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Review

# A Review on Variable Selection in Regression Analysis

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**Abstract:** In this paper, we investigate on 39 Variable Selection procedures to give an overview of the existing literature for practitioners. "Let the data speak for themselves" has become the motto of many applied researchers since the amount of data has significantly grew. Automatic model selection have been raised by the search for data-driven theories for quite a long time now. However while great extensions have been made on the theoretical side still basic procedures are used in most empirical work, eg. Stepwise Regression. Some reviews are already available in the literature for variable selection, but always focus on a specific topic like linear regression, groups of variables or smoothly varying coefficients. Here we provide a review of main methods and state-of-the art extensions as well as a topology of them over a wide range of model structures (linear, grouped, additive, partially linear and non-parametric). We provide explanations for which methods to use for different model purposes and what are key differences among them. We also review two methods for improving variable selection in the general sense.

**Keywords:** Variable Selection; Automatic Modelling; Sparse Models

**JEL Classification:** C50,C59

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## 1. Introduction

When building a statistical model the question of which variables to include arise very often. In practice is it true almost all the time. This can come from ignorance, competing theories, or whatever. Practitioners have now at their disposal a wide range of technologies to solve this issue. Literature on this topic started with Stepwise Regression (Breux 1967) and Autometrics (Hendry et al. 1987), moving to more advanced procedures from which the most famous are the Non Negative Garrotte (Breiman 1995), the Least Angle and Shrinkage Selection Operator (hereafter LASSO, Tibshirani (1996)) and the Sure Independence Screening (Fan and Zhang 2008). Many papers are available for empiricists to get an overview of the existing methods. Fan and Lv (2010) reviews most of the literature on linear and generalized models. A large part is devoted to penalized methods and algorithmic solutions, also the optimal choice of the parameter penalty is discussed. Breheny and Huang (2009) and Huang et al. (2012) gave a complete review of selection procedures in grouped variables models with great technical comparisons, especially in terms of rate of convergence. Castle et al. (2011) compared Autometrics to a wide range of other methods (Stepwise, Akaike Information Criterion, LASSO, etc. <sup>1</sup>) in terms of prediction accuracy under orthogonality of the regressors, with a particular attention given to dynamic models. In the same spirit as our paper Park et al. (2015) gave a very recent review of variable selection procedures but dealing only with varying-coefficient models. Fan and Lv (2017) provided a comprehensive review in the context of Sure Independence Screening major improvements. We can also cite more focusing papers like Fu (1998) who compared the Bridge and the LASSO theoretically but also empirically both through simulation and real data.

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<sup>1</sup> Some of them are not presented in this paper either because they are out of its scope, eg. bayesian framework, or because they are special cases of other ones.

32 [Epprecht et al. \(2013\)](#) that compared Autometrics and the LASSO according to prediction and selection accuracy.

33  
34 The contribution of this paper is threefold. First, 39 procedures are considered, these are listed and clearly  
35 classified. Secondly, we establish a topology of procedures under different model structures. We consider major  
36 ones: Linear Models, Grouped Variables Models, Additive Models, Partial Linear Models and Non-parametric  
37 Models. Thirdly, we describe and compare state-of-the-art papers in the literature. We give contexts where each  
38 procedure should be used, to which specific problem they answer and compare them on this ground. In this sense  
39 any practitioner with enough knowledge in Statistics can refer to our paper as a methodological guide for doing  
40 variable selection. It gives a wider view of existing technologies than the other reviews we mentioned.

41  
42 The paper is organized as follows, in section 2 we introduce the three main categories of variable selection  
43 procedures and we provide a typological table of these ones on the ground of model structures. Descriptions as  
44 well as comparisons are discussed along the sections 3 to 7. Each of these sections focuses on a particular model  
45 structure. Section 8 is devoted to two general methods for improving model selection, both can be applied on all  
46 the procedures presented across the paper. In the final section we make few critics on actual procedures and  
47 give insight on future area of research.

## 48 2. Typology of Procedures

49 In this section we propose a typology of state-of-the-art selection methods in many different frameworks,  
50 there are many types of models that can be considered. For this aim, Table 1 provides the classification of  
51 statistical methods available in the literature and that will be discussed in the paper. From the latter we have  
52 determined 3 main categories of algorithms:

- 53 ● Tests-based
- 54 ● Penalty-based
- 55 ● Screening-based

56 Originally, the first developed are based on statistical tests. The work was to automate standard tests in  
57 Econometrics (like testing residuals for normality, t-tests etc.) for choosing among candidate variables. It  
58 includes Stepwise Regression and Autometrics for example.

59 Then there are Penalty-based procedures. Imposing a constraint on parameters directly inside estimation  
60 encourages sparsity among them. For instance LASSO and Ridge belongs to this category.

61 The last are Screening procedures, they are not all designed to do selection intrinsically but rather ranking  
62 variables by importance. The main advantage is that it applies more easily to very large dimensional problems,  
63 when number of regressors is diverging with the number of observations (eg. cases with  $p \gg n$ ). This is mainly  
64 true because it considers additive models (linear or not) and so variables can be treated separately.

65 We discuss this distinction more deeply in subsections below and give brief description of their main features.

### 66 2.1. Tests-Based

67 This is the most classical way of handling variable selection in statistical models. It was also the first  
68 attempt of variable selection. Everything started with Stepwise Regression ([Breux 1967](#)), one of the latest of  
69 this kind is Autometrics ([Hendry et al. 1987](#))<sup>2</sup>. We focus on Stepwise Regression and Autometrics for two  
70 reasons. The first is that Stepwise Regression is the most well-known and the most widespread method for  
71 choosing variables in a model. Despite it dates back to 1967 many empiricists still practice it. The second is that  
72 Autometrics has integrated many features of Econometrics to achieve the highest degree of completeness for an  
73 automatic procedure. Authors have considered endogeneity, non-linearities, unit-roots and many others, trying to  
74 overcome most issues a statistician can face.

75 Stepwise Regression is the most simple and most straightforward way of doing model selection by just retrieving

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<sup>2</sup> Even though it started in 1987 there are still improvements nowadays.

76 insignificant variables (backward approach) or adding significant ones (forward approach) based on some  
77 statistical criterion. Therefore it is pretty easy to use it empirically because implementation is straightforward.  
78 However in several situations this does not ensure consistent selection. Its selection properties have been  
79 investigated in Wang (2009). On the contrary Autometrics is a complete philosophy of modelling, but comes at  
80 the cost of a quite complex algorithm and many tuning parameters are required, making its use more difficult for  
81 non-expert.

## 82 2.2. Penalty-Based

83 Thanks to the work of Tibshirani (1996) it became a quite common strategy in empirics. This kind of  
84 methods involves applying a penalty on parameters to encourage sparsity (i.e. some are set exactly to zero).  
85 Sparsity is a necessary condition for situations of unidentifiability ie. where  $p > n$ . Such a problem can be  
86 solved using penalties on parameters to make inference possible. These parameters can come from parametric  
87 models or from non-parametric models, so penalty based method can be applied on both structures. This kind  
88 of procedure started with the Non Negative Garrote (NNG of Breiman (1995)) in an Ordinary Least Squares  
89 framework up now to much complex model structure like varying coefficients and two-ways interactions ANOVA  
90 non-parametric models. The idea of producing sparse models is a convenient way of integrating a test inside  
91 the estimation. Inference of such models requires the prior assumption that some variables are not relevant, this  
92 is the test part, and penalty-based methods helps estimating the coefficients, this is the inference part. So both  
93 procedures are merged in an unified framework giving rise to a novel conception of statistical modelling. Maybe  
94 the most famous in this category is the LASSO of Tibshirani (1996).

## 95 2.3. Screening-Based

96 Screening is actually the most effective way of dealing with very high dimensional features (large  $p$ ). Few  
97 other selection methods can be as computationally efficient as these ones. However Screening often does not  
98 perform model selection itself, it rather ranks variables. To do so they have to be mixed up with other procedures,  
99 in the literature they are mainly penalty-based. Even if it does not select variables reducing the candidate set is an  
100 important aspect of the variable selection and screening methods are powerful in this task. In this respect it is  
101 worth mentioning the Sure Independence Screening (hereafter SIS, Fan and Lv (2008)) that is the first of this  
102 kind.

