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Abstract

We adapt Breiman's (1995) nonnegative garrote method to perform variable selection in nonparametric additive models. The technique avoids methods of testing for which no reliable distributional theory is available. In addition it removes the need for a full search of all possible models, something which is computationally intensive, especially when the number of variables is moderate to high. The method has the advantages of being conceptually simple and computationally fast. It provides accurate predictions and is effective at identifying the variables generating the model. For illustration, we consider both a study of Boston housing prices as well as two simulation settings. In all cases our methods perform as well or better than available alternatives like the Component Selection and Smoothing Operator (COSSO).

Keywords: cross-validation; nonnegative garrote; nonparametric regression; shrinkage methods; variable selection.

1 Introduction

Variable selection is an important issue in any statistical analysis, whether parametric or nonparametric in nature. Practically speaking, one is interested in determining the strongest effects that explain the response variable. Statistically speaking, variable selection is a way of reducing the complexity of the model, in some cases by admitting a small amount of bias to improve accuracy. For example, consider the study of the Boston Housing Data (available from the University of California at Irvine Repository Of Machine Learning Database at http://www.ics.uci.edu/~mlearn/MLRepository.html, aimed at describing the relationship between housing values in suburbs of Boston and different attributes as shown in Table 1. The data (originally from Harrison and Rubinfeld, 1978) have been considered by Belsley, Kuh, and Welsch (1980), among others, with various transformations proposed for the predictors. These data are therefore a good candidate with which to illustrate a nonparametric regression approach. The sample size is 506.

The full model (containing all available explanatory variables) for the Boston Housing Data can be written as:

$$log(medv) = \alpha + f_1(crim) + f_2(zn) + f_3(indus) + f_4(nox) + f_5(rm) + f_6(age) + f_7(dis) + f_8(rad) + f_9(tax) + f_{10}(ptratio) + f_{11}(b) + f_{12}(lstat) + \beta chas + \epsilon.$$
(1)

Note that **chas** is a dummy variable and consequently does not require any smoothing. Also, we could have chosen to use Bk, where Bk is the proportion of blacks by town, rather than $b = 1000(Bk - .63)^2$ due to the nonparametric nature of the analysis but instead elected to remain consistent with the original analysis in this regard. These data are analyzed in Section 2.

A nonparametric framework is more challenging than a parametric approach because of the lack of underlying assumptions that makes it difficult to define a general test approach for variable selection. Some notable exceptions exist, but only with strong restrictions: in special situations or for particular smoothers (see, e.g. Bock and Bowman, 1999 for local polynomials; Cantoni and Hastie, 2002 for smoothing splines).

Subset selection is a well-known approach to variable selection: it selects a model containing a subset of available variables, according to a given optimality criterion and requires that one visit all possible models. This approach quickly becomes infeasible when the dimension is too large even when efficient algorithms exist (e.g. *leaps and bounds* in the case of linear regression, see Furnival and Wilson, 1974). Stepwise procedures are a working compromise as they reduce the number of models for comparison. However, they

medv	median value of owner occupied homes in \$1000's
crim	per capita crime rate by town
zn	proportion of residential land zoned for lots over 25,000 sq.ft.
indus	proportion of non-retail business acres per town
nox	nitric oxides concentration (parts per 10 million)
rm	average number of rooms per dwelling
age	proportion of owner-occupied units built prior to 1940
dis	weighted distances to five Boston employment centres
rad	index accessibility to radial highways
tax	full-value property-tax rate per \$10,000
ptratio	pupil-teacher ratio by town
b	$1000(Bk - 0.63)^2$ where Bk is the proportion of blacks by town
lstat	proportion of the population that is lower status
chas	Charles River dummy variable $(=1 \text{ if tract bounds river}; 0 \text{ otherwise})$

Table 1: Boston Housing Data description.

suffer from dependence on the path chosen through the variable space and may be inconsistent. In addition, both subset selection and stepwise selection are discrete processes that either retain or discard one variable and therefore shrinkage methods (e.g. ridge regression in the case of linear models) should be preferred because of their continuity in this regard, which leads to lower variability.

