner and Fu \(1980\)](#).

More generally for the family of GLM models similar considerations about selection bias and computational complexity apply. [Hosmer, Jovanovic, and Lemeshow \(1989\)](#) discuss an approximate method for best subsets in logistic regression. No doubt there is scope for the development of more efficient branch-and-bound algorithms for the problem of subset selection in GLM models. See [Brusco and Stahl \(2009\)](#) for a recent monograph of the statistical applications of the branch-and-bound algorithm. We use the lexicographical method suggested by [Morgan and Tatar \(1972\)](#) for the all subsets regression problem to enumerate the loglikelihoods for all possible GLM model. Assuming there are  $p$  inputs, there are then  $2^p$  possible subsets which may be enumerated by taking  $i = 0, \dots, 2^p - 1$  and using the base-2 representation of  $i$  to determine the subset. This method is quite feasible on present PC workstations for  $p$  not too large.

### 1.1. Prostate Cancer Example

As an illustrative example of the subset regression problem we consider the prostate data discussed by [Hastie \*et al.\* \(2009\)](#). In this dataset there are 97 observations on men with prostate cancer. The object is to predict and to find the inputs most closely related with the outcome variable Prostate-Specific Antigen (psa). In the general male population, the higher the psa, the greater the chance that prostate cancer is present.

To facilitate comparison with the results given in the textbook as well as with other techniques such as LARS, we have standardized all inputs. The standardized prostate data is available in `zprostate` in our **bestglm** package and is summarized below,

```
R> library(bestglm)
R> data(zprostate)

R> str(zprostate)

'data.frame':      97 obs. of  10 variables:
 $ lcavol : num  -1.637 -1.989 -1.579 -2.167 -0.508 ...
 $ lweight: num  -2.006 -0.722 -2.189 -0.808 -0.459 ...
 $ age    : num  -1.862 -0.788 1.361 -0.788 -0.251 ...
 $ lbph   : num  -1.02 -1.02 -1.02 -1.02 -1.02 ...
 $ svi    : num  -0.523 -0.523 -0.523 -0.523 -0.523 ...
 $ lcp    : num  -0.863 -0.863 -0.863 -0.863 -0.863 ...
 $ gleason: num  -1.042 -1.042 0.343 -1.042 -1.042 ...
 $ pgg45  : num  -0.864 -0.864 -0.155 -0.864 -0.864 ...
 $ lpsa   : num  -0.431 -0.163 -0.163 -0.163 0.372 ...
 $ train  : logi   TRUE TRUE TRUE TRUE TRUE TRUE ...
```

The outcome is `lpsa` which is the logarithm of the psa. In [Hastie \*et al.\* \(2009, Table 3.3\)](#) only the training set portion is used. In the training portion there are  $n = 67$  observations.

Using `regsubsets` in **leaps** we find subsets of size  $m = 1, \dots, 8$  which have the smallest residual sum-of-squares.

```
R> train <- (zprostate[zprostate[, 10], ])[, -10]
R> X <- train[, 1:8]
R> y <- train[, 9]
R> out <- summary(regsubsets(x = X, y = y, nvmax = ncol(X)))
R> Subsets <- out$which
R> RSS <- out$rss
```

```
R> cbind(as.data.frame(Subsets), RSS = RSS)
```

	(Intercept)	lcavol	lweight	age	lbph	svi	lcp	gleason	pgg45	RSS
1	TRUE	TRUE	FALSE	FALSE	FALSE	FALSE	FALSE	FALSE	FALSE	44.52858
2	TRUE	TRUE	TRUE	FALSE	FALSE	FALSE	FALSE	FALSE	FALSE	37.09185
3	TRUE	TRUE	TRUE	FALSE	FALSE	TRUE	FALSE	FALSE	FALSE	34.90775
4	TRUE	TRUE	TRUE	FALSE	TRUE	TRUE	FALSE	FALSE	FALSE	32.81499
5	TRUE	TRUE	TRUE	FALSE	TRUE	TRUE	FALSE	FALSE	TRUE	32.06945

6	TRUE	TRUE	TRUE	FALSE	TRUE	TRUE	TRUE	FALSE	TRUE	30.53978
7	TRUE	TRUE	TRUE	TRUE	TRUE	TRUE	TRUE	FALSE	TRUE	29.43730
8	TRUE	TRUE	TRUE	TRUE	TRUE	TRUE	TRUE	TRUE	TRUE	29.42638

The residual sum-of-squares decreases monotonically as the number of inputs increases.

## 1.2. Overview of bestglm Package

**bestglm** uses the simple exhaustive search algorithm (Morgan and Tatar 1972) for GLM and the **regsubsets** function in the **leaps** package to find the GLM models with smallest sum of squares or deviances for size  $k = 0, 1, \dots, p$ . Size  $k = 0$  corresponds to intercept only. The exhaustive search requires more computer time but this is usually not an issue when  $p \leq 10$ . For example, we found that a logistic regression with  $p = 10$  requires about 12.47 seconds as compared with only 0.04 seconds for a comparably size linear regression. The timing difference would not be important in typical data analysis applications but could be a concern in simulation studies. In this case, if a multi-core PC or even better a computer cluster is available, we may use the **Rmpi** package. Our vignette Xu and McLeod (2009) provides an example of using **Rmpi** with **bestglm**.

## 1.3. Package Options

The arguments and their default values are:

```
R> args(bestglm)
```

```
function (Xy, family = gaussian, IC = "BIC", t = "default", CVArgs = "default",
  qLevel = 0.99, TopModels = 5, method = "exhaustive", intercept = TRUE,
  weights = NULL, nvmax = "default", RequireFullEnumerationQ = FALSE,
  ...)
```

```
NULL
```

The argument **Xy** is usually a data-frame containing in the first  $p$  columns the design matrix and in the last column the response. For binomial GLM, the last two columns may represent counts  $S$  and  $F$  as in the usual **glm** function when the **family=binomial** option is used.

When **family** is set to **gaussian**, the function **regsubsets** in **leaps** is used provided that all inputs are quantitative or that there are no factor inputs with more than two levels. When factor inputs at more than two levels are present, the exhaustive enumeration method is used and in this case the R function **lm** is used in the **gaussian** case. For all non-Gaussian models, the R function **glm** is used with the exhaustive enumeration method.

The arguments **IC**, **t**, **CVArgs**, **qLevel** and **TopModels** are used with various model selection methods. The model selection methods available are based on either an information criterion or cross-validation. The information criteria and cross-validation methods are discussed in the Sections 2 and 3.

The argument **method** is simply passed on to the function **regsubsets** when this function from the **leaps** package is used. The arguments **intercept** and **nvmax** are also passed on to **regsubsets** or may be used in the exhaustive search with a non-Gaussian GLM model is fit. These two arguments are discussed briefly in Sections 1.4 and 1.5.

The argument `RequireFullEnumerationQ` is provided to force the use of the slower exhaustive search algorithm when the faster algorithm in the **leaps** package would normally be used. This is provided only for checking.

The output from `bestglm` is a list with named components

```
R> Xy <- cbind(as.data.frame(X), lpsa = y)
R> out <- bestglm(Xy)
R> names(out)
```

```
[1] "BestModel"    "BestModels"  "Bestq"       "qTable"      "Subsets"
[6] "Title"       "ModelReport"
```

The components `BestModel`, `BestModels`, `Subsets`, `qTable` and `Bestq` are of interest and are described in the following table.

name	description
<code>BestModel</code>	lm or glm object giving the best model
<code>BestModels</code>	a $T \times p$ logical matrix showing which variables are included in the top $T$ models
<code>Bestq</code>	matrix with 2 rows indicating the upper and lower ranges
<code>Subsets</code>	a $(p + 1) \times p$ logical matrix showing which variables are included for subset sizes $k = 0, \dots, p$ have the smallest deviance
<code>qTable</code>	a table showing all possible model choices for different intervals of $q$ .

#### 1.4. Intercept Term

Sometimes it may be desired not to include an intercept term in the model. Usually this occurs when the response to the inputs is thought to be proportional. If the relationship is multiplicative of the form  $Y = e^{\beta_1 X_1 + \dots + \beta_p X_p}$  then a linear regression through the origin of  $\log Y$  on  $X_1, \dots, X_p$  may be appropriate.

Another, but not recommended use, of this option is to set `intercept` to `FALSE` and then include a column of 1's in the design matrix to represent the intercept term. This will enable one to exclude the intercept term if it is not statistically significant. Usually the intercept term is always included even if it is not statistically significant unless there are prior reasons to suspect that the regression may pass through the origin.

Cross-validation methods are not available in the regression through the origin case.

#### 1.5. Limiting the Number of Variables

The argument `nvmax` may be used to limit the number of possible explanatory variables that are allowed to be included. This may be useful when  $p$  is quite large. Normally the information criterion will eliminate unnecessary variables automatically and so when the default setting is used for `nvmax` all models up to an including the full model with  $p$  inputs are considered.

Cross-validation methods are not available when `nvmax` is set to a value less than  $p$ .

#### 1.6. Forcing Variables to be Included

In some applications, the model builder may wish to require that some variables be included in all models. This could be done by using the residuals from a regression with the required variables as inputs with a design matrix formed from the optional variables. For this reason, the optional argument `force.in` used in `leaps` is not implemented in `bestglm`.

## 2. Information criteria

Information criteria or cross-validation is used to select the best model out of these  $p + 1$  model cases,  $k = 0, 1, \dots, p$ . The information criteria include the usual AIC and BIC as well as two types of extended BIC (Chen and Chen 2008; Xu and McLeod 2009). These information criteria are discussed in the Section 2.

When the information criterion approach is used, it is possible to select the best  $T$  models out of all possible models by setting the optional argument `TopModels = T`.