103 Screening makes the use of a ranking measure, either linear or not so it can be applied in both frameworks. Some  
104 may rely on specific models (like a linear model) while others are model-free. The major differences among  
105 procedures in this category relies on the choice of the ranking measure. Correlation coefficients are the first  
106 coming to mind, these are mainly used. One limitation in screening is that they usually treats variables by pairs to  
107 compute their measure of association, so every effect is considered as additive and does not correct for the presence  
108 of interactions effects. This is not necessarily true, especially in the non-parametric settings. Sophisticated  
109 correlations such as distance correlation or canonical kernel correlation are employed in a multivariate framework  
110 and account for such interactions even if they do not model them explicitly. However in this case they may loose  
111 their computational efficiency compared to independence screening ones. As said before, a brief review of some  
112 SIS methods can be found in Fan and Lv (2017).

**Table 1.** Topology of Variable Selection Methods

	Screening	Penalty	Testing
Linear	SIS SFR CASE FA-CAR	SparseStep LASSO Ridge BRidge SCAD MCP NNG SHIM	Stepwise Autometrics
Group		gLASSO gBridge gSCAD gMCP ElasticNet	
Additive	NIS CR-SIS	SpAM penGAM	
Partial Linear		kernelLASSO adaSVC DPLSE PSA PEPS	SP-GLRT
Non-Parametric	DC-SIS HSIC-SIS KCCA-SIS Gcorr MDI MDA RODEO	VANISH COSSO	MARS

### 113 3. Linear Models

We began with the first model structure: the linear model. It is described as:

$$y = X\beta + \varepsilon \quad (1)$$

114 The variable to be explained  $y$  (sometimes also called the output, the response or the dependent variable) is a  
 115 one dimensional vector of length  $n$ , corresponding to the number of observations. The matrix  $X$  contains the  
 116 explanatory variables (sometimes also called the inputs, the regressors or the independent variables) of length  $n$   
 117 and dimension  $p$  which is the number of candidate variables. Therefore the one dimensional vector  $\beta$  of length  $k$   
 118 contains the parameters of interest. The residuals (sometimes called also the error term) are denoted  $\varepsilon$ , even if it  
 119 could be of interest we do not solely focus on their properties and consequences on variable selection in this  
 120 paper. This notation will be held constant throughout the paper. Notice that all of the three methodologies are  
 121 able to handle linear models, while this is not necessarily true for other structures (e.g. additive models).

#### 122 3.1. Testing

123 Stepwise Regression (Breux 1967) is the first model selection procedure. This approach have been  
 124 motivated when statisticians started to consider model uncertainty. This means that among  $p$  variables we can  
 125 possibly construct  $2^p$  models, so we should maybe take them all into account. To test all possibilities we have  
 126 to compute "all-subsets". This cannot be achieved for large  $p$ . In order to overcome this problem and reduce  
 127 the search, stepwise regression investigates only a subset of all possible regressions with the hope to end with  
 128 the true model. There exist two approaches: Backward and Forward. Either the process starts from a null  
 129 model (only an intercept) and introduces variables one by one, this is the forward step. Or it starts from the  
 130 full model (all variables) and deletes them one by one, this is the backward step. One improvement is also to

131 consider both. Usually the selection within each step is made according to some criterion. One consider all  
 132 one-variable increments from the actual model and choose the best move according to this criterion, it might be  
 133 the lowest p-value, highest adjusted  $R^2$ , lowest Mallows'  $C_p$ , lowest AIC, lowest prediction error, leave-one-out  
 134 cross validation, etc.

135 You can imagine any criterion to perform this job, but the main issue arising from Stepwise Regression does not  
 136 come from the choice of the criterion. Interesting critics (Doornik 2009) arise from the developers of Autometrics.  
 137 The main one is the lack of search. Stepwise regression proceeds step by step along a single path. Then, there is  
 138 no backtesting. That is the procedure never considers testing again variables that have been removed after each  
 139 step. Such an idea is present using the forward backward combination but it is restricted to the previous step only.  
 140 Obviously they are not the only one to express admonitions about Stepwise Regression. We can mention many  
 141 papers from Hurvich and Tsai (1990), Steyerberg et al. (1999), Whittingham et al. (2006) or Flom and Cassell  
 142 (2007) where they all prove biased estimation and inconsistent selection of Stepwise Regression.  
 143 However even if used as a selection method it behaves poorly, used a screening method it showed better results.  
 144 This has been developed by Wang (2009) and is detailed in the next subsection.

145 On the other side is Autometrics, an algorithm for model selection developed by Hendry et al. (1987)  
 146 under the famous Theory of Encompassing and the LSE (London School of Economics) type of Econometrics.  
 147 This method has been created as early as 1987 and is still under development. The basis of its methodology is  
 148 the General-to-Specific approach. Theory of Encompassing states that the researcher should start from a very  
 149 large model (called the GUM: General Unrestricted Model) encompassing all other possible models and then  
 150 reduce it to a simpler but congruent specification. This idea is somehow related to the backward specification in  
 151 Stepwise Regression. His work is an automation of standard way of testing for relevance in Econometrics such  
 152 as t-tests and F-tests and major concerns deal with power of tests, repeated testing but also outliers detection,  
 153 non-linearities, high dimensional features (with  $p > n$ ) and parameter invariance.

154 Tests come with some hyperparameters specifying the size of the battery of tests (t-tests, F-tests, normality  
 155 checks, etc.).

156 Repeated testing occurs when a variable that has been deleted under a certain specification that has now changed  
 157 is reintroduced and tested again. The absence of such a thing in Stepwise Regression is a severe drawback and  
 158 the main reason why it fails pretty often.

159 Non-linearities are handled using Principal Components Analysis (see Castle and Hendry (2010)) that makes the  
 160 design matrix orthogonal. Such a decomposition allows to introduce squares and cubics of the transformed  
 161 variables which are linear combination of the original ones. Orthogonality limits the number of non-linear terms  
 162 since it already accounts for interaction using components. In simple words a polynomial of degree  $d$  with  $p$   
 163 variable results in  $\binom{d+p}{d} - 1$  terms, while their methods reduces to  $d \times p$  which is very much less. It is advocated  
 164 that it can reproduce non-linear functions often met in Economics and Social Sciences. However the class of  
 165 functions that it can reproduce may be restricted compared to standard non-parametric methods<sup>3</sup>.

166 High dimensional features and non-identifiability ( $p > n$ ) of the GUM is solved in a very simple way called  
 167 "Block Search". Regressors are divided in different blocks until the size of each block is lower than  $p$ . Then  
 168 tests are applied in each block, some variables are discarded, the remaining blocks are merged and the process  
 169 continues. This idea is based on the fact that the methodology is still consistent under separability. This idea is  
 170 quite similar to the Split-and-Conquer methodology of Chen and Xie (2014) to solve ultra-high dimensional  
 171 problems.

172 Outliers can be detected using the Impulse Indicator Saturated Selection (IIS) developed by Hendry et al. (2006).  
 173 This is in the same spirit as the Block-Search (or Split-and-Conquer) approach defined previously. A set of  
 174 indicator is added to the GUM for every observation, and tests are applied in a Block-Search manner to remove  
 175 observations that are not consistent with the model, identified as outliers.

176

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<sup>3</sup> This should be investigated more deeply, to the best of our knowledge no papers have tried to compare their non-linear regression to the very well-known non-parametric procedures like Kernels or Splines. An obvious link can be made with Projection Pursuit Regression (PPR), in this respect we claim that Autometrics may be a special case of PPR.

177 Stepwise Regression and Autometrics are serial procedures where selection and estimation are performed  
 178 sequentially. In some sense Penalty-Based methods aim at performing both at the same time. One can view  
 179 penalty-based procedures as the direct implementation of tests inside inference.

### 180 3.2. Penalty

181 Penalty-based methods can be divided in two categories: penalties on the norm and concave ones. The  
 182 shape of the penalty may have a great influence on the selected set of variables and their estimates. Sparse model  
 183 is achieved because we reduce nearly zero coefficients to zero in estimation. The penalty parameter plays the  
 184 role of a threshold but in a non-orthogonal framework. To understand better the origins of these penalty one  
 185 should refer to threshold methods in [Kowalski \(2014\)](#). For that reason the penalty also introduces shrinkage of  
 186 the coefficients, making them biased. The literature is focused on the choice of the penalty in terms of selection  
 187 consistency and bias properties.

