lmSubsets: Exact Variable-Subset Selection in Linear Regression for R

Marc Hofmann
University of Oviedo
Cyprus University of Technology

Cristian Gatu
"Alexandru Ioan Cuza"
University of Iasi

Erricos J. Kontoghiorghes
Cyprus University of Technology
Birkbeck, University of London

Ana Colubi
University of Oviedo

Achim Zeileis
Universität Innsbruck

Abstract

An R package for computing the all-subsets regression problem is presented. The proposed algorithms are based on computational strategies recently developed. A novel algorithm for the best-subset regression problem selects subset models based on a predetermined criterion. The package user can choose from exact and from approximation algorithms. The core of the package is written in C++ and provides an efficient implementation of all the underlying numerical computations. A case study and benchmark results illustrate the usage and the computational efficiency of the package.

Keywords: linear regression, model selection, variable selection, best subset regression, R.

1. Introduction

An important problem in statistical modeling is that of subset selection regression or, equivalently, of finding the best regression equation (Clarke 1981; Hastie *et al.* 2001). Given a set of possible variables to be included in the regression, the problem consists in selecting a subset that optimizes some statistical criterion. The evaluation of the criterion function typically involves the estimation of the corresponding submodel (Miller 2002). Consider the standard regression model

$$y = X\beta + \epsilon, \tag{1}$$

where $y \in \mathbb{R}^M$ is the output variable, $X \in \mathbb{R}^{M\times N}$ is the regressor matrix of full column rank, $\beta \in \mathbb{R}^N$ is the coefficient vector, and $\epsilon \in \mathbb{R}^M$ is the noise vector. The ordinary least squares (OLS) estimator of β is the solution of

$$\widehat{\beta}_{\text{OLS}} = \underset{\beta}{\operatorname{argmin}}\, \text{RSS}(\beta), \tag{2}$$

where the residual sum of squares (RSS) of β is given by

$$\text{RSS}(\beta) = \|y - X\beta\|_2^2. \tag{3}$$

That is, $\widehat{\beta}_{\text{OLS}}$ minimizes the norm of the residual vector. The regression coefficients β do not

need to be explicitly computed in order to determine the RSS, which can be obtained through numerically stable orthogonal matrix decomposition methods (Golub and Van Loan 1996).

Let $V = \{1, \ldots, N\}$ denote the set of all independent variables. A subset model (or submodel) is denoted by S, $S \subseteq V$. Given a criterion function f, the best-subset selection problem consists in solving

$$S^* = \operatorname*{argmin}_{S \subseteq V} f(S). \tag{4}$$

Here, the value $f(S) = F(n, \rho)$ is seen as a function of $n = |S|$ and $\rho = \mathrm{RSS}(S)$, the number of selected variables and the RSS of the OLS estimator for S, respectively. Furthermore, it is assumed that $f(S)$ is monotonic with respect to $\mathrm{RSS}(S)$ for fixed n, that is

$$\mathrm{RSS}(S_1) \leq \mathrm{RSS}(S_2) \Rightarrow f(S_1) \leq f(S_2), \quad \text{when} \quad |S_1| = |S_2|. \tag{5}$$

Common selection criteria exhibit this property, such as those belonging to the AIC family defined by the formula

$$\mathrm{AIC}_k = M + M \log 2\pi + M \log(\mathrm{RSS}/M) + k(n+1), \tag{6}$$

where the scalar k represents a penalty per parameter ($k > 0$). The usual AIC and BIC are obtained for $k = 2$ and $k = \log M$, respectively (Miller 2002). It follows that (4) is equivalent to

$$S^* = S^*_\nu, \quad \text{where} \quad \nu = \operatorname*{argmin}_n f(S^*_n)$$

and

$$S^*_n = \operatorname*{argmin}_{|S|=n} \mathrm{RSS}(S) \quad \text{for} \quad n = 1, \ldots, N. \tag{7}$$

Finding the solution to (7) is called the all-subsets selection problem. Thus, solving (4) can be seen as an indirect, two-stage procedure:

Stage 1 For each size n, find the subset S^*_n ($|S^*_n| = n$) with the smallest RSS.

Stage 2 Compute $f(S^*_n)$ for all n, and determine ν such that $f(S^*_\nu)$ is minimal.

Note that the computational strategy may be optimized for a specific selection criterion when solving the best-subset selection problem (4) directly, thus lowering the computational cost. On the other hand, by explicitly solving the all-subsets regression problem (7) once and for all (Stage 1), the list of all N submodels is made readily available for further exploration: evaluating multiple criterion functions (e.g., AIC and BIC), or conducting a more elaborate statistical inference, can be performed at a negligible cost (Stage 2). Thus, it can be advisable to adopt a two-stage approach within the scope of a broader and more thorough statistical investigation.

Brute-force (or exhaustive) search procedures that enumerate all possible subsets are often intractable even for a modest number of variables. Exact algorithms must employ techniques to reduce the size of the search space – i.e., the number of enumerated subsets – in order to tackle larger problems. Heuristic algorithms renounce optimality in order to decrease execution times: they are designed for solving a problem more quickly, but make no guarantees on the quality of the solution produced; genetic algorithms and simulated annealing count among the well-known heuristic algorithms. The solution returned by an approximation

algorithm, on the other hand, can be prroven to lie within well specified bounds of the optimum.

Several packages that deal with variable subset selection are available on the R platform. The package **leaps** (Lumley and Miller 2017) implements exact, non-exhaustive algorithms for subset regression based on Miller (2002). Exhaustive algorithms have been considered within the context of generalized linear models (package **bestglm**, McLeod and Xu 2017). The package **subselect** proposes simulated annealing algorithms based on the work of Duarte Silva (2001). Furthermore, genetic algorithms for generalized linear models have been implemented by Calcagno and de Mazancourt (2010, package **glmulti**) and Wolters (2015, package **kofnGA**). Non-exact algorithms for regularized estimation of parametric models with automatic variable selection performed by lasso or elastic net estimation for generalized linear models have been investigated by Friedman *et al.* (2010).