All the information criteria we consider are based on a penalized form of the deviance or minus twice the log-likelihood. In the multiple linear regression the deviance  $\mathcal{D} = -2 \log \mathcal{L}$ , where  $\mathcal{L}$  is the maximized log-likelihood,  $\log \mathcal{L} = -(n/2) \log \mathcal{S}/n$ , where  $\mathcal{S}$  is the residual sum of squares.

### 2.1. AIC

Akaike (1974) showed that  $\text{AIC} = \mathcal{D} + 2k$ , where  $k$  is the number of parameters, provides an estimate of the entropy. The model with the smallest AIC is preferred. Many other criteria which are essentially equivalent to the AIC have also been suggested. Several other asymptotically equivalent but more specialized criteria were suggested. In the context of autoregressive models, Akaike (1970) suggested the final prediction error criterion,  $\text{FPE} = \hat{\sigma}_k^2(1 + 2k/n)$ , where  $\hat{\sigma}_k^2$  is the estimated residual variance in a model with  $k$  parameters. and in the subset regression problem, Mallows (1973) suggested using  $C_k = S_k/\hat{\sigma}_2 + 2k - n$ , where  $S_k$  is the residual sum-of-squares for a model with  $k$  inputs and  $\hat{\sigma}_2$  is the residual variance using all  $p$  inputs. Nishii (1984) showed that minimizing  $C_k$  or FPE is equivalent to minimizing the AIC. In practice, with small  $n$ , these criteria often select the same model. From the results of (Shibata 1981), the AIC is asymptotically efficient but not consistent.

*Best AIC Model for Prostate Data*

```
R> bestglm(Xy, IC = "AIC")
```

AIC

BICq equivalent for q in (0.708764213288624, 0.889919748490004)

Best Model:

	Estimate	Std. Error	t value	Pr(> t )
(Intercept)	2.4668675	0.08760022	28.160516	6.632457e-36
lcavol	0.6764486	0.12383666	5.462426	9.883880e-07
lweight	0.2652760	0.09363348	2.833132	6.298761e-03
age	-0.1450300	0.09756540	-1.486490	1.424742e-01
lbph	0.2095349	0.10128348	2.068796	4.295574e-02
svi	0.3070936	0.12190105	2.519204	1.449125e-02

```
lcp          -0.2872242 0.15300241 -1.877253 6.543004e-02
pgg45        0.2522850 0.11562030  2.182013 3.310324e-02
```

The best subset model using AIC has 7 variables and two of them are not even significant at 5%.

## 2.2. BIC

The BIC criterion (Schwarz 1978) can be derived using Bayesian methods as discussed by Chen and Chen (2008). If a uniform prior is assumed of all possible models, the usual BIC criterion may be written,  $BIC = \mathcal{D} + k \log(n)$ . The model with the smallest BIC corresponds to the model with maximum posterior probability. The difference between these criterion is in the penalty. When  $n > 7$ , the BIC penalty is always larger than for the AIC and consequently the BIC will never select models with more parameters than the AIC. In practice, the BIC often selects more parsimonious models than the AIC. In time series forecasting experiments, time series models selected using the BIC often outperform AIC selected models (Noakes, McLeod, and Hipel 1985; Koehler and Murphree 1988; Granger and Jeon 2004). On the other hand, sometimes the BIC underfits and so in some applications, such as autoregressive-spectral density estimation and for generating synthetic riverflows and simulations of other types of time series data, it may be preferable to use the AIC (Percival and Walden 1993).

*Best BIC Model for Prostate Data*

```
R> bestglm(Xy, IC = "BIC")

BIC
BICq equivalent for q in (0.0176493852011195, 0.512566675362627)
Best Model:

              Estimate Std. Error   t value    Pr(>|t|)
(Intercept) 2.4773573 0.09304738 26.624687 2.475214e-36
lcavol      0.7397137 0.09318316  7.938277 4.141615e-11
lweight     0.3163282 0.08830716  3.582135 6.576173e-04
```

Note that IC="BIC" is the default.

## 2.3. BICg

The notation  $BIC_g$  and  $BIC_\gamma$  will be used interchangeably. In mathematical writing  $BIC_\gamma$  is preferred but in our R code the parameter is denoted by  $BIC_g$ . Chen and Chen (2008) observed that in large  $p$  problems, the BIC tends to select models with too many parameters and suggested that instead of a prior uniform of all possible models, a prior uniform of models of fixed size. The general form of the  $BIC_\gamma$  criterion can be written,

$$BIC_\gamma = \mathcal{D} + k \log(n) + 2\gamma \log \binom{p}{k} \quad (2)$$

where  $\gamma$  is an adjustable parameter,  $p$  in the number of possible input variables not counting the bias or intercept term and  $k$  is the number of parameters in the model. Taking  $\gamma = 0$

reduces to the BIC. Notice that mid-sized models have the largest models, while  $k = 0$ , corresponding to only an intercept term and  $k = p$  corresponding to using all parameters are equally likely a priori. As pointed out in [Xu and McLeod \(2009\)](#) this prior is not reasonable because it is symmetric, giving large models and small models equal prior probability.

### *Best BICg Model for Prostate Data*

```
R> bestglm(Xy, IC = "BICg")

BICg(g = 1)
BICq equivalent for q in (0.0176493852011195, 0.512566675362627)
Best Model:
      Estimate Std. Error   t value    Pr(>|t|)
(Intercept) 2.4773573 0.09304738 26.624687 2.475214e-36
lcavol      0.7397137 0.09318316  7.938277 4.141615e-11
lweight     0.3163282 0.08830716  3.582135 6.576173e-04
```

## 2.4. BICq

As with the  $BIC_\gamma$  the notation  $BIC_q$  and  $BIC_q$  will be used interchangeably.

The  $BIC_q$  criterion ([Xu and McLeod 2009](#)) is derived by assuming a Bernoulli prior for the parameters. Each parameter has a priori probability of  $q$  of being included, where  $q \in [0, 1]$ . With this prior, the resulting information criterion can be written,

$$BIC_q = \mathcal{D} + k \log(n) - 2k \log q / (1 - q). \quad (3)$$

When  $q = 1/2$ , the  $BIC_q$  is equivalent to the BIC while  $q = 0$  and  $q = 1$  correspond to selecting the models with  $k = p$  and  $k = 0$  respectively. Moreover,  $q$  can be chosen to give results equivalent to the  $BIC_\gamma$  for any  $\gamma$  or the AIC [Xu and McLeod \(2009\)](#). When other information criteria are used with `bestglm`, the range of the  $q$  parameter that will produce the same result is shown. For example in [2.3.1](#), we see that  $q \in (0.0176493852011195, 0.512566675362627)$  produces an equivalent result.

For  $q = 0$ , the penalty is taken to be  $-\infty$  and so no parameters are selected and similarly for  $q = 1$ , the full model with all covariates is selected.

[Xu and McLeod \(2009\)](#) derive an interval estimate for  $q$  that is based on a confidence probability  $\alpha$ ,  $0 < \alpha < 1$ . This parameter may be set by the optional argument `qLevel` =  $\alpha$ . The default setting is with  $\alpha = 0.99$ .

### *Numerical Illustration q-Interval Computation*

In [Xu and McLeod \(2009, Table 1\)](#) we provided a brief illustrations of the computation of the intervals for  $q$  given by our Theorem.

```
R> set.seed(1233211235)
R> p <- 5
R> n <- 100
```



```

R> X <- matrix(rnorm(n * p), ncol = p)
R> err <- rnorm(n)
R> y <- 0.1 * (X[, 1] + X[, 2] + X[, 3]) + err
R> Xy <- as.data.frame(cbind(X, y))
R> names(Xy) <- c(paste("X", 1:p, sep = ""), "y")
R> ans <- bestglm(Xy)
R> ans$Subsets

```

	(Intercept)	X1	X2	X3	X4	X5	logLikelihood	BIC
0	TRUE	FALSE	FALSE	FALSE	FALSE	FALSE	-16.617205	33.23441
1*	TRUE	FALSE	FALSE	FALSE	FALSE	TRUE	-12.933572	30.47231
2	TRUE	FALSE	FALSE	TRUE	FALSE	TRUE	-11.149821	31.50998
3	TRUE	TRUE	FALSE	TRUE	FALSE	TRUE	-9.667975	33.15146
4	TRUE	TRUE	FALSE	TRUE	TRUE	TRUE	-9.608972	37.63862
5	TRUE	TRUE	TRUE	TRUE	TRUE	TRUE	-9.589967	42.20578

```

R> ans$qTable

```

	LogL	q1	q2	k
[1,]	-16.617205	0.0000000	0.2008406	0
[2,]	-12.933572	0.2008406	0.6268752	1
[3,]	-11.149821	0.6268752	0.6943933	2
[4,]	-9.667975	0.6943933	0.9040955	3
[5,]	-9.608972	0.9040955	0.9075080	4
[6,]	-9.589967	0.9075080	1.0000000	5

In [Xu and McLeod \(2009, Table 1\)](#) we added 20 to the value of the log-likelihood.

### *Best BIC<sub>q</sub> Model for Prostate Data*

Using the BIC<sub>q</sub> with its default choice for the tuning parameter  $q = t$ ,

```

R> data(zprostate)
R> train <- (zprostate[zprostate[, 10], ])[, -10]
R> X <- train[, 1:8]
R> y <- train[, 9]
R> Xy <- cbind(as.data.frame(X), lpsa = y)
R> out <- bestglm(Xy, IC = "BICq")

```

## 3. Cross-Validation

Cross-validation approaches to model selection are widely used and are also available in the `bestglm` function. The old standard, leave-one-out cross-validation (LOOCV) is implemented along with the more modern methods: K-fold and delete-d cross-validation (CV).

All CV methods work by first narrowing the field to the best models of size  $k$  for  $k = 0, 1, \dots, p$  and then comparing each of these models  $p+1$  possible models using cross-validation to select the best one. The best model of size  $k$  is chosen as the one with the smallest deviance.