#### 188 3.2.1. Norm Penalties

There are almost as many methods as there are norms, but generally the objective is to solve:

$$\min_{\beta} \|y - X\beta\|_2^2 + \lambda \|\beta\|_{\gamma}^2 \quad (2)$$

189 Each methods applies to different  $L_{\gamma}$  norms.

- 190 • SparseStep:  $\gamma = 0$
- 191 • LASSO :  $\gamma = 1$
- 192 • Ridge :  $\gamma = 2$

This methodology is gathered in the more general Bridge estimator ([Frank and Friedman 1993](#)) that considers any value for  $\gamma$ , but the authors did not say how to solve the problem. The advantage of Ridge ([Hoerl and Kennard 1970](#)) is that it has an analytical solution. However the solution is not sparse so it does not select variables (only shrinkage). The Least Absolute Shrinkage and Selection Operator (LASSO, [Tibshirani \(1996\)](#)) does because the  $L_1$  norm is singular at the origin. However both give bias estimates because they apply shrinkage to the coefficients. The zero norm used in SparseStep ([van den Burg et al. 2017](#)) is the counting norm, they penalize directly the number of non-zero elements in  $\beta$ , not their values (no shrinkage). Usually constraints on the number of non-zero elements require high computational costs (exhaustive search over the model space). Here they use an easy even though very precise continuous approximation from de Rooi and Eilers (2011) and that turns the problem into something computationally tractable.

[Meinshausen and Bühlmann \(2006\)](#) shown that LASSO tends to select noise variables using a penalty parameter optimally chosen for prediction. For this reason [Zou \(2006\)](#) developed AdaLASSO (Adaptive LASSO). His paper proved that the optimal estimation rate is not compatible with consistent selection. Moreover even sacrificing the estimation rate does not ensure that the LASSO will select the right variables with positive probability. This phenomenon is highlighted through a necessary condition on the covariance matrix of the regressors that cannot always be satisfied using the LASSO with a single penalty parameter. Therefore he introduced adaptive weights to the LASSO to make it consistent with variable selection.

$$\min_{\beta} \|y - X\beta\|_2^2 + \lambda \|w\beta\|_1 \quad (3)$$

The latest improvement on linear models is to allow for interactions terms. Even if it is possible, only adding them into a LASSO is not an efficient procedure because it greatly extends the dimensionality of the design matrix. The idea of the Strong Heredity Interaction Model (SHIM, [Choi et al. \(2010\)](#)) is to add interactions only if main effects are selected also (strong heredity property), this greatly reduces the search space and provides an efficient way of doing ANOVA-types of models. They consider a reparametrization of the two-ways interactions models:

$$y = X\beta + \sum_{j=1}^p \sum_{k \neq j} \gamma_{jk} \beta_j \beta_k x_j x_k \quad (4)$$

Introducing main effect parameters  $\beta$  on top of cross-effects  $\gamma$  ensures that the interaction will be non-zero if and only if both main effects are non-zeros. The problem is a composite LASSO of the following form:

$$\min_{\beta, \gamma} \|y - X\beta\|_2^2 + \lambda_\beta \|\beta\|_1 + \lambda_\gamma \|\gamma\|_1 \quad (5)$$

193 Solutions to these problems are numerous. Usually either it reduces to the LASSO and then algorithms like  
 194 Least Angle Regression (LARS) of [Efron et al. \(2004\)](#) are employed. Otherwise iterative algorithms like the  
 195 Local Quadratic Approximation [Fan and Li \(2001\)](#) can be used.

### 196 3.2.2. Concave Penalties

Norm penalties are very standard and easy to work with but there exists also other types of penalties. Thus we can consider penalties in a very general framework:

$$\min_{\beta} \|y - X\beta\|_2^2 + p_\lambda(\beta) \quad (6)$$

197 The difference will then lie in the choice of  $p_\lambda(\beta)$ .

- NonNegativeGarotte:

$$p_\lambda(\beta) = n\lambda \sum_{j=1}^p \left(1 - \frac{\lambda}{\beta_j^2}\right)_+ \quad (7)$$

- SCAD :

$$p_\lambda(\beta) = \begin{cases} \lambda, & \text{if } |\beta| \leq \lambda \\ \frac{a\lambda - |\beta|}{a-1}, & \text{if } \lambda < |\beta| < a\lambda \\ 0, & \text{if } |\beta| \geq a\lambda \end{cases} \quad (8)$$

- MCP :

$$p_\lambda(\beta) = \begin{cases} \lambda|\beta| - \frac{\lambda^2}{2\gamma}, & \text{if } |\beta| \leq \gamma\lambda \\ 0.5\gamma\lambda^2, & \text{if } |\beta| > \gamma\lambda \end{cases} \quad (9)$$

198 The Non Negative Garotte ([Breiman 1995](#)) was the first penalty of this kind, but because it has bad properties  
 199 (especially variables selection inconsistency) it was rapidly abandoned. SCAD (Smoothly Clipped Absolute  
 200 Deviation, [Fan and Li \(2001\)](#)) was the first penalty method that was consistent, continuous and unbiased for large  
 201 values of  $\beta$ . MCP (Minimax Convex penalty, [Zhang et al. \(2010\)](#)) has little difference with SCAD in terms of  
 202 selected variables. A comparative study between them can be found in [Zhang \(2007\)](#).

203 One thing with penalty method is that there are always some penalty parameters (eg  $\lambda$  in LASSO) that have to be  
 204 chosen. Usually they are set to optimal values according to some General Cross Validation (GCV) criterion or  
 205 out-of-sample predictions. This is crucial because results can be very sensitive to the choice of these parameters.  
 206 SCAD is more robust to this problem thanks to a bias-free property.<sup>4</sup>

### 207 3.3. Screening

208 Another methodology in variable selection is Screening. In fact these are ranking methods that rely on  
 209 some association measure between the dependent variable and the regressors. Very often this measure is taken to  
 210 be bivariate allowing then an extremely fast analysis.

---

<sup>4</sup> This is true only for large values of parameters, the reader can get intuitions of this phenomenon with threshold methods ([Kowalski 2014](#)).

### 211 3.3.1. Regressor Based

The Sure Independence Screening (SIS, [Fan and Lv \(2008\)](#)) is the first of this kind and almost all methods are derived from it. It uses simple correlation on standardized variables :  $\hat{\omega}(x_j, y) = \tilde{x}_j \tilde{y}$  and gives a ranking of the  $x_j$ . The set  $\hat{M}$  of relevant features is determined by a simple threshold:

$$\hat{M} = \{1 \leq j \leq p : |\hat{\omega}(x_j, y)| \text{ is among the top } d \text{ largest ones}\} \quad (10)$$

212 This set is reduced step by step until some moment. The method in itself does not select anything in fact, it just  
 213 remove the less correlated features from the set of candidates, but we are left with a candidate set where selection  
 214 has to apply. SIS needs a selection procedure in the end to obtain consistent results. The main advantage of the  
 215 method is that when the number of variables  $p$  is very large compared to the number of observations  $n$  usual  
 216 selection procedures tend to misbehave ([Fan and Lv 2008](#)). In their paper SIS has proven to lead to a set of  
 217 candidates that is manageable for LASSO and others in order to have good properties. SIS allows for ultrahigh  
 218 dimensional features, ultrahigh being defined as:  $\log(p) = \mathcal{O}(n^\alpha)$  with  $0 \leq \alpha \leq 1$ .

219 In this respect the screening properties of screening of Forward Regression ([Wang 2009](#)) have been investigated  
 220 and with little improvements proved to be consistent in variables selection. However it still requires a selection  
 221 procedure in the end, Forward Regression is just used for the screening part that is ranking and reducing the set  
 222 of candidates.

223 Because SIS may encounters issue for selecting weakly correlated variables (weak signal-to-noise ratio) [Fan and](#)  
 224 [Lv \(2008\)](#) introduced Iterative conditional SIS that is applying correlation ranking but conditional on selected  
 225 features. This is equivalent as looking through correlation between features and residuals from a model using  
 226 primarily selected variables instead of correlation with the dependent variable. This idea can be related to former  
 227 algorithms that were developed to infer the LASSO (eg. Forward Stagewise).