Shrinkage methods have emerged and gained popularity (especially in the parametric context) in recent years. In addition, methods that simultaneously address estimation and variable selection now exist (e.g. LASSO, see Tibshirani, 1996, and LARS, see Efron, Hastie, Johnstone, and Tibshirani, 2004). In the nonparametric setting, the method of COSSO has been proposed by Lin and Zhang (2003). It applies to the smoothing splines ANOVA framework as defined in Gu (2002). Efficient algorithms for model selection with shrinkage methods have been provided by Yuan and Lin (2006).

In this paper, we propose an approach to variable selection for nonparametric additive models based on the nonnegative garrote idea of Breiman (1995) which has simultaneously the properties of subset selection, shrinkage and stability as mentioned above. It also has the advantage of being conceptually simple (like its original parametric counterpart) and computationally cheap. Moreover, it can be used with any smoother. These desirable characteristics are not shared by alternative methods like COSSO with which we compare results.

As we shall see in Section 3, our proposal provides very accurate models

and is able to identify the true underlying model, with the procedure (C) (see Section 2.1) giving the best results in general. This is true when compared to COSSO as well as stepwise procedures.

The paper is organized as follows. We introduce the methodology in Section 2. Specifically, we discuss the automatic choice of the parameters involved (Sections 2.1 and 2.2) and provide guidelines for different options. In the same section we present an illustrative example, followed by results of a simulation study in Section 3. Both demonstrations provide strong evidence that our proposal works well under a variety of circumstances. A discussion (Section 4) closes the paper.

2 Methodology

A typical dataset of interest here will consist of p explanatory variables x_{1i}, \ldots, x_{pi} and a response variable Y_i for each of the $i = 1, \ldots, n$ independent individuals for which we postulate an additive model of the form

$$Y_i = \alpha + \sum_{k=1}^p f_k(x_{ki}) + \epsilon_i, \qquad (2)$$

for i = 1, ..., n.

Model (2) is often presented with only univariate functions for convenience, but it must be emphasized that this property is not necessary. In fact, component functions with two or more dimensions, as well as categorical variable terms (factors) and interactions between them can replace the univariate functions $f_k(x_k)$. Moreover, some of the functions in Model (2) may be defined parametrically, giving rise to a semiparametric model.

We suppose that the variables x_k have been centered by subtracting off their sample means. This is not a theoretical restriction, but rather for ease of implementation, see Section 2.3 for further details.

Given an initial estimate $\hat{g}_k^{h_k}(x_k)$ of each function $f_k(x_k)$, the nonnegative garrote approach solves

$$\min_{c_k} \sum_{i=1}^n \left(y_i - \alpha - \sum_{k=1}^p c_k \hat{g}_k^{h_k}(x_{ki}) \right)^2 \tag{3}$$

under the constraints $c_k \ge 0$ and $\sum_{k=1}^p c_k \le s$. The final estimate of $f_k(x_{ki})$ is $\hat{f}_k(x_{ki}) = c_k \hat{g}_k^{h_k}(x_{ki})$.

The set h_1, \ldots, h_p are referred to as the smoothing parameters of the initial function estimates $\hat{g}_1^{h_1}, \ldots, \hat{g}_p^{h_p}$. Alternatively one can consider the

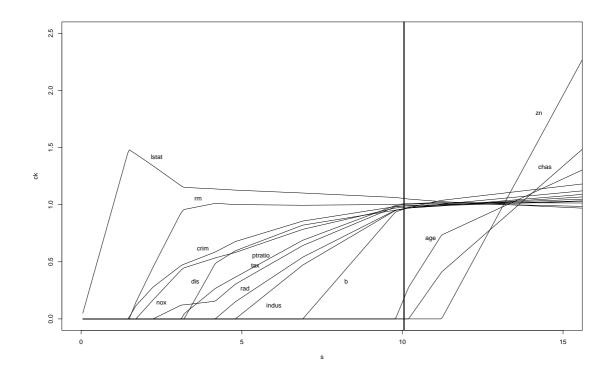


Figure 1: Shrinkage values c_k as a function of s for the Boston Housing data. The bold vertical line indicates the value of s chosen by 5-fold cross-validation.

degrees of freedom (see Hastie and Tibshirani, 1990, p. 128). Most smoothing techniques (e.g. splines, local polynomials), allow one parameter for each function [the AMlet technique (Sardy and Tseng, 2004) is an exception here in that it requires only a single parameter]. Note also that c_k depends on s, and s is regarded as an additional parameter. We will discuss the choice of these parameters in Sections 2.1 and 2.2 below.