### 3.1. Delete-d Cross-Validation

The delete-d method was suggested by [Shao \(1993\)](#). In the random sampling version of this algorithm, random samples of size  $d$  are used as the validation set. Many validation sets are generated in this way and the complementary part of the data is used each time as the training set. Typically 1000 validation sets are used.

When  $d = 1$ , the delete-d is similar to LOOCV (3.4) and should give the same result if enough validation sets are used.

[Shao \(1997\)](#) shows that when  $d$  increases with  $n$ , this method will be consistent. Note that  $K$ -fold cross-validation is approximately equivalent taking  $d \approx n/K$ . But [Shao \(1997\)](#) recommends a much larger cross-validation sample than is customarily used in  $K$ -fold CV. Letting  $\lambda_n = \log n$  as suggested [Shao \(1997, page 236, 4th line of last paragraph\)](#) and using [Shao \(1997, eqn. 4.5\)](#), we obtain

$$d^* = n(1 - (\log n - 1)^{-1}), \quad (4)$$

where  $n$  is the number of observations.

#### Comparison of size of validation samples for various sample sizes $n$ using delete- $d$ and $K$ -fold cross-validation.

$n$	$d^*$	$K = 10$	$K = 5$
50	33	5	10
100	73	10	20
200	154	20	40
500	405	50	100
1000	831	100	200

#### *Best Delete-d Model for Prostate Data*

The default cross-validation method is delete-d with 1000 replications, as with `bestglm(Xy, IC="CV")`. This takes about one minute to run, so in this vignette we set the optional tuning parameter `t=10` so only 10 replications are done.

The default for `IC="CV"` is delete-d with  $d$  as in eqn. (4) but in the example below, we set the optional tuning parameter `t=10`

```
R> set.seed(123321123)
R> bestglm(Xy, IC = "CV", t = 10)
```

```
CVd(d = 47, REP = 10)
```

```
No BICq equivalent
```

```
Best Model:
```

```
          Estimate Std. Error   t value    Pr(>|t|)
(Intercept) 2.4627121 0.08901202 27.667185 3.167240e-36
```

lcavol	0.5566392	0.11360017	4.899985	7.408246e-06
lweight	0.2415963	0.09467037	2.551974	1.323253e-02
lbph	0.1989292	0.10187183	1.952740	5.544293e-02
svi	0.2393565	0.11734589	2.039752	4.571228e-02
pgg45	0.1221447	0.10256941	1.190849	2.383261e-01

In practice though at least 1000 replications are usually needed to obtain convergence.

### 3.2. K-fold

Hastie *et al.* (2009) discuss  $K$ -fold CV. With this method, the data are divided, randomly, into  $K$  folds of approximately equal size.

For the prostate training data with  $n = 67$  and using  $K = 10$  folds,

```
R> set.seed(2377723)
R> ind <- sample(rep(1:10, length = 67))
R> ind
```

```
[1] 10  1  5 10  2  8  9  4  5  6  8  4  1  1  2  6  6  4  6  5  6  6  7  3  3
[26]  2  7  7  1  9 10  7 10  5  9  9  5  7  8  9  4  3  1  3  1  8  9  2  3 10
[51]  4  1  8  4  4  2  2  3 10  7  8  3  7  5  2  6  5
```

We see that the observations in  $\Pi_1$  are,

```
R> (1:67)[1 == ind]
```

```
[1]  2 13 14 29 43 45 52
```

and the values of  $N_k, k = 1, \dots, 10$  are:

```
R> tabulate(ind)
```

```
[1] 7 7 7 7 7 7 7 6 6 6
```

These folds form a partition of the the observations  $1, \dots, n$ . We will denote the set of elements in the  $k$ th partition by  $\Pi_k$ .

One fold is selected as the validation sample and the reamining to into the training sample. The performance is calibrated on the validation sample. This is repeated for each fold. The average performance over the  $K$  folds is determined.

Hastie *et al.* (2009) suggest using the *one-standard-deviation rule* with  $K$ -fold cross-validation. This makes the model selection more stable than simply selecting the model model with the best overall average performance. This rule was original defined in (Breiman, Freidman, Olshen, and Stone 1984, p. 79, Definition 3.19)) and used for selecting the best pruned CART.

For subset selection, this approach is implemented as follows. The validation sum-of-squares is computed for each of the  $K$  validation samples,

$$S_k = \sum_{i \in \Pi_k} \lim (\hat{e}^{(-k)_i})^2, \quad (5)$$

where  $e^{(-k)_i}$  denotes the prediction error when the  $k$ th validation sample is removed, the model fit to the remainder of the data and then used to predict the observations  $i \in \Pi_k$  in the validation sample. The final cross-validation score is

$$CV = \frac{1}{n} \sum_{k=1}^K S_k \quad (6)$$

where  $n$  is the number of observations. In each validation sample we may obtain the estimate of the cross-validation mean-square error,  $CV_k = S_k/N_k$ , where  $N_k$  is the number of observations in the  $k$ th validation sample. Let  $s^2$  be the sample variance of  $CV_1, \dots, CV_K$ . So an estimate of the sample variance of CV, the mean of  $CV_1, \dots, CV_K$  is  $s^2/K$ . Then an interval estimate for CV, using the one-standard-deviation rule, is  $CV \pm s/\sqrt{K}$ . When applied to model selection, this suggests that instead of selecting the model with the smallest CV, the most parsimonious adequate model will correspond to the model with the best CV score which is still inside this interval. Using this rule greatly improves the stability of k-fold CV.

This rule is implemented when the HTF CV method is used in our **bestglm** function.

```
R> set.seed(2377723)
R> out <- bestglm(Xy, IC = "CV", CVArgs = list(Method = "HTF", K = 10,
+       REP = 1))
R> out
```

```
CV(K = 10, REP = 1)
BICq equivalent for q in (0.0176493852011195, 0.512566675362627)
Best Model:
      Estimate Std. Error  t value    Pr(>|t|)
(Intercept) 2.4773573 0.09304738 26.624687 2.475214e-36
lcavol      0.7397137 0.09318316  7.938277 4.141615e-11
lweight     0.3163282 0.08830716  3.582135 6.576173e-04
```

In Figure 1 below we reproduce one of the graphs shown in (Hastie *et al.* 2009, page 62, Figure 3.3) that illustrates how the one-standard deviation rule works for model selection.

```
R> cverrs <- out$Subsets[, "CV"]
R> sdCV <- out$Subsets[, "sdCV"]
R> CVLo <- cverrs - sdCV
R> CVHi <- cverrs + sdCV
R> ymax <- max(CVHi)
R> ymin <- min(CVLo)
R> k <- 0:(length(cverrs) - 1)
R> plot(k, cverrs, xlab = "Subset Size", ylab = "CV Error", ylim = c(ymin,
```

```

+      ymax), type = "n", yaxt = "n")
R> points(k, cverrs, cex = 2, col = "red", pch = 16)
R> lines(k, cverrs, col = "red", lwd = 2)
R> axis(2, yaxp = c(0.6, 1.8, 6))
R> segments(k, CVLo, k, CVHi, col = "blue", lwd = 2)
R> eps <- 0.15
R> segments(k - eps, CVLo, k + eps, CVLo, col = "blue", lwd = 2)
R> segments(k - eps, CVHi, k + eps, CVHi, col = "blue", lwd = 2)
R> indBest <- oneSdRule(out$Subsets[, c("CV", "sdCV")])
R> abline(v = indBest - 1, lty = 2)
R> indMin <- which.min(cverrs)
R> fmin <- sdCV[indMin]
R> cutOff <- fmin + cverrs[indMin]
R> abline(h = cutOff, lty = 2)
R> indMin <- which.min(cverrs)
R> fmin <- sdCV[indMin]
R> cutOff <- fmin + cverrs[indMin]
R> min(which(cverrs < cutOff))

```

[1] 3

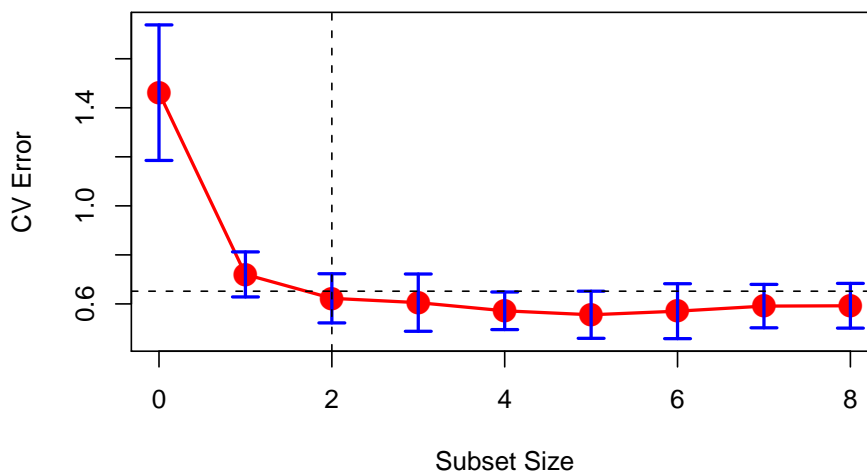


Figure 1: Model selection with 10-fold cross-validation and 1-sd rule

### 3.3. Bias Correction

[Davison and Hinkley \(1997, Algorithm 6.5, p.295\)](#) suggested an adjusted CV statistic which corrects for bias but this method has quite variable in small samples.