### 228 3.3.2. Covariance Based

229 The last approach is less common. The Covariate Assisted Screening Estimates (CASE, [Ke et al. \(2014\)](#)) is  
 230 a method that looks for sparse models but in the case where signals are rare and weak. All methods presented so  
 231 far work well if  $\beta$  is sparse (so rare) and has high values (strong signals). In this case methods like SCAD are  
 232 even bias-free. But if the signals are weak on top of rare then they won't manage to perform variable selection  
 233 very well. The idea in CASE is to sparsify the covariance matrix of the regressors using a linear filter and then  
 234 look for models inside this sparse covariance matrix using tests and penalties. Drawbacks are the choice of the  
 235 filter that is problem dependent and the power of the tests.

236 To improve on CASE when regressors are highly correlated, giving a very dense covariance structure, Factor  
 237 Adjusted-Covariate Assisted Ranking (FA-CAR, [Ke and Yang \(2017\)](#)) proposes using PCA to sparsify it. This is  
 238 in line with selecting appropriately the filter in CASE when the problem to solve includes strong collinearity. In  
 239 fact the covariance is assumed to have a sparse structure, hidden by latent variables. These are estimated by PCA  
 240 and then removed from the variables. The process does not change anything for the equation and the parameters  
 241 to be estimated does not require more technology than the simple OLS on the transformed decorrelated variables.  
 242 The main issue is to select the number of latent variables to be removed, this can be done via cross-validation for  
 243 instance, still it remains difficult.

## 244 4. Grouped Models

Depending on the application the model can come in a group structure form of the type:

$$y = \sum_{g=1}^G \sum_{j \in g} \beta_j x_j + \varepsilon \quad (11)$$

which can be rewritten in matrix-grouped notation:

$$y = \sum_{g=1}^G X_g \beta_g + \varepsilon \quad (12)$$

245 Within this framework there are 2 main possibilities. One can look for which group to be selected or which  
 246 variable is more relevant in which group. The former is referred to as single-level selection (sparse between group  
 247 estimates) and the latter as bi-level selection (sparse between and within group estimates). Technical reviews of  
 248 selection procedures with grouped variables can be found in [Breheny and Huang \(2009\)](#) and [Huang et al. \(2012\)](#).

#### 249 4.1. Penalty

##### 250 4.1.1. Single-level

The concept of group-penalty was introduced in [Yuan and Lin \(2006\)](#) (groupLASSO) in a LASSO framework. The objective is to solve a modified LASSO:

$$\min_{\beta} \|y - \sum_{g=1}^G \sum_{j \in g} \beta_j x_j\|_2^2 + \lambda \sum_{g=1}^G c_g (\beta_g' R_g \beta_g)^{1/2} \quad (13)$$

The parameters  $c_g$  are used to adjust for the group sizes in order to have selection consistency. The parameter  $\lambda$  controls for the penalty. The choice of  $R_g$  that weights each coefficients within the group is still challenging. A solution is to take  $R_g = (X_g' X_g) / n$  the Gram matrix of the grouped variables  $X_g$ . The effect is to scale the variables within groups and so make coefficients comparable in some sense. It can be easily shown that this lead to the LASSO solution with standardization of regressors when the group is formed with only one variable, such a thing is made pretty often empirically and is even advised by the LASSO's authors.

An obvious extension is to take into account any penalty, providing the following objective:

$$\min_{\beta} \|y - \sum_{g=1}^G \sum_{j \in g} \beta_j x_j\|_2^2 + p\left(\sum_{g=1}^G \|\beta_g\|_{R_g}; c_g \lambda, \gamma\right) \quad (14)$$

251 Where  $p(\cdot)$  can be taken to be the Bridge, the SCAD or the MCP criterion introducing then the groupBridge  
 252 ([Huang et al. 2009](#)), the groupSCAD [Wang et al. \(2007\)](#) and the groupMCP ([Breheny and Huang 2009](#))  
 253 respectively.

##### 254 4.1.2. Bi-level

Improvements have been made on norm penalties by considering mixed norms like the ElasticNet ([Zou and Hastie 2005](#)):

$$\min_{\beta} \|y - X\beta\|_2^2 + \lambda_1 \|\beta\|_1 + \lambda_2 \|\beta\|_2^2 \quad (15)$$

255 This method overcomes the issue of collinearity because it favours selection of correlated regressors  
 256 simultaneously while LASSO tends to select only on out of them. In fact the ElasticNet can be solved as a  
 257 LASSO using slight modification of the LARS algorithm. Since it is a mix of Ridge and LASSO, parameters can  
 258 be estimated by Ridge in a first step then apply the LASSO. A small correction due to the second penalty  $\lambda_2$  is  
 259 required. Originally the Elastic-net was not designed explicitly for grouped structure.

260 Also composite penalties have been considered in [Breheny and Huang \(2009\)](#) using the MCP criterion at both  
 261 stages (between and within).

262

263 Since there is a great literature of reviews on these method ([Breheny and Huang 2009](#), [Huang et al. 2012](#))  
 264 we do not spend time giving more details and advise readers interested in group models to have a look at them.

## 265 5. Additive Models

A step further in model structure complexity is to consider different non-parametric functions associated with each variables. The non-parametric additive model takes the following form:

$$y = \sum_{j=1}^p f_j(x_j) + \varepsilon \quad (16)$$

### 266 5.1. Penalty

The Sparse Additive Model (SpAM) of [Ravikumar et al. \(2007\)](#) applies to this kind of models. The idea is simply to apply the LASSO to functions non-parametrically fitted with parametric coefficients coming in top of them. This is obviously the most natural extension of LASSO to the additive structure. The main program to solve is:

$$\min_{\beta, f_j} \|y - \sum_{j=1}^p \beta_j f_j(x_j)\|_2^2 + \lambda \sum_{j=1}^p |\beta_j| \quad (17)$$

Even though the term  $\sum_{j=1}^p \beta_j f_j(x_j)$  remind us the very well-known Splines where the  $f_j$  would be the basis functions, the authors claim that any non-parametric method can be used for fitting them. The solution is given in the form of a backfitting algorithm (Breiman and Friedman 1985). Another approach have been investigated by [Meier et al. \(2009\)](#): the penalized General Additive Model (penGAM). It applies to the same models as before but are especially designed for splines estimation. In the same spirit the individual functions are penalized, but since each function can be represented as the sum of linear combinations of basis functions. It turns out to be a groupLASSO problem.

Their contribution is also to consider not only sparsity but also smoothness in the estimation. Because complex functions require many basis functions it is common in the splines settings to construct an over complete basis and then apply shrinkage on coefficients<sup>5</sup> to have a smooth estimates, this is known as smoothing splines. This takes the form of a Ridge regression so it can be easily integrated inside the procedure. The main objective is to solve:

$$\min_f \|y - f(X)\|_2^2 + J(f) \quad (18)$$

With the sparsity-smoothness penalty being:

$$J(f) = \lambda_1 \sqrt{\|f_j\|^2} + \lambda_2 \int (f_j''(x))^2 dx \quad (19)$$

and because we can rewrite each  $f_j(x) = \sum_{k=1}^K \beta_{j,k} b_{j,k}(x)$  as a sum of  $K$  basis  $b(\cdot)$  then the problem can be written as:

$$\min_{\beta} \|y - B\beta\|_2^2 + \lambda_1 \sum_{j=1}^p \sqrt{\beta_j' B_j' B_j \beta_j} + \lambda_2 \beta_j' \Omega_j \beta_j \quad (20)$$

267  $\Omega_j$  composed of the inner products of the second derivatives of the basis functions.