Our proposal (3) generalizes the original proposal of Breiman (1995) which is recovered with $\hat{g}_k^{h_k}(x_k) = \hat{\beta}_k x_{ki}$, where $\hat{\beta}_k$ are the ordinary least square estimates in the linear model $y_i = \alpha + \sum_{k=1}^p \beta_k x_{ki} + \epsilon_i$. In this parametric situation no choice of h_1, \ldots, h_p is required.

Given an initial estimate of all the additive functions in Model (2) and a value for s, the nonnegative garrote will automatically and in a single step provide a set of coefficients c_1, \ldots, c_p that will provide information on the importance of each variable in the model. For instance, if $c_k = 0$, the variable x_k is considered uninformative and can be removed from the model. Alternatively the variable contribution to the model will be shrunk by some proportion c_k or left unchanged (if $c_k = 1$). Decreasing s has the effect of increasing the shrinkage of the nonzeroed functions and making more of the c_k become zero. The nonnegative garrote can be viewed as a method for comparing all possible models, but unlike subset selection, it avoids fitting each model separately, therefore making its use possible at low computational cost even for large values of p.

For example, if we apply our proposal to the Boston Housing data (on log scale, see Equation (1)) with smoothing parameters h_1, \ldots, h_p automatically chosen according to Procedure (C) (see Section 2.1 below), we obtain the results as depicted in Figure 1. This plot identifies the strongest effects (the components that enter first in the model as s increases) which in this case are **1stat**, **crim** and **rm**. The bold vertical line shows the value of s automatically chosen by 5-fold cross-validation (see Section 2.2). Those c_k which are zero for this value of s (=10.05) identify the variables that can be removed from the final model: **zn** and **chas**. The significance of **age** is borderline. Although the model considered here is different, the conclusions are partly common with those of Belsley, Kuh, and Welsch (1980). Furthermore, the nonparametric model considered in our analysis is certainly a welcome alternative to their linear analysis given the strong nonlinear effects observed when the final model is plotted as shown in Figure 2.

2.1 Choice of h_1, \ldots, h_p

In order for the method to perform well, it is important that the smoothing parameters h_1, \ldots, h_p of the initial fits $\hat{g}_k^{h_k}$ be selected in a reasonable manner. They can either be set by the user (maybe on the basis of asymptotic results as in the plug-in approach) or selected automatically with a data driven approach (e.g. cross-validation); see, for example, Härdle (1990, Chapter 5). Note that until the recent contribution of Wood (2000), no satisfactory solution to the problem of automatic selection of the smoothing parameter has been available.

In our work, we will consider the following non exhaustive list of options with which to obtain an initial fit of the data:

- (A) Estimate h_1, \ldots, h_p automatically (by cross-validation, for example) on the basis of the *p* univariate nonparametric regressions $y_i = g_k(x_{ki}) + \epsilon_i$ for $k = 1, \ldots, p$, to produce $\hat{g}_k^{h_k}$.
- (B) Given starting values h_1^0, \ldots, h_p^0 provided by the user, estimate h_1, \ldots, h_p automatically (by cross-validation, for example) at each step of the backfitting algorithm (Hastie and Tibshirani, 1990, p. 91). This modified backfitting algorithm reads as follows:

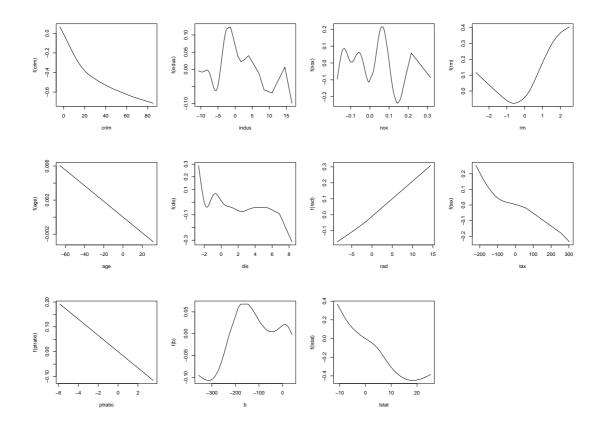


Figure 2: Fitted functions for the final model after variable selection by our nonparametric nonnegative garrote.

- 1. Initialize: $\hat{\alpha} = \bar{y}$, $h_k = h_k^0$ for $k = 1, \dots, p$, and $\hat{g}_k^{h_k} = \hat{g}_k^{h_k^0}$ for $k = 1, \dots, p$.
- 2. Cycle: j = 1, ..., p, 1, ..., p, ...Produce estimates $\hat{g}_j^{h_j}$ by smoothing the partial residuals $(Y_i - \hat{\alpha} - \sum_{k \neq j} \hat{g}_k^{h_k}(x_{ki}))$ on x_j , with h_j chosen automatically.
- 3. Continue Step 2 until the individual functions do not change.
- (C) Estimate h_1, \ldots, h_p automatically by minimizing a given criterion in the *p* dimensional space.

Procedure (C) is certainly the most desirable, but is not yet widely implemented in software packages. Procedure (A) is the simplest approach but neglects the correlation between covariates. Procedure (B) is a working compromise but is again effective only when there is little covariance between covariates. Note that the re-estimation of the smoothing parameter at each step of the backfitting algorithm might, in principle, affect the convergence of the backfitting algorithm. However, we never experienced this situation in our examples and simulations. We can expect procedure (C) to perform better than (B), which in turn would perform better than (A), but it is not clear a priori how large the differences will be.

2.2 Choice of s

The accuracy of the model can be measured through the (average) prediction error defined as

$$PE_s(\hat{\alpha}, \hat{f}_1^{h_1}(x_{1i}), \dots, \hat{f}_p^{h_p}(x_{pi})) = \frac{1}{n} \sum_{i=1}^n E\Big(Y_i^{new} - \hat{\alpha} - \sum_{k=1}^p \hat{f}_k^{h_k}(x_{ki})\Big)^2, \quad (4)$$

where $s = \sum_{k=1}^{p} c_k$, $\hat{f}_k^{h_k}(x_{ki}) = c_k \hat{g}_k^{h_k}(x_{ki})$ and the expectation on the right hand side of (4) is taken over Y_i^{new} . The best value of s is then defined as the minimizer of $PE_s(\hat{\alpha}, \hat{f}_1^{h_1}(x_{1i}), \dots, \hat{f}_p^{h_p}(x_{pi}))$. Of course, in practice $PE_s(\hat{\alpha}, \hat{f}_1^{h_1}(x_{1i}), \dots, \hat{f}_p^{h_p}(x_{pi}))$ is not observable and

Of course, in practice $PE_s(\hat{\alpha}, f_1^{h_1}(x_{1i}), \ldots, f_p^{n_p}(x_{pi}))$ is not observable and needs to be estimated. V-fold cross-validation is an approach used to mimic the behaviour of new observations coming into play, when only a single sample is available. It splits the data into V subsets. Denote by $\mathcal{I}_1, \ldots, \mathcal{I}_V$ the sets of the corresponding observation indices. For each value of s, the cross-validation estimate of (4) is then

$$\widehat{PE}_{s}(\hat{\alpha}, \hat{f}_{1}^{h_{1}}(x_{1i}), \dots, \hat{f}_{p}^{h_{p}}(x_{pi})) = \\ = \frac{1}{V} \sum_{v=1}^{V} \frac{1}{|\mathcal{I}_{v}|} \sum_{i \in \mathcal{I}_{v}} \left(Y_{i} - \hat{\alpha}^{(-v)} - \sum_{k=1}^{p} c_{k}^{(-v)} \hat{g}_{k}^{h_{k},(-v)}(x_{ki}) \right)^{2}, \quad (5)$$