Running the program 3 times produces 3 different results.

```
R> set.seed(2377723)
R> bestglm(Xy, IC = "CV", CVArgs = list(Method = "DH", K = 10, REP = 1))
```

```
CVAdj(K = 10, REP = 1)
```

```
No BICq equivalent
```

```
Best Model:
```

	Estimate	Std. Error	t value	Pr(> t )
(Intercept)	2.4627121	0.08901202	27.667185	3.167240e-36
lcavol	0.5566392	0.11360017	4.899985	7.408246e-06
lweight	0.2415963	0.09467037	2.551974	1.323253e-02
lbph	0.1989292	0.10187183	1.952740	5.544293e-02
svi	0.2393565	0.11734589	2.039752	4.571228e-02
pgg45	0.1221447	0.10256941	1.190849	2.383261e-01

```
R> bestglm(Xy, IC = "CV", CVArgs = list(Method = "DH", K = 10, REP = 1))
```

```
CVAdj(K = 10, REP = 1)
```

```
No BICq equivalent
```

```
Best Model:
```

	Estimate	Std. Error	t value	Pr(> t )
(Intercept)	2.4511950	0.08783569	27.906596	4.589425e-36
lcavol	0.6479821	0.12357416	5.243670	2.153436e-06
lweight	0.2412408	0.09315188	2.589758	1.203646e-02
lbph	0.1827709	0.10067001	1.815545	7.443814e-02
svi	0.3131270	0.12305547	2.544601	1.353129e-02
lcp	-0.2668206	0.15391392	-1.733570	8.813073e-02
pgg45	0.2126933	0.11363923	1.871654	6.613158e-02

```
R> bestglm(Xy, IC = "CV", CVArgs = list(Method = "DH", K = 10, REP = 1))
```

```
CVAdj(K = 10, REP = 1)
```

```
BICq equivalent for q in (0.708764213288624, 0.889919748490004)
```

```
Best Model:
```

	Estimate	Std. Error	t value	Pr(> t )
(Intercept)	2.4668675	0.08760022	28.160516	6.632457e-36
lcavol	0.6764486	0.12383666	5.462426	9.883880e-07
lweight	0.2652760	0.09363348	2.833132	6.298761e-03
age	-0.1450300	0.09756540	-1.486490	1.424742e-01
lbph	0.2095349	0.10128348	2.068796	4.295574e-02
svi	0.3070936	0.12190105	2.519204	1.449125e-02
lcp	-0.2872242	0.15300241	-1.877253	6.543004e-02
pgg45	0.2522850	0.11562030	2.182013	3.310324e-02

The results obtained after 1000 simulations are summarized in the table below.

Number of inputs selected	1	2	3	4	5	6	7	8
Frequency in 1000 simulations	0	0	23	61	64	289	448	115

When REP is increased to 100, the result converges the model with 7 inputs. It takes about 66 seconds. Using REP=100 many times, it was found that models with 7 inputs were selected 95

We conclude that if either this method (Davison and Hinkley 1997, Algorithm 6.5, p.295) or the method of Hastie *et al.* (2009) is used, many replications are need to obtain a stable result. In view of this, the delete-d of cross-validation is recommended.

### 3.4. Leave-one-out Cross-Validation

For completeness we include leave-one-out CV (LOOCV) but this method is not recommended because the model selection is not usually as accurate as either of the other CV methods discussed above. This is due to the high variance of this method (Hastie *et al.* 2009, Section 7.10).

In leave-one-out CV (LOOCV), one observation, say the  $i$ , is removed, the regression is refit and the prediction error,  $\hat{e}_{(i)}$  for the missing observation is obtained. This process is repeated for all observations  $i = 1, \dots, n$  and the prediction error sum of squares is obtained,

$$\text{PRESS} = \sum_{i=1}^n \hat{e}_{(i)}^2. \quad (7)$$

In the case of linear regression, leave-out-CV can be computed very efficiently using the PRESS method (Allen 1971),  $\hat{e}_{(i)} = \hat{e}_i$  where  $\hat{e}_i$  is the usual regression residual and  $h_{i,i}$  is the  $i$ -th element on the diagonal of the hat matrix  $H = XX'X)^{-1}X'$ . Stone (1977) showed that asymptotically LOOCV is equivalent to the AIC. The computation is very efficient.

#### *Best LOOCV Model for Prostate Data*

```
R> bestglm(Xy, IC = "LOOCV")
```

```
LOOCV
```

```
BICq equivalent for q in (0.708764213288624, 0.889919748490004)
```

```
Best Model:
```

	Estimate	Std. Error	t value	Pr(> t )
(Intercept)	2.4668675	0.08760022	28.160516	6.632457e-36
lcavol	0.6764486	0.12383666	5.462426	9.883880e-07
lweight	0.2652760	0.09363348	2.833132	6.298761e-03
age	-0.1450300	0.09756540	-1.486490	1.424742e-01
lbph	0.2095349	0.10128348	2.068796	4.295574e-02
svi	0.3070936	0.12190105	2.519204	1.449125e-02
lcp	-0.2872242	0.15300241	-1.877253	6.543004e-02
pgg45	0.2522850	0.11562030	2.182013	3.310324e-02

## 4. Examples from our BICq Paper

The following examples were briefly discussed in our paper “Improved Extended Bayesian Information Criterion” (Xu and McLeod 2009).

#### 4.1. Hospital Manpower Data

This dataset was used as an example in our paper (Xu and McLeod 2009, Example 1). We commented on the fact that both the AIC and BIC select the same model with 3 variables even though one of the variables is not even significant at the 5% level and has the incorrect sign.

```
R> data(manpower)
R> bestglm(manpower, IC = "AIC")
```

```
AIC
BICq equivalent for q in (0.258049145974038, 0.680450993834175)
Best Model:
```

	Estimate	Std. Error	t value	Pr(> t )
(Intercept)	1523.38923568	786.89772473	1.935943	7.492387e-02
Xray	0.05298733	0.02009194	2.637243	2.050318e-02
BedDays	0.97848162	0.10515362	9.305258	4.121293e-07
Stay	-320.95082518	153.19222065	-2.095086	5.631250e-02

```
R> bestglm(manpower, IC = "BIC")
```

```
BIC
BICq equivalent for q in (0.258049145974038, 0.680450993834175)
Best Model:
```

	Estimate	Std. Error	t value	Pr(> t )
(Intercept)	1523.38923568	786.89772473	1.935943	7.492387e-02
Xray	0.05298733	0.02009194	2.637243	2.050318e-02
BedDays	0.97848162	0.10515362	9.305258	4.121293e-07
Stay	-320.95082518	153.19222065	-2.095086	5.631250e-02

In this case the  $BIC_\gamma$  is completely useless selecting the full model when  $\gamma = 1$  or  $\gamma = 0.5$ .

```
R> bestglm(manpower, IC = "BICg")
```

```
BICg(g = 1)
BICq equivalent for q in (0.801591282573779, 1)
Best Model:
```

	Estimate	Std. Error	t value	Pr(> t )
(Intercept)	1962.94815647	1.071362e+03	1.8321993	0.09410839
Load	-15.85167473	9.765299e+01	-0.1623266	0.87399215
Xray	0.05593038	2.125828e-02	2.6309923	0.02336582
BedDays	1.58962370	3.092083e+00	0.5140947	0.61735574
AreaPop	-4.21866799	7.176557e+00	-0.5878401	0.56851117
Stay	-394.31411702	2.096395e+02	-1.8809148	0.08670281



```
R> bestglm(manpower, IC = "BICg", t = 0.5)
```

```
BICg(g = 0.5)
```

```
BICq equivalent for q in (0.258049145974038, 0.680450993834175)
```

```
Best Model:
```

	Estimate	Std. Error	t value	Pr(> t )
(Intercept)	1523.38923568	786.89772473	1.935943	7.492387e-02
Xray	0.05298733	0.02009194	2.637243	2.050318e-02
BedDays	0.97848162	0.10515362	9.305258	4.121293e-07
Stay	-320.95082518	153.19222065	-2.095086	5.631250e-02

Finally, with the  $BIC_q$  with its default choice,  $q = 0.25$ ,

```
R> out <- bestglm(manpower, IC = "BICq")
```

```
R> out
```

```
BICq(q = 0.25)
```

```
BICq equivalent for q in (0.00764992882308291, 0.258049145974038)
```

```
Best Model:
```

	Estimate	Std. Error	t value	Pr(> t )
(Intercept)	-68.31395896	228.44597086	-0.2990377	7.693043e-01
Xray	0.07486591	0.01913019	3.9134953	1.559779e-03
BedDays	0.82287456	0.08295986	9.9189488	1.033117e-07

The optimal range of  $q$  includes  $q = 0.25$ ,

```
R> out$Bestq
```

	q1	q2	selected	k
BICq1	0.007649929	0.2580491		2
BICq2	0.007649929	0.2580491		2

The calculations for the best  $q$  may be checked using

```
R> out$Subsets
```

	(Intercept)	Load	Xray	BedDays	AreaPop	Stay	logLikelihood	BICq
0	TRUE	FALSE	FALSE	FALSE	FALSE	FALSE	-146.0833	292.1667
1	TRUE	FALSE	FALSE	TRUE	FALSE	FALSE	-115.6360	236.3024
2*	TRUE	FALSE	TRUE	TRUE	FALSE	FALSE	-109.3540	228.7688
3	TRUE	FALSE	TRUE	TRUE	FALSE	TRUE	-106.8812	228.8538
4	TRUE	FALSE	TRUE	TRUE	TRUE	TRUE	-106.2205	232.5627
5	TRUE	TRUE	TRUE	TRUE	TRUE	TRUE	-106.2001	237.5525

and

```
R> out$qTable
```

	LogL	q1	q2	k
[1,]	-146.0833	0.000000e+00	2.466916e-13	0
[2,]	-115.6360	2.466916e-13	7.649929e-03	1
[3,]	-109.3540	7.649929e-03	2.580491e-01	2
[4,]	-106.8812	2.580491e-01	6.804510e-01	3
[5,]	-106.2205	6.804510e-01	8.015913e-01	4
[6,]	-106.2001	8.015913e-01	1.000000e+00	5