Here, the **lmSubsets** package (Hofmann *et al.* 2017) for exact variable-subset regression is presented. It offers methods for solving both the best-subset (4) and the all-subsets (7) selection problems. It implements the algorithms presented by Gatu and Kontoghiorghes (2006) and Hofmann *et al.* (2007). A branch-and-bound strategy is employed to reduce the size of the search space. A similar approach has been employed for exact least-trimmed-squares regression Hofmann *et al.* (2010). The package further proposes approximation methods that compute non-exact solutions very quickly while giving guarantees on the quality of the result. The core of the package is written in C++. The package is available for the R system for statistical computing (R Core Team 2017) from The Comprehensive R Archive Network at `https://CRAN.R-project.org/package=lmSubsets`.

Section 2 reviews the theoretical background and the underlying algorithms. The package's R interface is presented in Section 3. A usage example is given in Section 4, while benchmark results are illustrated in Section 5.

2. Computational strategies

The linear regression model (1) has 2^N possible subset models which can be efficiently organized in a regression tree. A dropping column algorithm (DCA) was devised as a straightforward approach to solve the all-subsets selection problem (7). The DCA evaluates all possible variable subsets by traversing a regression tree consisting of $2^{(N-1)}$ nodes (Gatu and Kontoghiorghes 2003; Gatu *et al.* 2007; Smith and Bremner 1989).

Each node of the regression tree can be represented by a pair (S, k), where $S = \{s_1, \ldots, s_n\}$ corresponds to a subset of n variables, $n = 0, \ldots, N$, and $k = 0, \ldots, n-1$. The subleading models are defined as $\{s_1, \ldots, s_{k+1}\}, \ldots, \{s_1, \ldots, s_n\}$, the RSS of which are computed for each visited node. The root node $(V, 0)$ corresponds to the full model. Child nodes are generated by dropping (deleting) a single variable:

$$\mathsf{drop}(S, j) = (S \setminus \{s_j\}, j-1), \quad j = k+1, \ldots, n-1.$$

Numerically, this is equivalent to downdating an orthogonal matrix decomposition after a column has been deleted (Golub and Van Loan 1996; Kontoghiorghes 2000; Smith and Bremner 1989). Givens rotations are employed to efficiently move from one node to another. The DCA maintains a subset table r with N entries, where entry r_n contains the RSS of the current-best submodel of size n (Gatu and Kontoghiorghes 2006; Hofmann *et al.* 2007). Figure 1

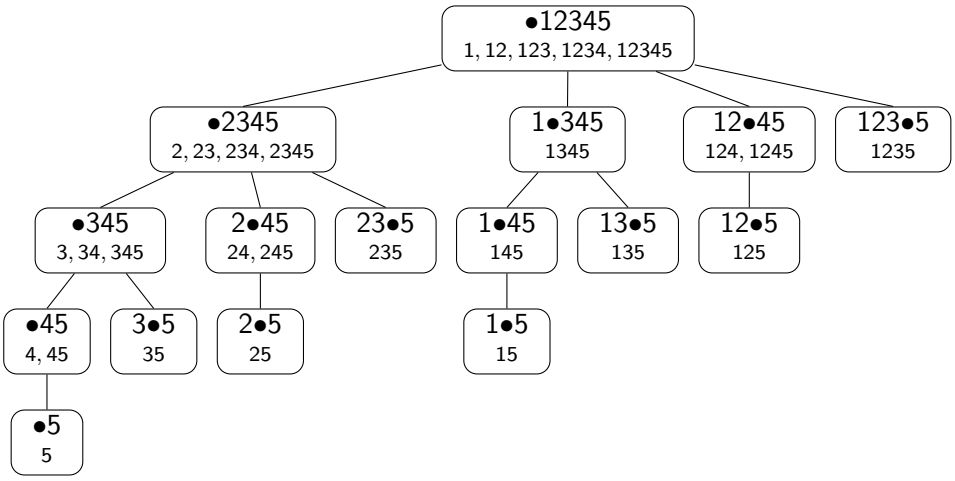


Figure 1: All-subsets regression tree for $N = 5$ variables. Nodes are shown together with their subleading models.

illustrates a regression tree for $N = 5$ variables. The index k is symbolized by a bullet (•). The subleading models are listed in each node.

The DCA is computationally demanding, with a theoretical time complexity of $O(2^N)$. A branch-and-bound algorithm (BBA) has been devised to reduce the number of generated nodes by cutting subtrees which do not contribute to the current-best solution. It relies on the fundamental property that the RSS increases when variables are deleted from a regression model, that is:

$$S_1 \subseteq S_2 \Rightarrow \mathrm{RSS}(S_1) \geq \mathrm{RSS}(S_2).$$

A cutting test is employed to determine which parts of the DCA tree are redundant: A new node $\mathsf{drop}(S, j)$ is generated only if $\mathrm{RSS}(S) < r_j$ $(j = k+1, \ldots, n-1)$. The quantity $\mathrm{RSS}(S)$ is called the bound of the subtree rooted in (S, k): no subset model extracted from the subtree can have a smaller RSS (Gatu and Kontoghiorghes 2006). Note that the BBA is an exact algorithm, i.e., it computes the optimal solution of the all-subsets regression problem (7).

To further reduce the computational cost, the all-subsets regression problem can be restricted to a range of submodel sizes (Hofmann *et al.* 2007). In this case, the problem (7) is reformulated as

$$S_n^* = \underset{|S|=n}{\operatorname{argmin}} \mathrm{RSS}(S) \quad \text{for} \quad n = n_{\min}, \ldots, n_{\max}, \tag{8}$$

where $n_{\min}$ and $n_{\max}$ are the subrange limits $(1 \leq n_{\min} \leq n_{\max} \leq N)$. The search will span only a part of the DCA regression tree. Specifically, nodes (S, k) are not computed if $|S| < n_{\min}$ or $k \geq n_{\max}$.

The size of subtrees rooted in the same level decreases exponentially from left to right. In order to encourage the pruning of large subtrees by the BBA cutting test, the variables in a given node can be ordered such that a child node will always have a larger RSS (i.e., bound) than its right siblings (Gatu and Kontoghiorghes 2006). This strategy can be applied in nodes of arbitrary depth. However, computing the variable bounds incurs a computational overhead. Thus, it is not advisable to indiscriminately preorder variables. A parameter – the

preordering radius p – has been introduced to control the degree of preordering (Hofmann *et al.* 2007). It accepts a value between $p = 0$ (no preordering) and $p = N$ (preordering in all nodes); when $p = 1$, preordering is performed in the root node only. Typically, $p = \lfloor N/3 \rfloor$ produces better results in terms of execution time.