where $\hat{\alpha}^{(-v)}$, $\hat{f}_k^{h_k,(-v)}$ and $c_k^{(-v)}$ are obtained from the sample containing all the observations but those in \mathcal{I}_v . Values of V between 5 and 10 produce satisfactory results and are known to be a good balance between bias and variance in the estimation of PE_s , that is between the high variance if V is large (e.g. V = n for leave-one out cross-validation) and the bias if V is smaller (because of the smaller size of the training set); see Breiman (1995) and Friedman, Hastie, and Tibshirani (2001, p. 214-7).

2.3 Implementation and software availability

Presently, considering all the procedures described in Section 2.1 (as well as COSSO) requires the use of several different software packages. There are essentially two parts to our approach: the initial fit followed by the nonnegative garrote for variable selection. The user has the following options:

Initial fit:

- Procedure (A): gam function of Splus or gam function of R (either from the gam or the mgcv library).
- Procedure (B): addreg function available from Statlib at http://lib.stat.cmu.edu/S/ or from the author's website (D. Ny-chka, see http://www.image.ucar.edu/~nychka/).
- Procedure (C) gam from the mgcv library in R.

Nonnegative garrote:

To implement our approach we adapted the Fortran code of L. Breiman publicly available by ftp from stat-ftp.berkeley.edu in the directory /pub/users/breiman. Redefinition of some of the input quantities was required. The algorithm makes use of a modification of the nonnegative least squares algorithm by Lawson and Hanson (1974). The predictors must be centered at zero by subtracting off their sample means. Note that for a given set of initial estimates $\hat{g}_k^{h_k}(x_k)$ for $k = 1, \ldots, p$, the nonnegative garrote Equation (3) is as simple as its parametric counterpart. We linked the Fortran code both within Splus and R and intend to distribute our routines as an R package.

The Matlab code for COSSO is available on the authors' website at http://www4.stat.ncsu.edu/~hzhang/pub.html. There is also an R version, but we have been unable to get it running properly.

3 Simulation Study

In this section we compare the different procedures available within our proposal to the COSSO (a direct competitor to our technique) as well as to a simpler and commonly used stepwise approach. Predictive accuracy and the ability to identify the significant explanatory variables are the criteria used for comparison. In Section 3.1 we reproduce the situation of Example 1 in Section 7 of Lin and Zhang (2003), whereas in Section 3.2 we generate a realistic dataset inspired by the Boston housing example in Section 1.

Our nonnegative garrote proposal makes available 4 different options. Procedures (A) and (B) as described in Section 2.1, and two versions of Procedure (C), hereafter referred to as Procedures (C1) and (C2). Procedure (C1) uses the smoothing parameters obtained from the initial fit with the entire dataset on the cross-validated samples (80% of the data if V = 5) and Procedure (C2) re-estimates the smoothing parameter automatically on each of the cross-validated samples. This same distinction is not necessary for Procedures (A) and (B) because the software allows the specification of the degrees of freedom (instead of the smoothing parameters) which don't need to vary with the sample size.

3.1 Example from Lin and Zhang

We consider here the generating process of Example 1 in Section 7 of Lin and Zhang (2003). It is a simple additive model in \mathcal{R}^{10} , where the underlying generating model for $i = 1, \ldots, 100$ is

$$Y_i = f_1(x_{1i}) + f_2(x_{2i}) + f_3(x_{3i}) + f_4(x_{4i}) + \epsilon_i,$$

and

$$f_1(t) = 5t, \quad f_2(t) = 3(2t-1)^2, \quad f_3(t) = \frac{\sin(2\pi t)}{2 - \sin(2\pi t)},$$

 $f_4(t) = 6 \left(0.1 \sin(2\pi t) + 0.2 \cos(2\pi t) + 0.3 \sin^2(2\pi t) + 0.4 \cos^3(2\pi t) + 0.5 \sin^3(2\pi t) \right).$