## 4.2. South African Heart Disease

The response variable, `chd`, indicates the presence or absence of coronary heart disease and there are nine inputs. The sample size is 462. Logistic regression is used. The full model is,

```
R> data(SAheart)
R> out <- bestglm(SAheart, IC = "BICq", t = 1, family = binomial)
```

Note: in this special case with BICq with  $t = 1$  only fitted model is returned. With  $t=1$ , full model is fitted.

```
R> out
```

```
BICq(q = 1)
Best Model:
```

	Estimate	Std. Error	z value	Pr(> z )
(Intercept)	-6.1507208650	1.308260018	-4.70145138	2.583188e-06
sbp	0.0065040171	0.005730398	1.13500273	2.563742e-01
tobacco	0.0793764457	0.026602843	2.98375801	2.847319e-03
ldl	0.1739238981	0.059661738	2.91516648	3.554989e-03
adiposity	0.0185865682	0.029289409	0.63458325	5.257003e-01
famhistPresent	0.9253704194	0.227894010	4.06052980	4.896149e-05
typea	0.0395950250	0.012320227	3.21382267	1.309805e-03
obesity	-0.0629098693	0.044247743	-1.42176449	1.550946e-01
alcohol	0.0001216624	0.004483218	0.02713729	9.783502e-01
age	0.0452253496	0.012129752	3.72846442	1.926501e-04

We find that the bounding interval for  $q$  is  $0.191 \leq q \leq 0.901$ . For values of  $q$  in this interval a model with 5 inputs: `tobacco`, `ldl`, `famhist`, `typea` and `age` and as expected all variables have very low  $p$ -values. Using  $q$  in the interval  $0.094 < q < 0.190$  results in a subset of the above model which excludes `ldl`. Using cross-validation [Hastie et al. \(2009, §4.4.2\)](#) also selected a model for this data with only four inputs but their subset excluded `typea` instead of `ldl`.

It is interesting that the subset chosen in [Hastie et al. \(2009, Section 4.4.2\)](#) may be found using two other suboptimal procedures. First using the  $BIC_q$  with  $q = 0.25$  and the R function `step`,

```
R> ans <- glm(chd ~ ., data = SAheart)
R> q <- 0.25
R> n <- nrow(SAheart)
R> k <- log(n) - 2 * log(q/(1 - q))
R> step(ans, k = k)
```

Start: AIC=585.74

```
chd ~ sbp + tobacco + ldl + adiposity + famhist + typea + obesity +
      alcohol + age
```

	Df	Deviance	AIC
- alcohol	1	79.919	577.49
- adiposity	1	79.945	577.64
- sbp	1	80.187	579.04
- obesity	1	80.350	579.98
<none>		79.904	585.74
- typea	1	81.480	586.43
- ldl	1	81.612	587.18
- tobacco	1	81.962	589.15
- age	1	82.002	589.38
- famhist	1	83.025	595.11

Step: AIC=577.49

```
chd ~ sbp + tobacco + ldl + adiposity + famhist + typea + obesity +
      age
```

	Df	Deviance	AIC
- adiposity	1	79.957	569.38
- sbp	1	80.192	570.73
- obesity	1	80.362	571.71
<none>		79.919	577.49
- typea	1	81.483	578.11
- ldl	1	81.677	579.21
- tobacco	1	81.979	580.92
- age	1	82.035	581.23
- famhist	1	83.025	586.78

Step: AIC=569.38

```
chd ~ sbp + tobacco + ldl + famhist + typea + obesity + age
```

	Df	Deviance	AIC
- sbp	1	80.248	562.73
- obesity	1	80.490	564.12
<none>		79.957	569.38
- typea	1	81.491	569.83
- ldl	1	81.921	572.26
- tobacco	1	82.025	572.84

```
- famhist 1 83.063 578.65
- age      1 83.232 579.59
```

Step: AIC=562.73

```
chd ~ tobacco + ldl + famhist + typea + obesity + age
```

	Df	Deviance	AIC
- obesity	1	80.686	556.91
<none>		80.248	562.73
- typea	1	81.736	562.88
- ldl	1	82.223	565.62
- tobacco	1	82.396	566.59
- famhist	1	83.331	571.81
- age	1	84.416	577.78

Step: AIC=556.91

```
chd ~ tobacco + ldl + famhist + typea + age
```

	Df	Deviance	AIC
- typea	1	82.043	556.28
<none>		80.686	556.91
- ldl	1	82.322	557.84
- tobacco	1	82.867	560.90
- famhist	1	83.725	565.66
- age	1	84.483	569.82

Step: AIC=556.28

```
chd ~ tobacco + ldl + famhist + age
```

	Df	Deviance	AIC
<none>		82.043	556.28
- ldl	1	83.914	558.36
- tobacco	1	84.351	560.76
- age	1	85.309	565.98
- famhist	1	85.368	566.30

```
Call: glm(formula = chd ~ tobacco + ldl + famhist + age, data = SAheart)
```

Coefficients:

(Intercept)	tobacco	ldl	famhistPresent	age
-0.237407	0.017263	0.032533	0.178173	0.006836

Degrees of Freedom: 461 Total (i.e. Null); 457 Residual

Null Deviance: 104.6

Residual Deviance: 82.04 AIC: 524.6

Even with  $q = 0.1$  in the above script only tobacco, famhist and age are selected. And using

$q = 0.5$  in the above script with `step` selects the same model the BICselects when exhaustive enumeration is done using `bestglm`. This example points out that using `step` for subset selection may produce a suboptimal answer.

Yet another way that the four inputs selected by [Hastie \*et al.\* \(2009, Section 4.4.2\)](#) could be obtained is to use least squares with `bestglm` to find the model with the best four inputs.

```
R> out <- bestglm(SAheart, IC = "BICq", t = 0.25)
```

Note: binary categorical variables converted to 0-1 so 'leaps' could be used.

```
R> out$Subsets
```

	(Intercept)	sbp	tobacco	ldl	adiposity	famhist	typea	obesity	alcohol
0	TRUE	FALSE	FALSE	FALSE	FALSE	FALSE	FALSE	FALSE	FALSE
1	TRUE	FALSE	FALSE	FALSE	FALSE	FALSE	FALSE	FALSE	FALSE
2	TRUE	FALSE	FALSE	FALSE	FALSE	TRUE	FALSE	FALSE	FALSE
3	TRUE	FALSE	TRUE	FALSE	FALSE	TRUE	FALSE	FALSE	FALSE
4*	TRUE	FALSE	TRUE	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE
5	TRUE	FALSE	TRUE	TRUE	FALSE	TRUE	TRUE	FALSE	FALSE
6	TRUE	FALSE	TRUE	TRUE	FALSE	TRUE	TRUE	TRUE	FALSE
7	TRUE	TRUE	TRUE	TRUE	FALSE	TRUE	TRUE	TRUE	FALSE
8	TRUE	TRUE	TRUE	TRUE	TRUE	TRUE	TRUE	TRUE	FALSE
9	TRUE	TRUE	TRUE	TRUE	TRUE	TRUE	TRUE	TRUE	TRUE

	age	logLikelihood	BICq
0	FALSE	343.1572	-686.3144
1	TRUE	377.7581	-747.1834
2	TRUE	387.4922	-758.3188
3	TRUE	394.0337	-763.0691
4*	TRUE	399.2435	-765.1559
5	TRUE	403.0944	-764.5248
6	TRUE	404.3510	-758.7053
7	TRUE	405.1909	-752.0524
8	TRUE	405.3023	-743.9423
9	TRUE	405.3439	-735.6928

## 5. Other Illustrative Examples

### 5.1. Nuclear Power Plant Data

```
R> data(znuclear)
R> bestglm(znuclear, IC = "AIC")
```

AIC

BICq equivalent for  $q$  in (0.349204366418954, 0.716418902103358)

Best Model:

	Estimate	Std. Error	t value	Pr(> t )
(Intercept)	-38.7480703	7.91826983	-4.893502	4.910313e-05
date	0.5620284	0.11445901	4.910303	4.701224e-05
capacity	0.4759804	0.07818015	6.088252	2.310934e-06
NE	0.6588957	0.19616044	3.358963	2.510375e-03
CT	0.3714664	0.15987847	2.323430	2.858187e-02
N	-0.2277672	0.10786682	-2.111560	4.489115e-02
PT	-0.5982476	0.30044058	-1.991235	5.748951e-02

## 5.2. Detroit Homicide Data

Our analysis will use the six inputs which generate the lowest residual sum of squares. These inputs are 1, 2, 4, 6, 7 and 11 as given in Miller (2002, Table 3.14). We have scaled the inputs, although this is not necessary in this example. Using backward step-wise regression in R, no variables are removed. But note that variables 1, 6 and 7 are all only significant at about 5%. Bearing in mind the selection effect, the true significance is much less.

```
R> data(Detroit)
R> X <- as.data.frame(scale(Detroit[, c(1, 2, 4, 6, 7, 11)]))
R> y <- Detroit[, ncol(Detroit)]
R> Xy <- cbind(X, HOM = y)
R> out <- lm(HOM ~ ., data = Xy)
R> step(out, k = log(nrow(Xy)))
```

Start: AIC=-11.34

HOM ~ FTP.1 + UEMP.2 + LIC.4 + CLEAR.6 + WM.7 + WE.11

	Df	Sum of Sq	RSS	AIC
<none>			1.3659	-11.3357
- WM.7	1	1.2724	2.6383	-5.3427
- CLEAR.6	1	1.3876	2.7535	-4.7871
- FTP.1	1	1.4376	2.8035	-4.5533
- WE.11	1	8.1170	9.4830	11.2888
- UEMP.2	1	16.3112	17.6771	19.3849
- LIC.4	1	20.6368	22.0027	22.2305

Call:

```
lm(formula = HOM ~ FTP.1 + UEMP.2 + LIC.4 + CLEAR.6 + WM.7 + WE.11, data = Xy)
```

Coefficients:

(Intercept)	FTP.1	UEMP.2	LIC.4	CLEAR.6	WM.7
25.127	1.724	2.570	5.757	-2.329	-2.452
WE.11					
6.084					

Same story with exhaustive search algorithm.

```
R> out <- bestglm(Xy, IC = "BIC")
R> out
```

BIC

BICq equivalent for q in (0.115398370069662, 1)

Best Model:

	Estimate	Std. Error	t value	Pr(> t )
(Intercept)	25.126923	0.1323333	189.875990	1.439772e-12
FTP.1	1.724110	0.6861084	2.512883	4.572467e-02
UEMP.2	2.569527	0.3035648	8.464511	1.485656e-04
LIC.4	5.757015	0.6046682	9.520948	7.657697e-05
CLEAR.6	-2.329338	0.9435019	-2.468822	4.853518e-02
WM.7	-2.452200	1.0372544	-2.364126	5.596776e-02
WE.11	6.083694	1.0188489	5.971144	9.892298e-04

We can use BICq to reduce the number of variables. The `qTable` let's choose q for other possible models.

```
R> out$qTable
```

	LogL	q1	q2	k
[1,]	-35.832829	0.000000e+00	5.144759e-08	0
[2,]	-17.767652	5.144759e-08	3.468452e-05	1
[3,]	-6.215995	3.468452e-05	1.039797e-04	2
[4,]	4.237691	1.039797e-04	7.680569e-02	3
[5,]	8.006726	7.680569e-02	1.153984e-01	4
[6,]	14.645170	1.153984e-01	1.000000e+00	6

This suggest we try  $q=0.05$

```
R> bestglm(Xy, IC = "BICq", t = 0.05)
```

BICq(q = 0.05)

BICq equivalent for q in (0.000103979673982901, 0.0768056921650389)

Best Model:

	Estimate	Std. Error	t value	Pr(> t )
(Intercept)	25.12692	0.2406075	104.43119	3.435051e-15
UEMP.2	3.38307	0.2601848	13.00257	3.876404e-07
LIC.4	8.20378	0.2802445	29.27365	3.090409e-10
WE.11	10.90084	0.2787164	39.11089	2.321501e-11

Or  $q=0.0005$ .

```
R> bestglm(Xy, IC = "BICq", t = 5e-05)
```

BICq(q = 5e-05)

BICq equivalent for q in (3.46845195655643e-05, 0.000103979673982901)

Best Model:

	Estimate	Std. Error	t value	Pr(> t )
(Intercept)	25.126923	0.5101048	49.258354	2.871539e-13
LIC.4	4.473245	0.6381795	7.009384	3.673796e-05
CLEAR.6	-13.386666	0.6381795	-20.976334	1.346067e-09

The above results agree with Miller (2002, Table 3.14). It is interesting that the subset model of size 2 is not a subset itself of the size 3 model. It is clear that simply adding and/or dropping one variable at a time as in the stepwise and stagewise algorithms will not work in moving either from model 2 to model 3 or vice-versa.

Using delete-d CV with d=4 suggests variables 2,4,6,11

```
R> set.seed(1233211)
```

```
R> bestglm(Xy, IC = "CV", CVArgs = list(Method = "d", K = 4, REP = 50))
```

CVd(d = 4, REP = 50)

BICq equivalent for q in (0.0768056921650389, 0.115398370069661)

Best Model:

	Estimate	Std. Error	t value	Pr(> t )
(Intercept)	25.126923	0.1909731	131.573114	1.244969e-14
UEMP.2	2.571151	0.3840754	6.694391	1.535921e-04
LIC.4	7.270181	0.4337409	16.761574	1.624771e-07
CLEAR.6	-3.250371	1.2964006	-2.507227	3.652839e-02
WE.11	8.329213	1.0492726	7.938083	4.617821e-05

### 5.3. Air Quality Data

Here is an example of a dataset with categorical variables at more than 2 levels. First we look at the full model,

```
R> data(AirQuality)
```

```
R> bestglm(AirQuality, IC = "BICq", t = 1)
```

Note: in this special case with BICq with t = 1 only fitted model is returned. With t=1, full model is fitted.

BICq(q = 1)

Best Model:

	Df	Sum Sq	Mean Sq	F value	Pr(>F)	
Solar.R	1	14780	14780	31.9857	1.815e-07	***
Wind	1	39969	39969	86.5007	8.147e-15	***
Temp	1	19050	19050	41.2273	6.239e-09	***
month	11	3713	338	0.7305	0.7066	
weekday	6	2703	451	0.9750	0.4469	
Residuals	90	41586	462			

---

Signif. codes: 0 '\*\*\*' 0.001 '\*\*' 0.01 '\*' 0.05 '.' 0.1 ' ' 1



Next we find the best AIC model,

```
R> bestglm(AirQuality, IC = "AIC")
```

Morgan-Tatar search since factors present with more than 2 levels.

AIC

Best Model:

	Df	Sum Sq	Mean Sq	F value	Pr(>F)
Solar.R	1	14780	14780	32.944	8.946e-08 ***
Wind	1	39969	39969	89.094	9.509e-16 ***
Temp	1	19050	19050	42.463	2.424e-09 ***
Residuals	107	48003	449		

---

Signif. codes: 0 '\*\*\*' 0.001 '\*\*' 0.01 '\*' 0.05 '.' 0.1 ' ' 1

## 5.4. Forest Fires

The forest fire data were collected during January 2000 to December 2003 for fires in the Montesinho natural park located in the Northeast region of Portugal. The response variable of interest was area burned in ha. When the area burned as less than one-tenth of a hectare, the response variable as set to zero. In all there were 517 fires and 247 of them recorded as zero.

The dataset was provided by [Cortez and Morais \(2007\)](#) who also fit this data using neural nets and support vector machines.

The region was divided into a 10-by-10 grid with coordinates X and Y running from 1 to 9 as shown in the diagram below. The categorical variable `xyarea` indicates the region in this grid for the fire. There are 36 different regions so `xyarea` has 35 df.

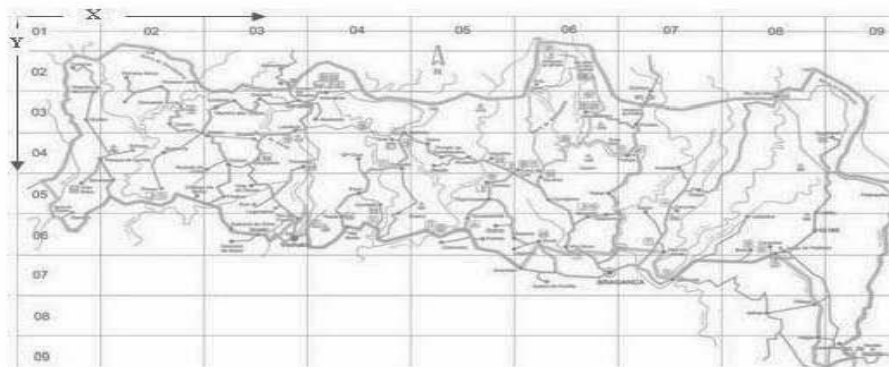


Figure 2: Montesinho Park

Fitting the best-AIC regression,

```
R> data(Fires)
R> bestglm(Fires, IC = "AIC")
```

Morgan-Tatar search since factors present with more than 2 levels.

AIC

Best Model:

	Df	Sum Sq	Mean Sq	F value	Pr(>F)
month	11	37.37	3.3970	1.7958	0.05195 .
DMC	1	6.31	6.3145	3.3381	0.06829 .
DC	1	4.85	4.8468	2.5622	0.11008
temp	1	8.92	8.9165	4.7136	0.03039 *
wind	1	3.94	3.9384	2.0820	0.14967
Residuals	501	947.72	1.8917		

---  
 Signif. codes: 0 '\*\*\*' 0.001 '\*\*' 0.01 '\*' 0.05 '.' 0.1 ' ' 1

## 6. Simulated Data

### 6.1. Null Regression Example

Here we check that our function handles the null regression case where there are no inputs to include in the model. We assume an intercept term only.

```
R> set.seed(123312123)
R> X <- as.data.frame(matrix(rnorm(50), ncol = 2, nrow = 25))
R> y <- rnorm(25)
R> Xy <- cbind(X, y = y)
R> bestglm(Xy)
```

BIC

BICq equivalent for q in (0, 0.540989544689166)

Best Model:

	Estimate	Std. Error	t value	Pr(> t )
(Intercept)	-0.3074955	0.2323344	-1.323504	0.1981378

### 6.2. Logistic Regression

As a check we simulate a logistic regression with  $K = 10$  inputs. The inputs are all Gaussian white noise with unit variance. So the model equation may be written,  $Y$  is IID Bernoulli distribution with parameter  $p$ ,  $p = \mathcal{E}(Y) = h(\beta_0 + \beta_1 X_1 + \dots + \beta_K X_K)$  where  $h(x) = (1 + e^{-x})^{-1}$ . Note that  $h$  is the inverse of the logit transformation and it may conveniently be obtained in R using `plogist`. In the code below we set  $\beta_0 = a = -1$  and  $\beta_1 = 3$ ,  $\beta_2 = 2$ ,  $\beta_3 = 4/3$ ,  $\beta_4 = 2\frac{2}{3}$  and  $\beta_i = 0, i = 5, \dots, 10$ . Taking  $n = 500$  as the sample size we find after fit with `glm`.

```
R> set.seed(231231)
R> n <- 500
```

```

R> K <- 10
R> a <- -1
R> b <- c(c(9, 6, 4, 8)/3, rep(0, K - 4))
R> X <- matrix(rnorm(n * K), ncol = K)
R> L <- a + X %*% b
R> p <- plogis(L)
R> Y <- rbinom(n = n, size = 1, prob = p)
R> X <- as.data.frame(X)
R> out <- glm(Y ~ ., data = X, family = binomial)
R> summary(out)