268

### 269 5.2. Screening

In an equivalent manner on the screening side the Non-parametric Independence Screening procedure (NIS) has been introduced by [Fan et al. \(2011\)](#) as a natural extension to SIS. Instead of marginal linear correlation they use the concept of "marginal utility", already defined in [Fan et al. \(2009\)](#) for generalized linear models, and here

---

<sup>5</sup> Usually the Ridge because it has an analytical solution.

set this marginal utility to be the sum of squared marginal residuals resulting from a non-parametric additive model.

$$\hat{\omega}_j = \sum_{i=1}^n (y_i - \hat{f}_j(x_{i,j}))^2 \quad (21)$$

The latter, with  $\hat{f}_j(x_{i,j})$  obtained by splines<sup>6</sup>, gives a ranking of variables in the same way as SIS:

$$\hat{M} = \{1 \leq j \leq p : \hat{\omega}_j > \delta\} \quad (22)$$

Where  $\delta$  is a predefined threshold. Usually this step does not ensures selection consistency so they rely on a external procedure, namely SpAM or penGAM. Because of the problem of weak signals Iterative Conditional SIS has been discussed exactly the same as Iterative Conditional SIS was for SIS, that is applying NIS on residuals, conditionally on primarily selected variables. It is worth mentioning the work of [Zhang et al. \(2017\)](#) who developed Correlation Ranked SIS (CR-SIS). The main purpose is to allow for any monotonic transformation of  $y$  by using its cumulative distribution as the dependent variable.

$$\begin{aligned} \omega_j &= Cov(f_j(x_j), G(y))^2 \\ G(y) &= \frac{1}{n} \sum_{i=1}^n I(y_i \leq y) \end{aligned} \quad (23)$$

270 The resulting model is less restricted allowing a non-linear response.

## 271 6. Partial Linear Models

A Partial Linear model takes the form:

$$y = X_1\beta + g(X_2) + \varepsilon \quad (24)$$

272 An important feature of these models is to assume two sets of variables. The  $X$  matrix is divided into  $X_1$  and  $X_2$   
 273 of dimension  $p_1$  and  $p_2$  respectively. The motivation behind this is to say that linearity is satisfactory enough for  
 274 some variables and treating these ones non-parametrically result in a loss of efficiency. So one should divide  
 275 the regressors according to their link function either it is parametric ( $X_1$ ) or not ( $X_2$ ). This section is divided in  
 276 two parts. The first one will concern Partial Linear models in their general form. Because a great literature has  
 277 focused on smoothly varying-coefficients the second part will focus only on them.

### 278 6.1. Standard

#### 279 6.1.1. Penalty

The Double-Penalized Least Squares Estimator (DPLSE) of [Ni et al. \(2009\)](#) is a method for selection of variables and selection between parametric and non-parametric parts. A penalty is imposed on the parametric part to select variables and splines are used for non-parametric estimation. Since in the splines settings one can rewrite this function as a linear combination of basis expansion:

$$g = [J, X_2] \delta + Ba \quad (25)$$

with  $J$  the unit vector  $a$  are the parameters of the basis expansion  $B$  and  $\delta$  is the overall parameter on  $X_2$ . The SCAD penalty is then applied on the vector  $\beta^* = [\beta, \delta]$  This can be viewed as a composite penalty where the key idea is to write everything as linear and perform usual model selection. Partial Splines with Adaptive penalty (PSA) of [Cheng et al. \(2015\)](#) try to achieve a sparse parametric part while having a non-parametric part aside

---

<sup>6</sup> Because of low computational costs, but it can be estimated with any non-parametric regression technology.

using a combination of Adaptive LASSO on the parametric part and Penalized Splines for the non-parametric. Therefore the problem to solve is:

$$\min_{\beta, f} \|y - X_1\beta - f(X_2)\|^2 + \lambda_1 \int_0^1 (f''(X_2))^2 dX_2 + \lambda_2 \sum_{j=1}^p \frac{|\beta_j|}{|\tilde{\beta}_j|^\gamma} \quad (26)$$

We remark the last term is exactly the penalty from the adaptive LASSO. This is in line with DPLSE, adding a smoothness penalty on top of the procedure. In this respect it is worth mentioning the Penalized Estimation with Polynomial Splines (PEPS) of [Lian et al. \(2015\)](#). The same objective is achieved in a quite similar fashion. The only difference is that the penalty is not adaptive:

$$\min_{\beta, f} \|y - B\beta\|^2 + n\lambda_1 \sum_{j=1}^p w_{1,j} \|\beta_j\|_{A_j} + n\lambda_2 \sum_{j=1}^p w_{2,j} \|\beta_j\|_{D_j} \quad (27)$$

280 Basis expansion is contained in  $B$  therefore exploiting once again the linear transformation provided in splines,  
 281 just like DPLSE introduced it. The whole thing is turned as a linear model on which penalties are applied  
 282 to achieve sparsity  $\|\beta_j\|_{A_j} = \|\sum_k \beta_{j,k} B_k(x_j)\|$  and linear parts are recovered from the smoothness penalty  
 283  $\|\beta_j\|_{D_j} = \|\sum_k \beta_{j,k} B_k''(x_j)\|$ .

284

285 In the end there is little difference between the 3 procedures. All exploits the linearity provided by splines.  
 286 PEPS improves on DPLSE adding a smoothness penalty and PSA improves on PEPS making the penalty adaptive  
 287 to achieve better selection consistency.

## 288 6.2. Varying Coefficients

Another usual structure for modelling is the semi-varying coefficient model, written as:

$$y = X_1\beta + X_2\alpha(Z) + \varepsilon \quad (28)$$

289 The coefficients  $\alpha$  associated to each  $x_{j \in 2}$  are supposed to vary smoothly along another variable  $Z$ . This can be  
 290 seen as a particular case of previous models where  $g(\cdot)$  has the specific varying coefficient form.

### 291 6.2.1. Penalty

The methods in this section do not use the semi-structure form, they work only with the varying-coefficient part.

$$y = X\beta(Z) + \varepsilon \quad (29)$$

The Kernel LASSO of [Wang and Xia \(2009\)](#) deals with this problem in the spirit of groupLASSO.

$$\min_{\beta} \sum_{t=1}^n \sum_{i=1}^n \{y_i - X_i\beta(Z_t)\}^2 K_h(Z_t - Z_i) + \sum_{j=1}^p \lambda_j \|\beta_j\| \quad (30)$$

The penalty enforces the procedure to reduce estimated varying coefficients close to zero to true zeros in a single-level group fashion.

Another improvement in this setting is the Adaptive Semi-Varying Coefficients (AdaSVC) of [Hu and Xia \(2012\)](#). Instead of all coefficients varying smoothly one may think that some don't (hence semi-varying). To avoid the loss of efficiency introduced by non-parametric estimation when the true underlying coefficient is constant the latter have to be identified. Their method can simultaneously identify and estimate such a model. Selection is done only over constant regressors. They do not consider sparsity as in Kernel LASSO. The idea is to impose a group penalty on the estimated varying-coefficients such that the penalty enforces nearly constant coefficients to

be truly constant. Their penalty is in line with the FusedLASSO of Tibshirani et al. (2005). The main idea is that nearly constant coefficients will become constant in a grouped fashion. The objective is to solve:

$$\min_{\beta} \sum_{t=1}^n \sum_{i=1}^n \{y_i - X_i \beta(Z_t)\}^2 K_h(Z_t - Z_i) + \sum_{j=1}^p \lambda_j \|b_j\| \quad (31)$$

with the penalty applied on a different norm than the Kernel LASSO:

$$\|b_j\| = \left\{ \sum_{t=2}^n (\beta_j(Z_t) - \beta_j(Z_{t-1}))^2 \right\}^{1/2} \quad (32)$$

## 292 6.2.2. Testing

The Semi-Parametric Generalized Likelihood Ratio Test (SP-GLRT) of Li and Liang (2008). It applies to semi-varying coefficients model. The purpose is both to identify relevant variables and whether if they belong to the non-linear or the linear component. The likelihood can be written as:

$$\mathcal{L}(\alpha, \beta) = l(\alpha, \beta) - n \sum_{j=1}^p p \lambda_j (|\beta_j|) \quad (33)$$

The two parts are estimated alternatively conditionally on the other. Then they introduce a novel generalized likelihood ratio test:

$$\mathcal{T}_{GLR} = r_K \{ \mathcal{R}(H_1) - \mathcal{R}(H_0) \} \quad (34)$$

with

$$\mathcal{R}(H_1) = \mathcal{Q}(X_1 \beta + X_2 \alpha(Z), y) \quad (35)$$

The conditional likelihood under  $H_1$  : at least one coefficient from the non-parametric part is non-zero.

$$\mathcal{R}(H_0) = \mathcal{Q}(X_1 \beta, y) \quad (36)$$

The conditional likelihood under  $H_0$  : the variable does not appear in the non-parametric part. where the conditional likelihood is given by:

$$\mathcal{Q}(\mu, y) = \int_{\mu}^y \frac{s-y}{V(s)} ds \quad (37)$$

293 The test is then evaluated using a Monte Carlo or Bootstrap methods to empirically estimates distribution of the  
294 statistics since the theoretical degrees of freedom tends to infinity preventing from a parametric test.