The computational efficiency of the BBA is improved by allowing the algorithm to prune non-redundant branches of the regression tree. The approximation branch-and-bound algorithm (ABBA) relaxes the cutting test by employing a set of tolerance parameters $\tau_n \geq 0$ ($n = 1, \ldots, N$), one for every submodel size. A node $\mathsf{drop}(S, j)$ is generated only if there exists at least one i such that

$$(1 + \tau_i) \cdot (\mathrm{RSS}(S) - \mathrm{RSS}_{\mathrm{full}}) < (r_i - \mathrm{RSS}_{\mathrm{full}}), \quad i = j, \ldots, n - 1, \tag{9}$$

where $\mathrm{RSS}_{\mathrm{full}} = \mathrm{RSS}(V)$ is the RSS of the full model. The algorithm is non-exact if $\tau_n > 0$ for any n, meaning that the computed solution is not guaranteed to be optimal. The greater the value of τ_n, the more aggressively the regression tree will be pruned, thus decreasing the computational load. The advantage of the ABBA over heuristic algorithms is that the relative error of the solution is bounded by the tolerance parameter (Gatu and Kontoghiorghes 2006; Hofmann *et al.* 2007), thus giving the user control over the tradeoff between solution quality and speed of execution.

The DCA and its derivatives report the N subset models with the lowest RSS, one for each subset size. The user can then analyze the list of returned subsets to determine the "best" subset, for example by evaluating some criterion function. This approach is practical but not necessarily the most efficient to solve the best-subset selection problem (4). Let f be a criterion function such that $f(S) = F(n, \rho)$, where $n = |S|$ and $\rho = \mathrm{RSS}(S)$, satisfying the monotonicity property (5). The f-BBA specializes the standard cutting test for f under the additional condition that F is non-decreasing in n. Specifically, a node $\mathsf{drop}(S, j)$ is generated if and only if

$$F(j, \mathrm{RSS}(S)) < r_f, \tag{10}$$

where r_f is the single current-best solution. This results in a more "informed" cutting test, and in a smaller number of generated nodes.

3. Implementation in R

The R package **lmSubsets** provides a library of methods for variable subset selection in linear regression. Two S3 classes are defined, namely "`lmSubsets`" and "`lmSelect`", that address all-subsets (7) and best-subset (4) selection, respectively. The package offers R's standard formula interface: linear models can be specified by means of a symbolic formula, and possibly a data frame. The model specification is resolved into a regressor matrix and a response vector, which are forwarded to low-level functions for actual processing, together with optional arguments which further specify the selection problem. A routine to extract the best submodels from an all-subsets regression solution (i.e., to convert an "`lmSubsets`" to an "`lmSelect`" object) is also provided. An overview of the package structure is given in Table 1.

3.1. Specifying the selection problem

The default methods are closely modeled after R's standard `lm()` function: they can be called with any entity that can be coerced to a `formula` object (Chambers and Hastie 1992). The

S3 class	Methods and functions	Description
"lmSubsets"	`lmSubsets()`	all-subsets selection (generic function)
	`lmSubsets.matrix()`	matrix interface
	`lmSubsets.default()`	standard formula interface
	`lmSubsets_fit()`	low-level matrix interface
"lmSelect"	`lmSelect()`	best-subset selection (generic function)
	`lmSelect.lmSubsets()`	conversion method
	`lmSelect.matrix()`	matrix interface
	`lmSelect.default()`	standard formula interface
	`lmSelect_fit()`	low-level matrix interface

Table 1: Package structure.

`formula` object declares the dependent and independent variables, which are typically taken from a `data.frame` specified by the user. For example, the call

```
lmSubsets(mortality ~ precipitation + temperature1 + temperature7 +
  age + household + education + housing + population + noncauc +
  whitecollar + income + hydrocarbon + nox + so2 + humidity,
  data = AirPollution)
```

specifies a response variable (`mortality`) and fifteen predictor variables, all taken from the `AirPollution` dataset (Miller 2002). It is common to shorten the call by employing R's practical "dot-notation":

```
lmSubsets(mortality ~ ., data = AirPollution),
```

where the dot (`.`) stands for "all variables not mentioned in the left-hand side of the formula". By default, an intercept term is included in the model; that is, the call in the previous example is equivalent to

```
lmSubsets(mortality ~ . + 1, data = AirPollution).
```

To discard the intercept, the call may be rewritten as follows:

```
lmSubsets(mortality ~ . - 1, data = AirPollution).
```

Submodels can be rejected based on the presence or absence of certain independent variables. The parameter `include` specifies that all submodels must contain one or several variables. In the following example, only submodels containing the variable `noncauc` are retained:

```
lmSubsets(mortality ~ ., include = "noncauc", data = AirPollution).
```

Conversely, the `exclude` parameter can be employed to discard a specific set of variables, as in the following example:

```
lmSubsets(mortality ~ ., exclude = "whitecollar", data = AirPollution).
```

The same effect can be achieved by rewriting the formula as follows:

```
lmSubsets(mortality ~ . - whitecollar, data = AirPollution).
```

The `include` and `exclude` parameters may be used in combination, and both may specify more than one variable (e.g., `include = c("noncauc", "whitecollar")`).

The criterion used for best-subset selection is evaluated following the expression

$$-2 \cdot \texttt{logLik} + \texttt{penalty} \cdot \texttt{npar},$$

where `penalty` is the penalty per model parameter defined in (6), `logLik` the log-likelihood of the fitted model, and `npar` the number of model parameters (including the error variance). The `penalty` value indicates how strongly model parameters are penalized, with large values favoring parsimonious models. When `penalty` $= 2$, the criterion corresponds to Akaike's information criterion (AIC, Akaike 1974); when `penalty` $= \log($`nobs`$)$, to Schwarz's Bayesian information criterion (BIC, Schwarz 1978), where `nobs` is the number of observations. For example, either one of

```
lmSelect(mortality ~ ., data = AirPollution, penalty = 2)
```

and

```
lmSelect(mortality ~ ., data = AirPollution, penalty = "AIC")
```

will select the best submodel according to the usual AIC; by default, `lmSelect()` employs the BIC. The user may also specify a custom criterion function

```
lmSelect(..., penalty = function (size, rss) ...),
```

where `size` is the number of regressors, and `rss` the residual sum of squares of the corresponding submodel. The user-specified function must be non-decreasing in both parameters.