```

Call:

```
glm(formula = Y ~ ., family = binomial, data = X)
```

Deviance Residuals:

	Min	1Q	Median	3Q	Max
	-2.80409	-0.28120	-0.02809	0.25338	2.53513

Coefficients:

	Estimate	Std. Error	z value	Pr(> z )
(Intercept)	-0.882814	0.182554	-4.836	1.33e-06 ***
V1	3.186252	0.325376	9.793	< 2e-16 ***
V2	1.874106	0.242864	7.717	1.19e-14 ***
V3	1.500606	0.215321	6.969	3.19e-12 ***
V4	2.491092	0.281585	8.847	< 2e-16 ***
V5	0.029539	0.165162	0.179	0.858
V6	-0.179920	0.176994	-1.017	0.309
V7	-0.047183	0.172862	-0.273	0.785
V8	-0.121629	0.168903	-0.720	0.471
V9	-0.229848	0.161735	-1.421	0.155
V10	-0.002419	0.177972	-0.014	0.989

---

Signif. codes: 0 '\*\*\*' 0.001 '\*\*' 0.01 '\*' 0.05 '.' 0.1 ' ' 1

(Dispersion parameter for binomial family taken to be 1)

Null deviance: 685.93 on 499 degrees of freedom  
 Residual deviance: 243.86 on 489 degrees of freedom  
 AIC: 265.86

Number of Fisher Scoring iterations: 7

### 6.3. Binomial Regression

As a further check we fit a binomial regression taking  $n = 500$  with  $K = 10$  inputs and with Bernoulli number of trials  $m = 100$ . So in this case the model equation may be

written,  $Y$  is IID binomially distributed with number of trials  $m = 10$  and parameter  $p$ ,  $p = \mathcal{E}(Y) = h(\beta_0 + \beta_1 X_1 + \dots + \beta_K X_K)$  where  $h(x) = (1 + e^{-x})^{-1}$ . We used the same  $\beta$ 's as in Section 6.2.

```
R> set.seed(231231)
R> n <- 500
R> K <- 8
R> m <- 100
R> a <- 2
R> b <- c(c(9, 6, 4, 8)/10, rep(0, K - 4))
R> X <- matrix(rnorm(n * K), ncol = K)
R> L <- a + X %*% b
R> p <- plogis(L)
R> Y <- rbinom(n = n, size = m, prob = p)
R> Y <- cbind(Y, m - Y)
R> dimnames(Y)[[2]] <- c("S", "F")
R> X <- as.data.frame(X)
R> out <- glm(Y ~ ., data = X, family = binomial)
R> summary(out)
```

Call:

```
glm(formula = Y ~ ., family = binomial, data = X)
```

Deviance Residuals:

	Min	1Q	Median	3Q	Max
	-2.77988	-0.70691	0.07858	0.75158	2.70323

Coefficients:

	Estimate	Std. Error	z value	Pr(> z )
(Intercept)	2.025629	0.016967	119.383	<2e-16 ***
V1	0.898334	0.015175	59.197	<2e-16 ***
V2	0.607897	0.012987	46.809	<2e-16 ***
V3	0.429355	0.013609	31.551	<2e-16 ***
V4	0.835002	0.014962	55.807	<2e-16 ***
V5	-0.006607	0.013867	-0.476	0.634
V6	-0.011497	0.013596	-0.846	0.398
V7	0.022112	0.013660	1.619	0.105
V8	0.000238	0.013480	0.018	0.986

---

Signif. codes: 0 '\*\*\*' 0.001 '\*\*' 0.01 '\*' 0.05 '.' 0.1 ' ' 1

(Dispersion parameter for binomial family taken to be 1)

```
Null deviance: 10752.23 on 499 degrees of freedom
Residual deviance: 507.19 on 491 degrees of freedom
AIC: 2451.8
```

Number of Fisher Scoring iterations: 4

In this example, one input V6 is significant at level 0.03 even though its correct coefficient is zero.

```
R> Xy <- cbind(X, Y)
R> bestglm(Xy, family = binomial)
```

Morgan-Tatar search since family is non-gaussian.

BIC

BICq equivalent for q in (0, 0.870630550022155)

Best Model:

	Estimate	Std. Error	z value	Pr(> z )
(Intercept)	2.0247237	0.01689493	119.84211	0.000000e+00
V1	0.8995804	0.01513694	59.42948	0.000000e+00
V2	0.6063199	0.01287612	47.08872	0.000000e+00
V3	0.4290062	0.01360140	31.54132	2.358219e-218
V4	0.8349437	0.01485556	56.20412	0.000000e+00

Using the default selection method, BIC, the correct model is selected.

## 6.4. Binomial Regression With Factor Variable

An additional check was done to incorporate a factor variable. We include a factor input representing the day-of-week effect. The usual corner-point method was used to parameterize this variable and large coefficients chosen, so that this factor would have a strong effect. Using the corner-point method, means that the model matrix will have six additional columns of indicator variables. We used four more columns of numeric variables and then added the six columns for the indicators to simulate the model.

```
R> set.seed(33344111)
R> n <- 500
R> K <- 4
R> m <- 100
R> a <- 2
R> dayNames <- c("Sunday", "Monday", "Tuesday", "Wednesday", "Friday",
+               "Saturday")
R> Days <- data.frame(d = factor(rep(dayNames, n))[1:n])
R> Xdays <- model.matrix(~d, data = Days)
R> bdays <- c(7, 2, -7, 0, 2, 7)/10
R> Ldays <- Xdays %*% bdays
R> b <- c(c(9, 6)/10, rep(0, K - 2))
R> X <- matrix(rnorm(n * K), ncol = K)
R> L <- a + X %*% b
R> L <- L + Ldays
R> p <- plogis(L)
```

```

R> Y <- rbinom(n = n, size = m, prob = p)
R> Y <- cbind(Y, m - Y)
R> dimnames(Y)[[2]] <- c("S", "F")
R> X <- as.data.frame(X)
R> X <- data.frame(X, days = Days)
R> out <- glm(Y ~ ., data = X, family = binomial)
R> anova(out, test = "Chisq")

```

Analysis of Deviance Table

Model: binomial, link: logit

Response: Y

Terms added sequentially (first to last)

	Df	Deviance	Resid. Df	Resid. Dev	P(> Chi )
NULL			499	5609.2	
V1	1	2992.36	498	2616.9	<2e-16 ***
V2	1	1253.89	497	1363.0	<2e-16 ***
V3	1	2.49	496	1360.5	0.1145
V4	1	1.91	495	1358.6	0.1668
d	5	797.44	490	561.1	<2e-16 ***

---

Signif. codes: 0 '\*\*\*' 0.001 '\*\*' 0.01 '\*' 0.05 '.' 0.1 ' ' 1

After fitting with `glm` we find the results as expected. The factor variable is highly significant as well as the first two quantitative variables.

Using `bestglm`, we find it selects the correct model.

```

R> Xy <- cbind(X, Y)
R> out <- bestglm(Xy, IC = "BICq", family = binomial)

```

Morgan-Tatar search since family is non-gaussian.

Note: factors present with more than 2 levels.

```
R> out
```

BICq(q = 0.25)

Best Model:

Response S :

	Df	Sum Sq	Mean Sq	F value	Pr(>F)
V1	1	24841.5	24841.5	792.61	< 2.2e-16 ***
V2	1	9110.0	9110.0	290.67	< 2.2e-16 ***
d	5	7473.4	1494.7	47.69	< 2.2e-16 ***

```

Residuals    492 15419.9    31.3
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

Response F :
      Df Sum Sq Mean Sq F value    Pr(>F)
V1      1 24841.5 24841.5  792.61 < 2.2e-16 ***
V2      1  9110.0  9110.0  290.67 < 2.2e-16 ***
d       5  7473.4  1494.7   47.69 < 2.2e-16 ***
Residuals 492 15419.9    31.3
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

```

## 6.5. Poisson Regression

```

R> set.seed(231231)
R> n <- 500
R> K <- 4
R> a <- -1
R> b <- c(c(1, 0.5), rep(0, K - 2))
R> X <- matrix(rnorm(n * K), ncol = K)
R> L <- a + X %*% b
R> lambda <- exp(L)
R> Y <- rpois(n = n, lambda = lambda)
R> X <- as.data.frame(X)
R> out <- glm(Y ~ ., data = X, family = poisson)
R> summary(out)

```

```

Call:
glm(formula = Y ~ ., family = poisson, data = X)

```

```

Deviance Residuals:
      Min       1Q   Median       3Q      Max
-2.1330  -0.8084  -0.4853   0.4236   2.6320

```

```

Coefficients:
      Estimate Std. Error z value Pr(>|z|)
(Intercept) -0.92423    0.07933 -11.650  <2e-16 ***
V1           0.97841    0.05400  18.119  <2e-16 ***
V2           0.51967    0.05707   9.107  <2e-16 ***
V3           0.03773    0.05525   0.683    0.495
V4           0.03085    0.04646   0.664    0.507
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

```

(Dispersion parameter for poisson family taken to be 1)

```
Null deviance: 880.73 on 499 degrees of freedom
Residual deviance: 427.49 on 495 degrees of freedom
AIC: 913.41
```

Number of Fisher Scoring iterations: 5

As expected the first two variables are highly significant and the next two are not.

```
R> Xy <- data.frame(X, y = Y)
R> bestglm(Xy, family = poisson)
```

Morgan-Tatar search since family is non-gaussian.

BIC

BICq equivalent for q in (0, 0.947443940310683)

Best Model:

	Estimate	Std. Error	z value	Pr(> z )
(Intercept)	-0.9292265	0.07955966	-11.679619	1.620199e-31
V1	0.9897770	0.05284046	18.731421	2.744893e-78
V2	0.5302822	0.05588287	9.489171	2.328782e-21

Our function `bestglm` selects the correct model.