295 This has to be noticed because this is one of the first attempt of introducing non-parametric and therefore automatic  
296 tests inside a selection procedure. While methods like Autometrics and Stepwise Regression relies on parametric  
297 tests, SP-GLRT uses data-driven tests to construct the model. This idea of exploiting the data themselves to  
298 conduct tests is certainly not new, but it was in model selection. This idea is the core of methodologies for  
299 improving model selection in section 8.

## 300 7. Non-Parametric Models

A fully non-parametric model takes the form of:

$$y = f(X) + \varepsilon \quad (38)$$

301 Where  $f(\cdot)$  is any multivariate function, linear or not, additive or not. This framework is very general therefore  
302 making it complicated for estimation. The most well known drawback is the Curse of Dimensionality. Briefly,  
303 it states that the number of observations required for estimation of this function grows exponentially with the  
304 dimension of  $X$  :  $p$ . It is already complicated to fit such a (maybe very non-linear) function non-parametrically  
305 in a reduced dimension, thus looking for a sparse representation is necessary when dealing with large  $p$ .

306 This time the different methods differ under several aspects. Testing ones like MARS shares similarities  
 307 with Stepwise Regression for example, in an ANOVA Splines settings. Penalty ones uses ANOVA models also,  
 308 the reason is that it limits interactions terms and gets closer to an additive model, this is indeed very common  
 309 when dealing with fully non-parametric regression. The screening based ones can be divided in two categories:  
 310 some make the use of generalized correlations to avoid using a model (DC-SIS,HSIC-SIS,KCCA-SIS,Gcorr)<sup>7</sup>  
 311 while others rely on a specific model ex ante (MDI,MDA,RODEO).<sup>8</sup>

### 312 7.1. Penalty

The Variable selection using Adaptive Nonlinear Interaction Structures in High dimensions (VANISH) of  
 Radchenko and James (2010). It is very similar to the SHIM of Choi et al. (2010) but in a non-linear framework.  
 In order to approach the complexity of the function it uses an ANOVA-type of model defined as:

$$f(X) = \sum_{j=1}^p f_j(x_j) + \sum_{j<k} f_{j,k}(x_j, x_k) + \dots + \varepsilon \quad (39)$$

Where  $f_j$  are the main effects,  $f_{j,k}$  are the two-way interactions and so on. Their approach is closely related to  
 the penGAM of Meier et al. (2009) generalized to include interaction terms<sup>9</sup> but with a different penalty. The  
 authors say that the penalty shouldn't be the same for main effect than for two-way interactions. They advocate  
 the fact that ceteris paribus including an interaction term add more regressors than a main effect and thus that they  
 are less interpretable. So interactions should be more penalized. Therefore this condition is a little bit different  
 from the "strong heredity constraint" introduced in Choi et al. (2010). The objective is to solve:

$$\min_f \|y - f(X)\|_2^2 + \tau^2 J(f) \quad (40)$$

With:

$$J(f) = \lambda_1 \sum_{j=1}^p \left( \|f_j\|^2 + \sum_{k \neq j} \|f_{j,k}\|^2 \right)^{1/2} + \lambda_2 \sum_{j=1}^p \sum_{k=j+1}^p \|f_{j,k}\| \quad (41)$$

The penalty is written so that the first part penalizes additional regressors while the second penalizes interactions  
 occurring without main effects. In the SHIM there was no possibility for that. Here this constraint is released  
 but a stronger penalty can be applied to restrict interactions without main effects, which are less interpretable.  
 Another approach for fitting this type of models is the Component Selection and Smoothing Operator (COSSO)  
 of Lin et al. (2006). It differs from VANISH in the penalty function. The key idea is to use a penalty term  
 written in terms of a sum of Reproducible Kernel Hilbert Space (RHKS) norms. In a model with only two-way  
 interactions it would be:

$$J(f) = \sum_{\alpha=1}^{p(p-1)/2} \|P^\alpha f\|^2 \quad (42)$$

313 This time the penalty is not designed to take into account the structure of the resulting model. There is no desire  
 314 to limit interactions. Since the heredity constraint is not present as before the model authors of VANISH claim it  
 315 has trouble with high dimensional settings. Nevertheless the heredity constraint can obviously be inadequate  
 316 in some applications where only interactions matter, in this type of settings COSSO is more advisable than  
 317 VANISH.

<sup>7</sup> Respectively Distance Correlation-SIS, Hilbert Schmidt Independence Criterion-SIS, Kernel Canonical Correlation Analysis and the Generalized Correlation.

<sup>8</sup> Respectively Mean Decrease Impurity, Mean Decrease Accuracy and the Regularization Of Derivative Expectation Operator.

<sup>9</sup> They also introduce it as SpIn (SpAM with INteractions) in their paper but claim that interactions would then not be treated efficiently.

318 *7.2. Testing*

Introduced by [Friedman \(1991\)](#) the Multivariate Adaptive Regression Splines is a method for building non-parametric fully non-linear ANOVA sparse models (39). The model is written in terms of splines as:

$$\hat{f}(x) = \sum_{k=1}^K c_k B_k(x) \quad (43)$$

The basis functions  $B_k$  are taken to be hinge functions. The form of these functions makes the model piecewise linear.

$$B_k(x, \alpha, \beta) = \beta \max(0, \alpha + x) \quad (44)$$

319 Therefore  $\alpha$  can be considered as "knots" like in standard splines. The  $\beta$  are parameters on which selection  
 320 will occur through a pretty complicated algorithm. The building process is quite comparable to the one of usual  
 321 Regression Trees and Stepwise Regression. Starting from a null model a forward step search over all possible  
 322 variables and determines by least squares the parameter  $\beta$  (thus it creates a new hinge function) and over all  
 323 possible values where to add a knot  $\alpha$  that reduces best the residuals sum of squares<sup>10</sup>. This process goes until  
 324 some stopping criterion is met. All combinations have to be taken into account, therefore it is computationally  
 325 intractable for high interactions effects. Friedman advises to limit the number of interactions  $m$  to a small value  
 326 like 2 such that the model can be build in a reasonable time. Selection of variables is part of the building process.  
 327 If using a fit based criterion like the sum of squares residuals, variables are selected only if they bring enough  
 328 explanatory power during the search. The same thing applies for Regression Trees on non-parametric models. In  
 329 this sense MARS is closely related to Stepwise Regression. Also MARS is available with a backward approach,  
 330 and a combination of both. This method is mainly used to fit high dimensional non-linear functions because since  
 331 it is piecewise linear, it does not suffer much from the Curse of Dimensionality. However its selection consistency  
 332 can be directly linked to the way variables are selected in trees, this is discussed in the next subsections. Used  
 333 directly MARS is more like a non-linear version of Stepwise Regression using piecewise functions.

334 *7.3. Screening*335 *7.3.1. Model-free*

336 In the screening literature of non-parametric methods we find a bunch of papers that deals with the same  
 337 core idea. They all define some association measure that generalizes usual linear correlation. Here is the list  
 338 of them as well as the criteria they use. In fact these methods are quite nested within each other. Considering  
 339 which one is the best is a question of computational complexity rather than in which case they apply. Otherwise  
 340 it seems that the last one (KCCA) should be selected.

- DC-SIS ([Li et al. 2012](#))

The Distance Correlation is a generalization of the Pearson Correlation Coefficient in terms of norm distances. It can be written as:

$$\omega_j = \frac{dcov(x,y)}{\sqrt{dcov(x,x)dcov(y,y)}} \quad (45)$$

Where:

$$\begin{aligned} dcov(x,y)^2 &= \mathbb{E}[\|X - X'\| \|Y - Y'\|] \\ &+ \mathbb{E}[\|X - X'\|] \mathbb{E}[\|Y - Y'\|] \\ &- 2\mathbb{E}[\mathbb{E}[\|X - X'\|] \mathbb{E}[\|Y - Y'\|]] \end{aligned} \quad (46)$$

---

<sup>10</sup> This is known as "Greedy Algorithms" where the optimal global solution is sought by taking optimal local solutions.