As a consequence there are 6 uninformative dimensions. The X's are built according to the following "compound symmetry" design: $X^{(j)} = (W^{(j)} + tU)/(1+t)$, where $W^{(1)}, \ldots, W^{(p)}$ and U are i.i.d. from Uniform(0,1) which results in $Corr(X^{(j)}, X^{(k)}) = t^2/(1+t^2)$ for $j \neq k$. The uniform design corresponds to the case where t = 0. The error term ϵ_i is generated according to a centered normal distribution with variance equal to 1.74 yielding a signal to noise ratio of 3.

To remain consistent with Lin and Zhang (2003) we measure the accuracy via the integrated squared error (ISE), where ISE = $E_X((\hat{f}(X) - f(X))^2)$,

	t=0	t=1	t=3
COSSO	0.73(0.03)	0.79(0.03)	0.91(0.04)
NNG - Proc. (A)	$1.71 \ (0.10)$	$1.24\ (0.06)$	$1.12 \ (0.05)$
NNG - $Proc.$ (B)	$0.81 \ (0.03)$	0.85(0.03)	0.95(0.04)
NNG - Proc. $(C1)$	0.72(0.03)	0.75(0.04)	0.71(0.03)
NNG - Proc. $(C2)$	0.65~(0.03)	0.64(0.04)	0.64(0.03)

Table 2: Average ISE (estimated by Monte Carlo over 10,000 points) over 100 simulations. V = 5 fold cross-validation is used. Empirical standard errors are given within parentheses. NNG stands for nonnegative garrote.

estimated by Monte Carlo using 10,000 test points generated from the same distribution as the training points.

We begin by examining the predictive ability of each method under three different designs: t = 0 which corresponds to a uniform independent design, and t = 1 and 3 which generates covariates with correlations of 0.5 and 0.9, respectively. Table 2 presents the average ISE over the 100 simulations. If we consider the COSSO results as a benchmark, we see that our proposal can produce similar or better results in its (C) versions. This is particularly true in the presence of correlation between the x's (t = 1 and t = 3) where Procedures (C1) and (C2) have significantly lower ISE. Procedure (B) behaves similarly (or slightly worse) than COSSO. Procedure (A) should be avoided, even though a somewhat strange and unexpected behavior seems to appear: the results get better in the presence of higher correlation.

Table 3 displays the number of times (out of the 100 simulations) that each variable has been selected to appear in the final model. Generally, COSSO tends to include less extra covariates but at the same time misses significant covariates more often. In contrast, our approaches are more effective at identifying the signal. In keeping with Shao (1993), who considers *good models* as those which contain the true generating model, our approaches should be preferred. Note also that the presence of some extra variables doesn't seem to impact the predictive ability of our approaches (see Table 2 above).

One has to be careful when reading the results in Table 3 for t = 1 and t = 3 since the X's are correlated in these cases, and as a result substitution can arise. We decide nevertheless to report the results in this manner, given that all of the compared methods are affected in the same way.

We also ran the nonnegative garrote procedures with V = 10 folds. The results (not reported here) were very similar.

Design	Technique	X1	X2	Х3	X4	X5	X6	X7	X8	X9	X10
t=0	COSSO	100	98	100	100	2	1	0	1	0	3
	NNG - Proc. (A)	100	100	100	100	23	21	21	15	23	23
	NNG - Proc. (B)	100	100	100	100	23	20	27	22	33	15
	NNG - Proc. (C1)	100	100	100	100	28	27	35	35	22	30
	NNG - Proc. $(C2)$	100	100	100	100	19	16	19	20	13	19
t=1	COSSO	95	74	100	100	3	12	4	5	10	3
	NNG - $Proc.$ (A)	100	100	100	100	13	22	24	28	20	20
	NNG - $Proc.$ (B)	99	100	100	100	34	29	32	32	29	28
	NNG - $Proc.$ (C1)	100	100	100	100	45	44	37	35	37	32
	NNG - Proc. (C2)	99	100	100	100	24	24	22	15	18	18
t=3	COSSO	56	79	94	100	19	23	18	19	20	20
	NNG - $Proc.$ (A)	80	100	100	100	33	29	34	35	40	36
	NNG - $Proc.$ (B)	87	100	100	100	36	43	34	44	37	46
	NNG - Proc. (C1)	90	100	100	100	46	38	39	40	36	41
	NNG - Proc. (C2)	79	100	100	100	24	22	23	26	19	22

Table 3: Frequency of appearance of the variables in 100 simulations.