3.2. Core functions

The high-level interface methods process the model specification before dispatching the call to one of two low-level core functions, passing along a regressor matrix `x` and a response vector `y`, together with problem-specific arguments. The core functions act as wrappers around the C++ library, and are declared as

```
lmSubsets_fit(x, y, weights = NULL, offset = NULL, include = NULL,
  exclude = NULL, nmin = NULL, nmax = NULL, tolerance = 0,
  nbest = 1, ..., pradius = NULL)
```

and

```
lmSelect_fit(x, y, weights = NULL, offset = NULL, include = NULL,
  exclude = NULL, penalty = "BIC", tolerance = 0,
  nbest = 1, ..., pradius = NULL).
```

Parameter	Description	Canonical representation	
`x`	data matrix	`double[nobs,nvar]`	
`y`	response variable	`double[nobs]`	
`weights`	model weights	`double[nobs]`	
`offset`	model offset	`double[nvar]`	
`include`	regressors to force in	`logical[nvar]`	
`exclude`	regressors to force out	`logical[nvar]`	
`nmin`	min. number of regressors	`integer[1]`	`lmSubsets()` only
`nmax`	max. number of regressors	`integer[1]`	`lmSubsets()` only
`penalty`	penalty per parameter	`double[1]`	`lmSelect()` only
	or criterion function	`function[1]`	
`tolerance`	ABBA tolerance parameter	`double[nvar]`	`lmSubsets()`
		`double[1]`	`lmSelect()`
`nbest`	number of best subsets	`integer[1]`	
`pradius`	preordering radius	`integer[1]`	

Table 2: Core parameters for `lmSubsets()` and `lmSelect()`.

The parameters are summarized in Table 2.

The `weights` and `offset` parameters correspond to the homonymous parameters of the `lm()` function. The `include` and `exclude` parameters allow the user to specify variables that are to be included in, or excluded from all candidate models. They are either logical vectors – with each entry corresponding to one variable – or automatically expanded if given in the form of an integer vector (i.e., set of variable indices) or character vector (i.e., set of variable names).

For a large number of variables (see Section 5), execution times may become prohibitive. In order to speed up the execution, either the search space can be reduced, or one may settle for a non-exact solution. In the first approach, the user may specify values for the `nmin` and `nmax` parameters as defined in (8), in which case submodels with less than `nmin` or more than `nmax` variables are discarded. Well-defined regions of the regression tree can be ignored by the selection algorithm, and the search space is thus reduced.

In the second approach, expectations with respect to the solution quality are lowered, i.e., non-optimal solutions are tolerated. The numeric value – typically between 0 and 1 – passed as the `tolerance` argument indicates the degree of "over-pruning" performed by the ABBA cutting test (9). The solution produced by the ABBA satisfies the following relationship:

$$f(S) - f(V) \leq (1 + \texttt{tolerance}) \cdot (f(S^*) - f(V)),$$

where S is the returned solution, V the full model, S^* the optimal (theoretical) solution, and f the cost of a submodel (e.g., deviance, AIC). The `lmSubsets_fit()` function accepts a vector of tolerances, with one entry for each subset size.

The `nbest` parameter controls how many submodels (per subset size) are retained. In the case of `lmSubsets_fit()`, a two-dimensional result set is constructed with `nbest` submodels for each subset size, while in the case of `lmSelect_fit()`, a one-dimensional sequence of `nbest` submodels is handed back to the user.

Component	Description	Canonical representation
`nobs`	number of observations	`integer[1]`
`nvar`	number of regressors	`integer[1]`
`intercept`	intercept flag	`logical[1]`
`include`	regressors forced in	`logical[nvar]`
`exclude`	regressors forced out	`logical[nvar]`
`size`	covered subset sizes	`integer[]`
`tolerance`	tolerances used	`double[nvar]`
`nbest`	number of best subsets	`integer[1]`
`submodel`	submodel information	`data.frame`
`subset`	selected variables	`data.frame`

Table 3: Components of "`lmSubsets`" and "`lmSelect`" objects.

The `pradius` parameter serves to specify the desired preordering radius. The algorithm employs a default value of $\lfloor \texttt{nvar}/3 \rfloor$. The need to set this parameter directly should rarely arise; please refer to Section 2 for further information.

3.3. Extracting submodels

The user is handed back a result object that encapsulates the solution to an all-subsets (class "`lmSubsets`") or best-subset (class "`lmSelect`") selection problem. An object of class "`lmSubsets`" represents a two-dimensional `nvar` × `nbest` set of submodels; an object of class "`lmSelect`", a linear sequence of `nbest` submodels. Problem-specific information is stored alongside the selected submodels. Table 3 summarizes the components of the result objects.

A wide range of standard methods to visualize, summarize, and extract information are provided (see Table 4). The `print()`, `plot()`, and `summary()` methods give the user a compact overview – either textual or graphical – of the information gathered on the selected submodels in order to help identify "good" candidates. The remaining extractor functions can be used to extract variable names, coefficients, covariance matrices, fitted values, etc.

In order to designate a submodel, "`lmSubsets`" methods provide two parameters to specify the number of regressors and the ranking of the desired submodel, namely `size` and `best`, respectively. For "`lmSelect`" methods, the `size` parameter has no meaning and is not defined. Some methods – i.e., `variable.names()`, `deviance()`, `sigma()`, `logLik()`, `AIC()`, `BIC()`, and `coef()` – can extract more than one submodel at a time if passed a numeric vector as an argument to either `size` (e.g., `size = 5:10`) or `best` (e.g., `best = 1:3`). The shape of the return value can be controlled with the `drop` parameter: a `numeric` or `character` vector (in some cases, a `logical` or `numeric` matrix) is returned if `drop` is `TRUE`; otherwise, a `data.frame` object is handed back.

4. Case study: Variable selection in weather forecasting

Advances in numerical weather prediction (NWP) have played an important role in the increase of weather forecast skill over the past decades (Bauer *et al.* 2015). Numerical models simulate physical systems that operate at a large, typically global, scale. The horizontal (spa-

Method	Description
`print()`	print object
`plot()`	plot RSS or penalty
`image()`	heatmap of selected regressors
`summary()`	summary statistics
`variable.names()`	extract variables names
`formula()`	extract formula object
`model.frame()`	extract (full) model frame
`model.matrix()`	extract model matrix
`model_response()`	extract model response
`refit()`	fit sub-"`lm`"
`deviance()`	extract deviance (RSS)
`sigma()`	extract residual standard deviation
`logLik()`	extract log-likelihood
`AIC()`	extract AIC values
`BIC()`	extract BIC values
`coef()`	extract regression coefficients
`vcov()`	extract covariance matrix
`fitted()`	extract fitted values
`residuals()`	extract residual values

Table 4: S3 methods for "`lmSubsets`" and "`lmSelect`" objects.

tial) resolution is limited by the computational power available today. To obtain forecasts for specific locations, the NWP outputs are post-processed to correct for local and unresolved effects (Wilks 2006, p. 220). Model output statistics (MOS, Glahn and Lowry 1972) develops a statistical relationship between a meteorological variable to be predicted (observed quantity) and variables from the numerical model at some lead time (forecasted quantities). MOS employs variable-subset selection to determine which NWP outputs to include in the regression model for a specific location.