- HSIC-SIS (Balasubramanian et al. 2013)

The Hilbert Schmidt Independence Criterion generalizes the previous one as it defines a maximum distance metric in a RKHS space:

$$\begin{aligned}\omega_{(k)}^2 &= \mathbb{E}[k_{\mathcal{X}}(X, X')k_{\mathcal{Y}}(Y, Y')] \\ &\quad + \mathbb{E}[k_{\mathcal{X}}(X, X')]\mathbb{E}[k_{\mathcal{Y}}(Y, Y')] \\ &\quad - 2\mathbb{E}[\mathbb{E}[k_{\mathcal{X}}(X, X')]\mathbb{E}[k_{\mathcal{Y}}(Y, Y')]]\end{aligned}\quad (47)$$

We recognize again the form of the usual correlation but this time written in terms of kernels. In order to avoid the choice of the bandwidths in kernels, they decided to use the sup of the criterion over a family of Kernel  $\mathcal{K}$ .

$$\gamma = \sup \left\{ \omega_{(k)} : k \in \mathcal{K} \right\} \quad (48)$$

Empirically the ranking measure is simpler to compute:

$$\hat{\omega} = \frac{1}{n} \sup_{k_{\mathcal{X}}, k_{\mathcal{Y}}} \sqrt{\text{trace}(K_{\mathcal{X}} H K_{\mathcal{Y}} H)} \quad (49)$$

341 with  $H = I - (1/n)JJ'$ ,  $I$  being the  $n \times n$  unit matrix and  $J$  the  $n \times 1$  unit vector.

- KCCA-SIS Liu et al. (2016)

The Kernel Canonical Correlation Analysis is the last improvement in the field of Non-parametric Screening. It encompasses SIS as it can handle non-linearities. Unlike DC-SIS it is scale-free and does not rely on the Gaussian assumption. However even if it shares many aspects of the HSIC-SIS it differs in one aspect: HSIC is based on maximum covariance between the transformations of two variables, while KCCA uses the maximum correlation between the transformations by removing the marginal variations. Their measure is defined as:

$$\mathcal{R}_{YX} = \Sigma_{YY}^{-1/2} \Sigma_{YX} \Sigma_{XX}^{-1/2} \quad (50)$$

Because the covariance matrices may not be invertible they introduce a ridge penalty  $\varepsilon$ :

$$\mathcal{R}_{YX} = (\Sigma_{YY} + \varepsilon I)^{-1/2} \Sigma_{YX} (\Sigma_{XX} + \varepsilon I)^{-1/2} \quad (51)$$

The correlation measure is then defined as the norm of the correlation operator:

$$\omega(\varepsilon)_j = \|\mathcal{R}_{YX_j}\| \quad (52)$$

342 Empirical estimates of covariance matrices  $\Sigma$  are obtained after singular decomposition of kernel matrices  
343 (the latter being the same as in HSIC). While bandwidths in kernels can be chosen optimally ex ante,  $\varepsilon$   
344 has to be estimated via GCV over a grid of values.

For each one the variables are ranked along marginal association measures  $\hat{\omega}_j$  between  $y$  and  $x_j$  and one defines the set of relevant features after applying a threshold. The latter's value differs among them.

$$\hat{M} = \{1 \leq j \leq p : \hat{\omega}_j \geq \delta\} \quad (53)$$

- 345 • DC-SIS:  $\delta = cn^{-k}$
- 346 • HSIC-SIS:  $\delta = cn^{-k}$
- 347 • KCCA-SIS:  $\delta = cn^{-k}\varepsilon^{-3/2}$

348 with  $0 \leq k \leq 1/2$ .

349

Another of the same kind is the Generalized Correlation Screening (Gcorr) of [Hall and Miller \(2009\)](#) that was introduced as a more general method than NIS. The general correlation coefficient is used as the measure of non-linear relationship. It can be defined as:

$$\hat{\omega}_j = \sup_{h \in \mathcal{H}} \frac{\sum_{i=1}^n \{h(x_{i,j}) - \bar{h}_j\} (y_i - \bar{y})}{\sqrt{n \sum_{i=1}^n \{h(x_{i,j})^2 - \bar{h}_j^2\}}} \quad (54)$$

350 Then these estimates are tested using bootstrap confidence interval instead of threshold like the others usually do.  
 351 Finally significant ones are ranked. Even though their method seems very general, empirically  $h(\cdot)$  are chosen to  
 352 be polynomial functions. This can be restrictive in some situations and less non-parametric in some sense.

### 353 7.3.2. Model Based

The Regularization Of Derivative Expectation Operator (RODEO) of [Lafferty et al. \(2008\)](#), named in reference to the LASSO, applies in the framework of Multivariate Kernel Methods. In kernel regression a specific attention is given to the choice of the bandwidth. We recall that this hyperparameter defines the width of the support for the regression, the lower it is the less observations enter the local regression, leading to less bias but more variance and conversely for a high bandwidth. The authors here state that for variables that are important in the model the derivative of the estimated function with respect to the bandwidth  $h$  is higher than for useless variables. A change in bandwidth affects the estimation if the variable intervenes in the model, it affects the bias-variance trade-off. For an irrelevant variable a change in bandwidth has no effect since more or less observations does not change the fitted curve. For a Gaussian kernel we have:

$$\begin{aligned} \frac{\partial f_h(x)}{\partial h_j} &= e'(X'WX)^{-1}X' \frac{\partial W}{\partial h_j} (y - X\hat{\beta}) \\ \frac{\partial W}{\partial h_j} &= WL_j \\ L_j &= \frac{1}{h_j^3} \text{diag}((x_{1,j} - \bar{x}_j)^2, \dots, (x_{n,j} - \bar{x}_j)^2) \end{aligned} \quad (55)$$

354 Note that it refers to a specific point in the sample  $\bar{x}$ . The derivative is not computed over the whole sample. The  
 355 authors propose an extension of local RODEO to a global procedure where the derivative is computed in every  
 356 point and then averaged.

357 The idea is to exploit this derivative iteratively, starting from a high bandwidth value and adapted in each step  
 358 according to a certain rate of decay. Important variables should have low bandwidth, so the derivative is greater  
 359 and the bandwidth reduces more quickly. Variables then can be ranked according to the final value of their  
 360 bandwidth. One can apply some threshold on these to end up with a sparse solution. In this respect RODEO can  
 361 be classified as a screening procedure. RODEO is based on a full estimation via Kernel, therefore it suffers the  
 362 Curse of Dimensionality mentioned earlier. RODEO may not be able to deal with high dimensional feature space.

363

A large part of the literature focuses on a quite restricted set of regression methods for doing selection such as Ordinary Least Squares for linear models, Splines and Kernels for non-linear ones. However there exists other ways for doing regression from which model selection procedures intuitively arise. In a Bayesian framework<sup>11</sup> one will consider a collection of models called an Ensemble. There is a distribution of them and we are uncertain on which one is the truth<sup>12</sup>. Still we can exploit this distribution across these different models to assign probabilities to each variables since they may not all appear in every models. This idea has also been developed in the frequentist approach by [Breiman \(2001\)](#) who introduced Random Forest. From an Ensemble of Regression Trees (called a Forest) he derived two types of variables importance measures : Mean Decrease

<sup>11</sup> Which is out of the scope of this paper but still very important.

<sup>12</sup> This relates obviously to the problem raised when discussing Stepwise Regression. Here the Ensemble is a subset of the model space.