## 6.6. Gamma Regression

To simulate a Gamma regression we first write a function `GetGammaParameters` that translates mean and standard deviation into the shape and scale parameters for the function `rgamma`.

```
R> GetGammaParameters <- function(muz, sdz) {
+   phi <- (sdz/muz)^2
+   nu <- 1/phi
+   lambda <- muz/nu
+   list(shape = nu, scale = lambda)
+ }
R> set.seed(321123)
R> test <- rnorm(20)
R> n <- 500
R> b <- c(0.25, 0.5, 0, 0)
R> b0 <- 0.3
R> K <- length(b)
R> sdz <- 1
R> X <- matrix(rnorm(n * K), ncol = K)
R> L <- b0 + X %*% b
R> muHat <- exp(L)
R> gp <- GetGammaParameters(muHat, sdz)
R> zsim <- rgamma(n, shape = gp$shape, scale = gp$scale)
```



```
R> Xy <- data.frame(as.data.frame.matrix(X), y = zsim)
R> out <- glm(y ~ ., data = Xy, family = Gamma(link = log))
R> summary(out)
```

Call:

```
glm(formula = y ~ ., family = Gamma(link = log), data = Xy)
```

Deviance Residuals:

Min	1Q	Median	3Q	Max
-5.6371	-0.7417	-0.1968	0.2237	3.2105

Coefficients:

	Estimate	Std. Error	t value	Pr(> t )
(Intercept)	0.313964	0.044124	7.115	3.93e-12 ***
V1	0.191957	0.040983	4.684	3.64e-06 ***
V2	0.558321	0.042485	13.142	< 2e-16 ***
V3	0.018709	0.044939	0.416	0.677
V4	0.004252	0.043367	0.098	0.922

---

Signif. codes: 0 '\*\*\*' 0.001 '\*\*' 0.01 '\*' 0.05 '.' 0.1 ' ' 1

(Dispersion parameter for Gamma family taken to be 0.944972)

Null deviance: 792.56 on 499 degrees of freedom  
 Residual deviance: 621.67 on 495 degrees of freedom  
 AIC: 1315.9

Number of Fisher Scoring iterations: 9

```
R> bestglm(Xy, family = Gamma(link = log))
```

Morgan-Tatar search since family is non-gaussian.

BIC

BICq equivalent for q in (0.000599916119599198, 0.953871171759292)

Best Model:

	Estimate	Std. Error	t value	Pr(> t )
(Intercept)	0.3110431	0.04353445	7.144757	3.229210e-12
V1	0.1931868	0.04098936	4.713096	3.172312e-06
V2	0.5560244	0.04226866	13.154531	4.011556e-34

As expected, `bestglm` selects the correct model.

## 7. Simulation Experiment

Please see the separate vignette [Xu and McLeod \(2009\)](#) for a discussion of how the simulation experiment reported in [Xu and McLeod \(2009, Table 2\)](#) was carried out as well for more

detailed results of the simulation results themselves. The purpose of the simulation experiment reported on in [Xu and McLeod \(2009, Table 2\)](#) and described in more detail in the accompanying vignette [Xu and McLeod \(2009\)](#) was to compare different information criteria used in model selection.

Similar simulation experiments were used by [Shao \(1993\)](#) to compare cross-validation criteria for linear model selection. In the simulation experiment reported by [Shao \(1993\)](#), the performance of various CV methods for linear model selection were investigated for the linear regression,

$$y = 2 + \beta_2 x_2 + \beta_3 x_3 + \beta_4 x_4 + \beta_5 x_5 + e, \quad (8)$$

where  $e \sim \text{NID}(0, 1)$ . A fixed sample size of  $n = 40$  was used and the design matrix used is given in ([Shao 1993, Table 1](#)) and the four different values of the  $\beta$ 's are shown in the table below,

Experiment	$\beta_2$	$\beta_3$	$\beta_4$	$\beta_5$
1	0	0	4	0
2	0	0	4	8
3	9	0	4	8
4	9	6	4	8

The table below summarizes the probability of correct model selection in the experiment reported by [Shao \(1993, Table 2\)](#). Three model selection methods are compared: LOOCV (leave-one-out CV), CV(d=25) or the delete-d method with d=25 and APCV which is a very efficient computation CV method but specialized to the case of linear regression.

Experiment	LOOCV	CV(d=25)	APCV
1	0.484	0.934	0.501
2	0.641	0.947	0.651
3	0.801	0.965	0.818
4	0.985	0.948	0.999

The CV(d=25) outperforms LOOCV in all cases and it also outperforms APCV by a large margin in Experiments 1, 2 and 3 but in case 4 APCV is slightly better.

In the code below we show how to do our own experiments to compare model selection using the BIC,  $\text{BIC}_\gamma$  and  $\text{BIC}_q$  criteria.

```
R> testCorrect <- function(ans, NB) {
+   NBfit <- names(coef(ans))[-1]
+   ans <- ifelse(length(NBfit) == length(NB) & (!any(is.na(match(NBfit,
+     NB))))), 1, 0)
+   ans
+ }
R> NSIM <- 5
R> data(Shao)
R> set.seed(123321123)
R> X <- as.matrix.data.frame(Shao)
R> BETA <- list(b1 = c(0, 0, 4, 0), b2 = c(0, 0, 4, 8), b3 = c(9,
+   0, 4, 8), b4 = c(9, 6, 4, 8))
R> NamesBeta <- list(b1 = c("x4"), b2 = c("x4", "x5"), b3 = c("x2",
+   "x4", "x5"), b4 = c("x2", "x3", "x4", "x5"))
R> hitsBIC <- hitsEBIC <- hitsQBIC <- numeric(4)
```

```

R> startTime <- proc.time()[1]
R> for (iB in 1:4) {
+   b <- BETA[[iB]]
+   NB <- NamesBeta[[iB]]
+   for (iSIM in 1:NSIM) {
+     y <- 2 + X %*% b + rnorm(40)
+     Xy <- cbind(Shao, y)
+     hitsBIC[iB] <- hitsBIC[iB] + testCorrect(bestglm(Xy,
+       IC = "BIC")$BestModel, NB)
+     hitsEBIC[iB] <- hitsEBIC[iB] + testCorrect(bestglm(Xy,
+       IC = "BICg")$BestModel, NB)
+     hitsQBIC[iB] <- hitsQBIC[iB] + testCorrect(bestglm(Xy,
+       IC = "BICq")$BestModel, NB)
+   }
+ }
R> endTime <- proc.time()[1]
R> totalTime <- endTime - startTime
R> ans <- matrix(c(hitsBIC, hitsEBIC, hitsQBIC), byrow = TRUE, ncol = 4)
R> dimnames(ans) <- list(c("BIC", "BICg", "BICq"), 1:4)
R> ans <- t(ans)/NSIM
R> ans

```

```

      BIC BICg BICq
1 0.6  0.8  0.8
2 1.0  0.8  1.0
3 1.0  0.8  1.0
4 1.0  1.0  1.0

```

```
R> totalTime
```

```

user.self
      1.02

```

Increasing the number of simulations so NSIM=10000, the following result was obtained,

```

      BIC  BICg  BICq
1 0.8168 0.8666 0.9384
2 0.8699 0.7741 0.9566
3 0.9314 0.6312 0.9761
4 0.9995 0.9998 0.9974

```

## 8. Controlling Type 1 Error Rate

Consider the case where there are  $p$  input variables and it we wish to test the null hypothesis  $\mathcal{H}_0$ : the output is not related to any inputs. By adjusting  $q$  in the  $BIC_q$  criterion, we can control the Type 1 error rate. Using simulation, we can determine for any particular  $n$  and

$p$ , what value of  $q$  is needed to achieve a Type 1 error rate for a particular level, such as  $\alpha = 0.05$ .

We compare the performance of information selection criteria in the case of a null model with  $p = 25$  inputs and  $n = 30$  observations. Using 50 simulations takes about 30 seconds. Since there is no relation between the inputs and the output, the correct choice is the null model with no parameters. Using the BICq criterion with  $q = 0.05$  works better than AIC, BIC or BICg. We may consider the number of parameters selected as the frequency of Type 1 errors in an hypothesis testing framework. By adjusting  $q$  we may adjust the Type 1 error rate to any desired level. This suggests a possible bootstrapping approach to the problem of variable selection.

```
R> set.seed(123321123)
R> startTime <- proc.time()[1]
R> NSIM <- 5
R> p <- 25
R> n <- 30
R> ans <- numeric(4)
R> names(ans) <- c("AIC", "BIC", "BICg", "BICq")
R> for (iSim in 1:NSIM) {
+   X <- matrix(rnorm(n * p), ncol = p)
+   y <- rnorm(n)
+   Xy <- as.data.frame(cbind(X, y))
+   names(Xy) <- c(paste("X", 1:p, sep = ""), "y")
+   bestAIC <- bestglm(Xy, IC = "AIC")
+   bestBIC <- bestglm(Xy, IC = "BIC")
+   bestEBIC <- bestglm(Xy, IC = "BICg")
+   bestQBIC <- bestglm(Xy, IC = "BICq", t = 0.05)
+   ans[1] <- ans[1] + length(coef(bestAIC$BestModel)) - 1
+   ans[2] <- ans[2] + length(coef(bestBIC$BestModel)) - 1
+   ans[3] <- ans[3] + length(coef(bestEBIC$BestModel)) - 1
+   ans[4] <- ans[4] + length(coef(bestQBIC$BestModel)) - 1
+ }
R> endTime <- proc.time()[1]
R> totalTime <- endTime - startTime
R> totalTime

user.self
  4.54

R> ans

AIC  BIC BICg BICq
58   13    0    0
```

## 9. Concluding Remarks

The subset regression problem is related to the subset autoregression problem that as been discussed by McLeod and Zhang (2006, 2008) and implemented in the **FitAR** R package available on CRAN. The **FitAR** has been updated to include the new  $BIC_q$  criterion.

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