In the following, package **lmSubsets** is used to build a MOS regression model predicting temperature at Innsbruck Airport, Austria, based on data from the Global Ensemble Forecast System (Hamill *et al.* 2013). The data frame `IbkTemperature` contains 1824 daily cases for 42 variables: the temperature at Innsbruck Airport (observed), 36 NWP outputs (forecasted), and 5 deterministic time trend/season patterns. The NWP variables include quantities pertaining to temperature (e.g., 2-meter above ground, minimum, maximum, soil), precipitation, wind, and fluxes, among others. See `?IbkTemperature` for more details.

First, the dataset is loaded and the few missing values are omitted for simplicity.

```
R> data("IbkTemperature", package = "lmSubsets")
R> IbkTemperature <- na.omit(IbkTemperature)
```

A simple output model for the observed temperature (`temp`) is constructed, which will serve as the reference model. It consists of the 2-meter temperature NWP forecast (`t2m`), a linear trend component (`time`), as well as seasonal components with annual (`sin`, `cos`) and bi-annual (`sin2`, `cos2`) harmonic patterns.

	MOS0		MOS1		MOS2	
(Intercept)	-72.102	(109.212)	-393.434***	(95.349)	-388.550***	(95.225)
t2m	0.318***	(0.016)	0.055.	(0.029)		
time	0.132*	(0.054)	0.149**	(0.047)	0.147**	(0.047)
sin	-1.234***	(0.126)	0.522***	(0.147)	0.811***	(0.120)
cos	-6.329***	(0.164)	-0.812**	(0.273)		
sin2	0.240*	(0.110)	-0.794***	(0.119)	-0.870***	(0.118)
cos2	-0.332**	(0.109)	-1.067***	(0.101)	-1.128***	(0.097)
sshnf			0.016***	(0.004)	0.018***	(0.004)
vsmc			20.200***	(3.115)	20.181***	(3.106)
tmax2m			0.145***	(0.037)	0.181***	(0.023)
st			1.077***	(0.051)	1.142***	(0.043)
wr			0.450***	(0.109)	0.505***	(0.103)
t2pvu			0.064***	(0.011)	0.149***	(0.028)
mslp					-0.000***	(0.000)
p2pvu					-0.000**	(0.000)
AIC	9493.602		8954.907		8948.182	
BIC	9537.650		9031.992		9025.267	
RSS	19506.469		14411.122		14357.943	
Sigma	3.281		2.825		2.820	
R-sq.	0.803		0.854		0.855	

Table 5: Estimated regression coefficients (along with standard errors) and summary statistics for models `MOS0`, `MOS1`, and `MOS2`.

```
R> MOS0 <- lm(temp ~ t2m + time + sin + cos + sin2 + cos2,
+    data = IbkTemperature)
```

The estimated coefficients (and standard errors) are shown in Table 5. It can be observed that despite the inclusion of the NWP variable `t2m`, the coefficients for the deterministic components remain significant, which indicates that the seasonal temperature fluctuations are not fully resolved by the numerical model.

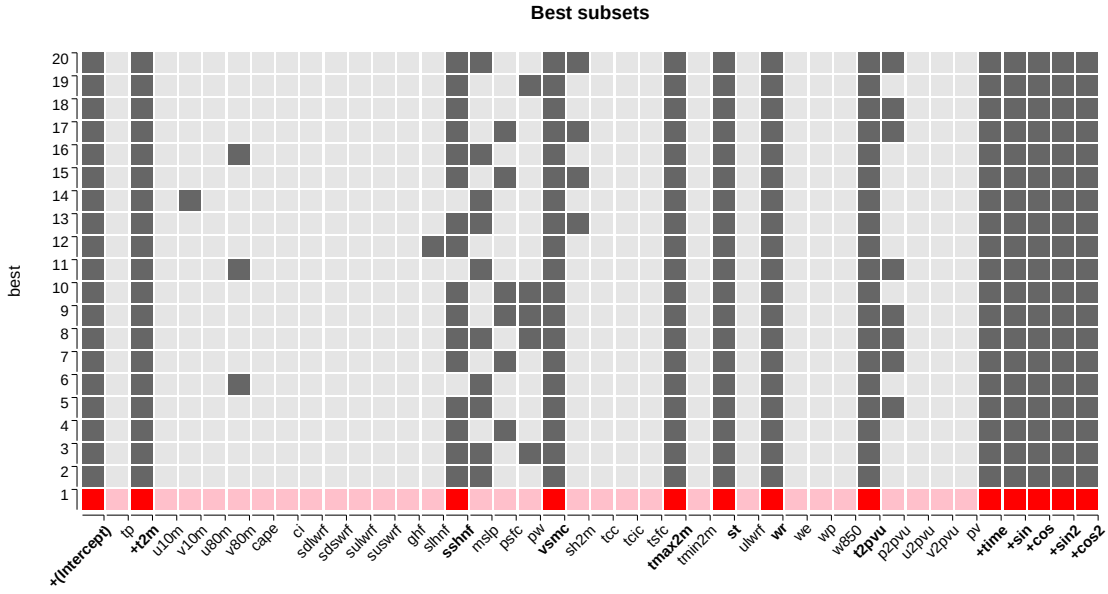
Next, the reference model is extended with selected regressors taken from the remaining 35 NWP variables.

```
R> MOS1_best <- lmSelect(temp ~ ., data = IbkTemperature,
+    include = c("t2m", "time", "sin", "cos", "sin2", "cos2"),
+    penalty = "BIC", nbest = 20)
R> MOS1 <- refit(MOS1_best)
```