Impurity (MDI) and Mean Decrease Accuracy (MDA). We recall briefly that a tree is constructed as a recursive partitioning over the sample space. Simple Regression Trees allows for constant estimation in subregions, this is closely related to the Nadaraya-Watson local constant kernel estimator. Splits are chosen according to an impurity criterion that describes the degree of similarity<sup>13</sup> of the data in the partition.

$$MDI(x_j) = \frac{1}{N_t} \sum_T \sum_{t \in T} \frac{N_t}{N} \left( i(t) - \frac{N_{t_{left}}}{N_t} i(t_{left}) - \frac{N_{t_{right}}}{N_t} i(t_{right}) \right) \quad (56)$$

364 The importance of variable  $j$  is computed as the average decrease in impurity among each node  $t$  in tree  $T$ . The  
 365 idea is to show the decrease in impurity caused by a split in this variable. It is computed as the impurity in the  
 366 node minus the sum of impurity in the child nodes weighted by their respective sizes. This gain is weighted in  
 367 the end by the number of observations entering the node. MDI can be easily extended to an Ensemble of Trees  
 368 (i.e. a Forest).

The second measure relies on the predictive power of the model instead of the impurity inside nodes. From a statistical point of view it is equivalent as focusing on out-of-sample fit rather than in-sample fit. Since it does not rely on an inside criterion it is only defined for a tree and therefore applies only for an ensemble of them.

$$VI^T(x_j) = \frac{\sum_{i \in \mathcal{B}(T)} I(y_i = y_i^{(T)})}{|\mathcal{B}(T)|} - \frac{\sum_{i \in \mathcal{B}(t)} I(y_i = y_{i,\pi_j}^{(T)})}{|\mathcal{B}(T)|} \quad (57)$$

$$MDA(x_j) = \frac{\sum_{T \in F} VI^T(x_j)}{N_T} \quad (58)$$

369 The importance of variable  $j$  is computed as the average decrease in accuracy among each tree  $T$  in the forest  
 370  $F$ . The idea is that if a variable is uninformative then the prediction accuracy should be unchanged under  
 371 permutation. The difference between actual prediction and permuted prediction give sthe decrease in accuracy  
 372 for each variable and the whole is a weighted average of each tree in the forest.

## 373 8. Improving on Variable Selection

374 This last section is devoted to general methodologies designed for improving model selection procedures.  
 375 Based on bootstrap or resampling, the core idea is to exploit randomness to account for uncertainty in the  
 376 modelling. Usual model selection procedures may suffer from inconsistency under some conditions. For example  
 377 we remember the LASSO where the regularization parameter  $\lambda$  can not be chosen optimally<sup>14</sup> so that it ensures  
 378 correct identification. This has lead to the adaptive LASSO (Zou 2006), but this problem can also be solved using  
 379 these procedures.

### 380 8.1. Stability Selection

The Stability Selection (Stabsel) has been introduced by Meinshausen and Bühlmann (2010) to improve on selection. Given a specific selection procedure a variable is said to be stable if its selection probability under subsampling<sup>15</sup> (number of times it has been selected among the random samples) exceeds a specified threshold  $\delta$ . The selection probabilities for a variable  $j$  to belong to the set  $S^\lambda$  of selected variables for a given regularization parameter  $\lambda$  is:

$$\Pi_j^\lambda = \mathbb{P}(j \subseteq S^\lambda) \quad (59)$$

The set of stable variables is then:

$$S^{Stable} = \{j : \max_{\lambda \in \Lambda} \Pi_j^\lambda \geq \delta\} \quad (60)$$

<sup>13</sup> In case of a regression: How well the subregion can be approximated by a constant.

<sup>14</sup> Both from an estimation and a predictive point of view

<sup>15</sup> Without replacement, random samples have to be non-overlapping.

This is given by the underlying selection procedure, it can be the LASSO or whatever, but the methodology aims at improving a procedure, not being one itself.

Another way for randomness that is almost equivalent is to divide the sample in two non-overlapping parts of sizes  $\lfloor n/2 \rfloor$  and look for variables that are selected simultaneously in both. This is more computationally efficient. The threshold can be selected appropriately so that the expected number of false inclusion  $V$  is bounded.

$$\mathbb{E}[V] \leq \frac{1}{2\delta - 1} \frac{q_\lambda^2}{p} \quad (61)$$

Thus one will ensure  $\mathbb{P}(V > 0) \leq \alpha$  by setting for example:

$$\begin{aligned} \delta &= 0.9 \\ q_\lambda &= \sqrt{0.8\alpha p} \end{aligned} \quad (62)$$

381 The results are then presented as stability paths:  $\Pi_j^\lambda$  as a function of  $\lambda$ . This is in contrast to regularization paths  
382 of LASSO:  $\beta_j$  as a function of  $\lambda$ .

383 Extensions to Stabsel are proposed in [Bach \(2008\)](#) and [Shah and Samworth \(2013\)](#). The first uses bootstrap with  
384 replacement instead of resampling without while the latter uses subsampling of complementary pairs.

## 385 8.2. Ranking-Based Variable Selection

The Ranking-Based Variable Selection (RBVS) of [Baranowski and Fryzlewicz \(2016\)](#) is a screening procedure based on bootstrap and permutation tests. Contrary to Stabsel it does not rely on any threshold nor any assumptions.

Given a metric to assess the strength of the relationship denoted  $\omega$  and then using the  $m$ -out-of- $n$  bootstrap of Bickel et al. (2012) they construct a permutation ranking  $\mathcal{R}$ .

$$\mathcal{R} = (\mathcal{R}_1, \dots, \mathcal{R}_p) \text{ satisfying } \omega_{\mathcal{R}_1} \geq \dots \geq \omega_{\mathcal{R}_p} \quad (63)$$

The metric can be anything like the Pearson Correlation, the LASSO coefficients, etc. The probability of the set of the  $k$  top-ranked variables  $\mathcal{A}_k$  is defined as:

$$\pi(\mathcal{A}_k) = \mathbb{P}(\{\mathcal{R}_1, \dots, \mathcal{R}_k\} = \mathcal{A}) \quad (64)$$

This value is approximated with using the  $m$ -out-of- $n$  bootstrap procedure involving random draws without replacements of the observations.

In fact selection can be performed on the set of top-ranked variables  $\mathcal{A}$  from which the number of terms  $k^*$  can be determined automatically without threshold. The idea is not to look for a threshold  $\delta$  that would cut in the ranking of  $\omega$ . As an alternative they try to estimate  $k^*$  as:

$$k^* = \operatorname{argmin}_{k=0, \dots, p-1} \frac{\pi(\mathcal{A}_{k+1, m})}{\pi(\mathcal{A}_{k, m})} \quad (65)$$

386 That is the number of terms for which the differences among the  $\pi(\mathcal{A})$  is the greater. This is equivalent to look  
387 for a threshold that best separates assuming there are two sets: the relevant and the irrelevant. It has the advantage  
388 of being totally non-parametric. Just like the SIS has its iterative counterpart they introduce the Iterative RBVS  
389 that accounts for marginally related variables with low Signal-to-Noise and for the multicollinearity problem.

## 390 9. Discussion

391 In this article, we provide a review for 39 state-of-the-art procedures to perform variable  
392 selection over a wide range of model structures going from the simple linear one to the complex  
393 non-parametric one. Procedures have been classified in three groups: Tests-Based, Penalty-Based  
394 and Screening-Based. They have been described and compared on the ground of model structures.

395 The main difference consists of modelling purposes and objectives rather than their strength as oracles. In  
 396 an empirical work the choice between two strategies should rely on the form of the model, data specificities  
 397 (collinearity, groups, etc..) and objectives (in other words understandability).

398

399 Selection consistency for widely used methods in empirical work have been discussed and several  
 400 improvements were presented. Far beyond Stepwise Regression and the LASSO, empiricists have access to  
 401 more advanced technologies that we claim are not much more complicated than the basic ones. The limits  
 402 in main methods (LASSO, Stepwise Regression) are now well understood and various answers have come to light.

403

404 The area of model selection is still very investigated, much more now that amounts of data have become  
 405 available. Nevertheless, methods for handling large number of variables are restricted in terms of model  
 406 complexity. This is mainly due to the Curse of Dimensionality and it prevents from looking for very complex  
 407 models in high dimensions. Sure Independence Screening is a powerful tool in linear models but have lower  
 408 dataset capacities when it comes to non-linearities. Also, the literature is lacking from very complete algorithmic  
 409 solutions. To the best of our knowledge, no statistical procedure have been developed to reach the level of  
 410 completeness of Autometrics. Other methods are only parts of the statistical work and do not cover as many  
 411 problems as Autometrics do.

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413

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