3.2 Simulated example

In this section we construct a model based upon the introductory example on the Boston Housing Data. The aim is to compare the four versions of our technique to common stepwise approaches. We will evaluate the ability of each approach to extract the true underlying model.

We consider the fitted functions of the final model of Section 2 (see Figure 2) to be the "true" functions. The linear predictor is then constructed with the variables crim, rm, dis, rad, tax, ptratio, and lstat. Finally we added a normally distributed error term (mean=0, sd=0.1) to simulate the responses. Variables nox, indus, age, zn and b are considered non informative. Note that we discard variable chas given its binary nature and our interest in nonparametric fits. In summary, we arrive at a simulated dataset with 7 informative dimensions out of 12.

In Table 4 we summarize the results of 100 simulations by classifying the final model obtained into one of the following categories: Missing ≥ 2 , Missing 1, True, Extra 1, Extra ≥ 2 , or Other. The title of each category indicates the number of missing or extra variables appearing in the final model as compared to the true generating model. Note that the last category, Other, may for example include a final model where a generating variable is missing, but where a variable not used in the construction of the model appears. Procedures (A), (B), (C1) and (C2), as described earlier, are based on our

	$Missing \ge 2$	Missing 1	True	Extra 1	Extra ≥ 2	Other
Proc. (A)	0	0	43	36	21	0
Proc. (B)	2	0	17	30	50	1
Proc. $(C1)$	0	0	8	26	66	0
Proc. $(C2)$	0	0	21	34	45	0
Step. (A)	0	0	0	2	35	63
Step. (B)	0	0	1	2	61	36

Table 4: Percentage of models in each category.

nonnegative garrote approach. Step. (A) and (B) refer to stepwise backward variable selection procedures based on an initial choice of the degrees of freedom as per procedure (A) and (B), respectively. They are both conducted on the basis of an F-test. These latter two approaches are included so as to compare results with what is often done in practice. The four versions contained in our nonnegative garrote approach clearly outperform both stepwise approaches in identifying the underlying signal.

In Figure 3 we present a series of boxplots to show the variability of the c_k values across the 100 simulations. For the informative variables these boxplots are centered around 1, whereas for the non informative variables they are shrunken down toward 0. Note that the median of the c_k for the noninformative variables is always zero while the median of the c_k for the informative variables is very close to 1.

4 Discussion

We have proposed a model selection approach based on nonnegative garrote for variable selection in nonparametric regression. We have compared (via simulations) the performance of its four versions to existing methods, e.g. COSSO and stepwise. In terms of predictive ability, versions (C1) and (C2) of our approach perform very well and better than COSSO. Alternative versions (A) and (B) are not as good with respect to predictive ability, but are quite effective in identifying the underlying model, although additional spurious variables are included at times. In contrast, COSSO tends to select smaller models, sometimes missing important variables. Stepwise approaches show a tendency to select very large models, including non significant variables.

Wood and Augustin (2002) suggested an ad-hoc procedure to try to obtain a variable selection procedure from the automatic smoothing parameter selection. Their approach is based essentially on 3 criteria (see their Section 3.3). This involves some manual tuning and is very difficult to implement on a

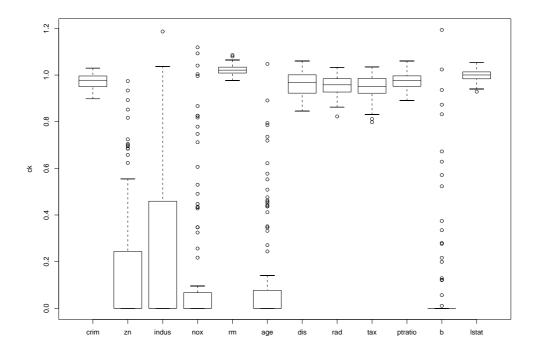


Figure 3: Boxplot of the values of the c_k over 100 simulations for each variable for procedure (C2).

large scale.