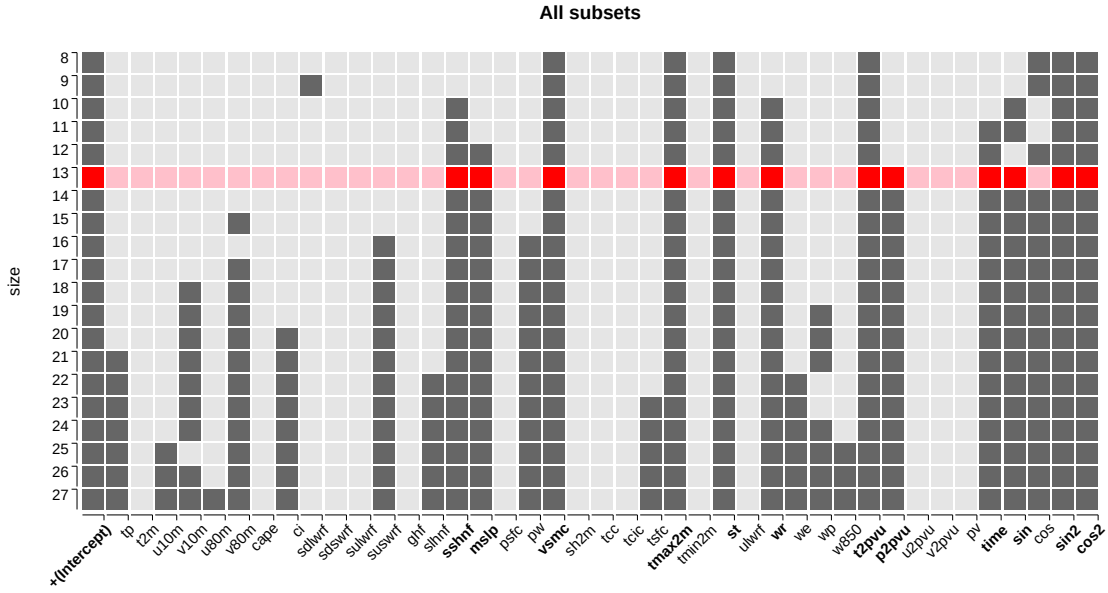
Best-subset regression is employed to determine pertinent veriables in addition to the regressors already found in `MOS0`. The 20 best submodels with respect to the BIC are computed. The selected subsets and the corresponding BIC values are illustrated in Figures 2a and 3a, respectively. The "`lm`" object for the best submodel is extracted (`MOS1`). Selected coefficients and summary statistics for `MOS1` are listed in Table 5.

Finally, an all-subsets regression is conducted on all 41 variables without any restrictions.

```
R> MOS2_all <- lmSubsets(temp ~ ., data = IbkTemperature)
R> MOS2 <- refit(lmSelect(MOS2_all, penalty = "BIC"))
```



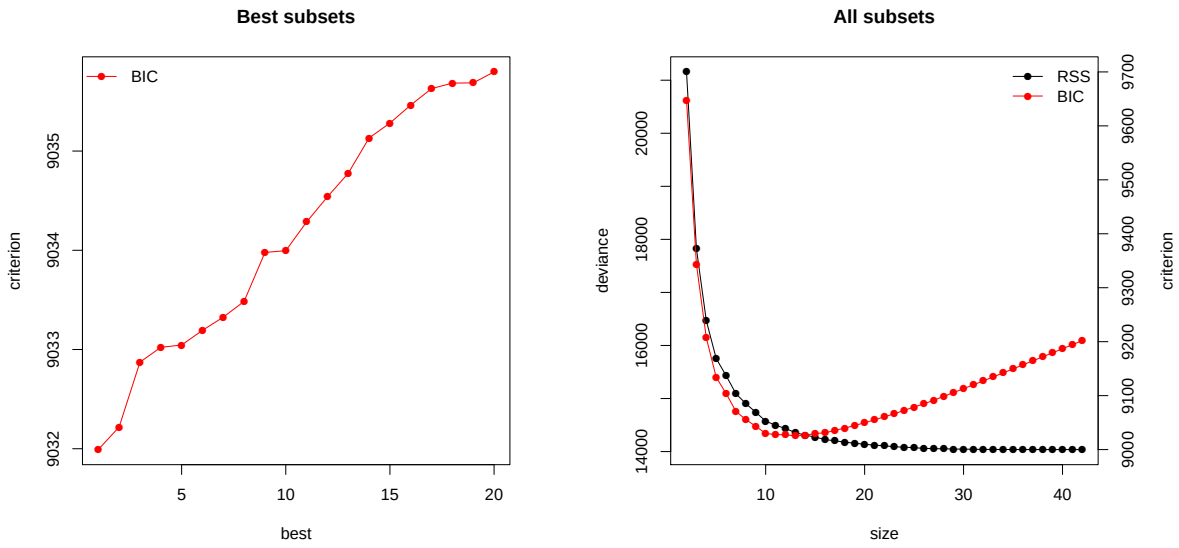
(a) `MOS1_best`



(b) `MOS2_all`

Figure 2: Variables selected in `MOS1_best` and `MOS2_all`. Submodels `MOS1` and `MOS2` are highlighted in red.

The results are illustrated in Figures 2b and 3b. Here, all-subsets regression is employed – instead of the cheaper best-subsets regression – in order to give insights into possible variable selection patterns over a range of submodel sizes. The "`lm`" object for the submodel with the lowest BIC is extracted (`MOS2`). See Table 5 for `MOS2` summary statistics.



(a) `MOS1_best` (b) `MOS2_all`

Figure 3: BIC (and RSS) for submodels in `MOS1_best` and `MOS2_all`.

The best-BIC models `MOS1` and `MOS2` both have 13 regressors. The deterministic trend and all but one of the harmonic seasonal components are retained in `MOS2`. In addition, `MOS1` and `MOS2` share six NWP outputs relating to temperature (`tmax2m`, `st`, `t2pvu`), pressure (`mslp`, `p2pvu`), hydrology (`vsmc`, `wr`), and heat flux (`sshnf`). However, and most remarkably, `MOS1` does not include the direct 2-meter temperature output from the NWP model (`t2m`). In fact, `t2m` is not included by any of the 20 submodels (sizes 8 to 27) shown in Figure 2b, whereas the temperature quantities `tmax2m`, `st`, `t2pvu` are included by all. The summary statistics reveal that both `MOS1` and `MOS2` significantly improve over the simple reference model `MOS0`, with `MOS2` being slightly better than `MOS1`.

In summary, this case study illustrates how **lmSubsets** can be used to easily identify relevant variables beyond the direct model output for MOS regressions, yielding substantial improvements in forecasting skill. A full meteorological application would require further testing using cross-validation or other out-of-sample assessments. Recently, there has been increasing interest in MOS models beyond least-squares linear regression, e.g., to take into account the effects of heteroscedasticity, censoring, and truncation. In this context, other selection techniques – such as boosting (Messner *et al.* 2016, 2017) – can be considered.

5. Benchmark tests

Comparative tests are conducted to evaluate the computational efficiency of the proposed methods for exact all-subsets and exact best-subset regression. The `regsubsets()` method from package **leaps** (Lumley and Miller 2017), and the `bestglm()` method from package **bestglm** (McLeod and Xu 2017) serve as benchmarks, respectively.

Datasets which contain a "true" model are simulated, with `nobs` observations and `nvar` independent variables. The dependent variable `y` is constructed from a linear combination of

sigma	nvar	leaps	leaps1	lmSubsets	(speedup)	(speedup1)
0.05	20	0.009	0.004	0.021	0.4	0.2
	25	0.072	0.033	0.011	6.4	2.9
	30	0.829	0.474	0.027	31.2	17.8
	35	12.309	5.084	0.067	182.6	75.4
	40	172.613	82.566	0.313	550.8	263.5
0.10	20	0.008	0.004	0.007	1.1	0.6
	25	0.064	0.031	0.010	6.2	3.0
	30	0.970	0.457	0.027	36.5	17.2
	35	9.912	4.792	0.068	146.2	70.7
	40	208.998	93.101	0.334	626.5	279.1
0.50	20	0.009	0.004	0.007	1.2	0.6
	25	0.081	0.031	0.011	7.5	2.9
	30	0.995	0.462	0.026	38.0	17.6
	35	12.751	4.995	0.068	187.5	73.4
	40	204.834	82.710	0.312	656.9	265.3
1.00	20	0.008	0.004	0.007	1.2	0.6
	25	0.070	0.033	0.011	6.6	3.1
	30	0.971	0.461	0.026	37.6	17.9
	35	13.066	4.560	0.066	198.6	69.3
	40	171.499	62.978	0.277	620.0	227.7
5.00	20	0.008	0.004	0.007	1.1	0.5
	25	0.058	0.019	0.010	5.7	1.9
	30	0.588	0.198	0.021	28.5	9.6
	35	6.951	2.455	0.053	131.7	46.5
	40	117.859	30.252	0.193	609.4	156.4

Table 6: Average execution times (in seconds) of `leaps()` with and without preordering, and `lmSubsets()`; the speedup of `lmSubsets()` with respect to `leaps()` is also shown.

`ntrue` randomly selected independent variables, a noise vector `e`, and the intercept:

$$\mathtt{y} = \mathtt{X} \cdot \mathbb{1}_{\text{true}} + \mathtt{e} + 1, \quad \mathtt{e} \sim (0, \mathtt{sigma}^2),$$

were `X` is a `nobs` $\times$ `nvar` matrix of random data, and $\mathbb{1}_{\text{true}}$ a (random) indicator function evaluating to 1 if the corresponding column of `X` belongs to the "true" model. All tests were conducted on a Dell XPS15 laptop with 8GB (7.4 GiB) of memory and an Intel Core i7-6700HQ CPU@2.60GHz×8 processor, running a Ubuntu 64bit operating system.

Benchmark 1 concerns itself with all-subsets selection. The `lmSubsets()` method is compared to `regsubsets()`, hereafter denoted by `leaps()`. Data configurations with varying sizes (`nvar` $= 20, 25, 30, 35, 40$) and degrees of noise (`sigma` $= 0.05, 0.10, 0.50, 1.00, 5.00$) are considered; in all cases, `nobs` $= 1000$ and `ntrue` $= \lfloor$`nvar`$/2 \rfloor$. For each configuration, five random datasets are generated, giving rise to five runs per method over which average execution times are determined. The performance of `leaps()` can be improved by "manually" preordering the dataset in advance (Hofmann *et al.* 2007). The average running times are summarized in Table 6, where `leaps` denotes the "vanilla" `leaps()` function, and `leaps1` the modified version with preordering. The same setup is used in Benchmark 2, where methods for best-subset selection are compared, namely `bestglm()` and `lmSelect()`. As in the previous benchmark, average execution times are determined for `bestglm()` with and without preordering. The results are illustrated in Table 7.

It is not surprising that `bestglm()` is very close to `leaps()` in terms of execution time, as the former post-processes the results returned by the latter; in fact, `bestglm()` implements the

sigma	nvar	bestglm	bestglm1	lmSelect	(speedup)	(speedup1)
0.05	20	0.021	0.017	0.006	3.4	2.7
	25	0.083	0.046	0.008	10.4	5.7
	30	0.835	0.489	0.008	99.4	58.2
	35	12.270	5.110	0.010	1202.9	501.0
	40	174.041	83.399	0.012	14503.4	6949.9
0.10	20	0.020	0.016	0.007	3.0	2.5
	25	0.074	0.045	0.007	10.1	6.1
	30	0.974	0.471	0.009	110.7	53.5
	35	9.875	4.777	0.010	949.5	459.3
	40	210.076	93.968	0.012	17219.3	7702.3
0.50	20	0.020	0.017	0.006	3.3	2.7
	25	0.093	0.044	0.008	12.2	5.8
	30	1.004	0.474	0.009	114.1	53.8
	35	12.744	5.067	0.011	1158.5	460.7
	40	205.744	83.268	0.012	17145.4	6939.0
1.00	20	0.021	0.017	0.006	3.2	2.7
	25	0.082	0.046	0.007	11.0	6.3
	30	0.979	0.474	0.008	119.3	57.8
	35	13.002	4.568	0.011	1182.0	415.2
	40	172.923	63.283	0.012	14907.2	5455.4
5.00	20	0.020	0.016	0.006	3.2	2.6
	25	0.070	0.032	0.008	9.3	4.3
	30	0.598	0.212	0.009	63.6	22.6
	35	6.942	2.467	0.012	588.3	209.1
	40	118.004	30.404	0.018	6555.8	1689.1

Table 7: Average execution times (in seconds) of `bestglm()` with and without preordering, and `lmSelect()`; the speedup of `lmSelect()` with respect to `bestglm()` is also shown.