Further work includes the extension of this approach to the entire GAM (non normal) class of models and the consideration of resistance-robustness aspects building on work by Cantoni and Ronchetti (2001) and Cantoni, Mills Flemming, and Ronchetti (2005).

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References

- Belsley, D. A., Kuh, E., and Welsch, R. E. (1980). *Regression Diagnostics: Identifying Influential Data and Sources of Collinearity*. New York: Wiley.
- Bock, M. and Bowman, A. W. (1999). Comparing bivariate nonparametric regression models. Technical Report 99-1, Department of Statistics, University of Glasgow, Scotland.
- Breiman, L. (1995). Better subset regression using the nonnegative garrote. *Technometrics*, **37**, 373–384.
- Cantoni, E. and Hastie, T. (2002). Degrees of freedom tests for smoothing splines. *Biometrika*, 89, 251–263.
- Cantoni, E., Mills Flemming, J., and Ronchetti, E. (2005). Variable selection for marginal longitudinal generalized linear models. *Biomet*rics, **61**, 507–514.
- Cantoni, E. and Ronchetti, E. (2001). Resistant selection of the smoothing parameter for smoothing splines. *Statistics and Computing*, **11**, 141–146.
- Efron, B., Hastie, T., Johnstone, I., and Tibshirani, R. (2004). Least angle regression. *The Annals of Statistics*, **32**, 407–451.
- Friedman, J. H., Hastie, T., and Tibshirani, R. (2001). The Elements of Statistical Learning. Berlin/New York: Springer-Verlag.
- Furnival, G. M. and Wilson, Robert W., J. (1974). Regression by leaps and bounds. *Technometrics*, 16, 499–511.

- Gu, C. (2002). *Smoothing spline ANOVA models*. Berlin/New York: Springer-Verlag.
- Härdle, W. (1990). *Applied Nonparametric Regression*. Cambridge: Cambridge University Press.
- Harrison, D. and Rubinfeld, D. L. (1978). Hedonic prices and the demand for clean air. Journal of Environmental Economics and Management, 5, 81–102.
- Hastie, T. J. and Tibshirani, R. J. (1990). *Generalized Additive Models*. London: Chapman & Hall.
- Lawson, C. and Hanson, R. (1974). Solving Least Squares Problems. Englewood Cliffs, NJ: Prentice-Hall.
- Lin, Y. and Zhang, H. H. (2003). Component selection and smoothing in smoothing spline analysis of variance models - COSSO. Technical Report 2556, Institute of Statistics, North Carolina State University.
- Sardy, S. and Tseng, P. (2004). AMlet, RAMlet, GAMlet: Automatic nonlinear fitting of additive models, robust and generalized, with wavelets. *Journal of Computational and Graphical Statistics*, **13**, 283–309.
- Shao, J. (1993). Linear model selection by cross-validation. Journal of the American Statistical Association, 88, 486–494.
- Tibshirani, R. (1996). Regression shrinkage and selection via the Lasso. Journal of the Royal Statistical Society, Series B, Methodological, 58, 267–288.
- Wood, S. N. (2000). Modelling and smoothing parameter estimation with multiple quadratic penalties. Journal of the Royal Statistical Society, Series B, Methodological, 62,(2), 413–428.
- Wood, S. N. and Augustin, N. H. (2002). GAMs with integrated model selection using penalized regression splines and applications to environmental modelling. *Ecological Modelling*, **157**, 157–177.
- Yuan, M. and Lin, Y. (2006). Model selection and estimation in regression with grouped variables. *Journal of the Royal Statistical Society, Series B*, *Methodological*, **68**, 49–67.

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