				tolerance = 0.0			tolerance = 0.1		
sigma	nvar	nmin	nmax	lmSubsets	lmSelect	(speedup)	lmSubsets	lmSelect	(speedup)
0.05	20	-	-	0.021	0.022	1.0	0.006	0.007	1.0
	40	-	-	0.327	0.012	26.8	0.227	0.012	18.6
	60	-	-	217.028	0.020	10961.0	101.557	0.020	5181.5
	80	30	50	413.982	0.032	12936.9	163.629	0.031	5312.6
0.10	20	-	-	0.007	0.006	1.1	0.007	0.007	1.0
	40	-	-	0.315	0.012	26.2	0.220	0.012	18.4
	60	-	-	208.721	0.020	10332.7	97.096	0.020	4953.9
	80	30	50	465.824	0.031	14835.2	185.665	0.031	5989.2
0.50	20	-	-	0.007	0.007	1.0	0.007	0.007	1.0
	40	-	-	0.336	0.012	28.0	0.231	0.012	19.2
	60	-	-	197.147	0.020	9956.9	93.936	0.020	4744.2
	80	30	50	486.858	0.032	15406.9	195.240	0.031	6217.8
1.00	20	-	-	0.007	0.006	1.1	0.007	0.007	1.0
	40	-	-	0.290	0.012	24.2	0.205	0.012	17.1
	60	-	-	228.710	0.020	11668.9	106.009	0.019	5464.4
	80	30	50	374.452	0.032	11701.6	148.421	0.043	3467.8
5.00	20	-	-	0.007	0.007	1.1	0.007	0.007	1.0
	40	-	-	0.196	0.017	11.4	0.146	0.015	9.5
	60	-	-	89.244	0.195	458.1	47.399	0.114	416.5
	80	30	50	154.836	8.056	19.2	58.246	3.012	19.3

Table 8: Average execution times (in seconds) of `lmSubsets()` and `lmSelect()`, for `tolerance` = 0.0 and 0.1; the speedup of `lmSelect()` with respect to `lmSubsets()` is also shown.

two-stage approach to solving the best-subset selection problem, where Stage 1 is tackled by `leaps()` (see Section 1 for further details). Manually preordering the variables improves the performance of `leaps()` (and hence, of `bestglm()`) by a factor of approx. 2; for `nvar` = 40 and a high level of noise (`sigma` = 5.00), by a factor of almost 4. In Table 6, the speedup of `lmSubsets()` with respect to `leaps()` and `leaps1()` is reported in columns `speedup` and `speedup1`, respectively; likewise, the speedup of `lmSelect()` with respect to `bestglm()` is reported in Table 7. In the tests conducted here, `lmSubsets()` is two orders of magnitude faster than `leaps()`, even with preordering; `lmSelect()` is three orders of magnitude faster than `bestglm()`.

Benchmark 3 pits all-subsets and best-subset selection, exact and approximation algorithms against one another. The average execution times of `lmSubsets()` and `lmSelect()`, for `tolerance` = 0.0 and 0.1, are illustrated in Table 8. Note that for large datasets (`nvar` = 80), subsets computed by `lmSubsets()` are restricted to sizes between `nmin` = 30 and `nmax` = 50 variables; the restriction does not apply to `lmSelect()`.

In the case of `lmSubsets()`, the approximation algorithm (`tolerance` = 0.1) is 2–3 times faster than the exact algorithm. The speedup of `lmSelect()` with respect to `lmSubsets()` is four orders of magnitude for the exact, three orders of magnitude for the approximation algorithm. It is interesting to note, that the computational performance of `lmSubsets()` increases for high levels of noise (`sigma` = 5.00), contrary to `lmSelect()`. Under these conditions, the relative speedup of `lmSelect()` is significantly lower. As the noise increases, the information in the data is "blurred", rendering the cutting test (10) – which depends on the information criterion – less effective; in this the respect, `lmSubsets()` is more robust, as it only depends on the RSS.

nvar	ic	nbest 1	5	10	15	20
100	AIC	2.159	2.334	2.457	2.557	2.639
	BIC	0.051	0.058	0.068	0.074	0.079
200	BIC	23.987	49.622	82.175	104.860	119.064

Table 9: Average execution times (in seconds) of `lmSelect()` by number of computed subset models (`nbest`).

nvar	penalty 1.0	2.0	4.0	8.0	16.0	32.0
80	0.293	0.300	0.050	0.033	0.032	0.068
100	4.223	0.894	0.084	0.048	0.054	0.341
120	14.178	6.420	0.531	0.085	0.168	3.925

Table 10: Average execution times (in seconds) of `lmSelect()` for varying AIC penalty per parameter (`penalty`).

In Benchmark 4, the effects of the `nbest` parameter (number of computed best submodels) on the execution times of `lmSelect()` are investigated. Two information criteria are considered (`ic` = `AIC` and `BIC`). The noise level used in the benchmark is `sigma` = 1.0. Average execution times are reported in Table 9 for `nbest` $= 1, 5, 10, 15, 20$. Finally, Benchmark 5 investigates how the AIC penalty per parameter (`penalty`) affects the performance of `lmSelect()`. Table 10 summarizes the results for `penalty` $= 1.0, 2.0, 4.0, 8.0, 16.0, 32.0$. Note that `penalty` = 2.0 and `penalty` = `log`(1000) ≈ 6.9 correspond to the usual AIC and BIC, respectively (here, `nobs` = 1000). The results reveal that the execution time of `lmSelect()` increases linearly with `nbest`, and – from the values considered here – is minimal for `penalty` = 8.0, which is close to the BIC.

6. Conclusions

An R package for all-subsets variable selection is presented. It is based on threoretical strategies that have been recently developed. A novel algorithm for best-subset variable selection is proposed, which selects the best variable-subset model according to a pre-determined search criterion. It performs considerably faster than all-subsets variable selection algorithms that rely on the residual sum of squares only. Approximation algorithms allow to further increase the size of tackled datasets. The package implements R's standard formula interface. A case study is presented, and the performance of the package is illustrated in a benchmark with various configurations of simulated datasets.

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Affiliation:

Marc Hofmann
Institute of Natural Resources and Territorial Planning
University of Oviedo
33600 Mieres, Spain
E-mail: marc.hofmann@gmail.com, marc.indurot@uniovi.es
URL: http://www.indurot.uniovi.es/