Multi-Model Ensemble Optimization

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Abstract

Methodology and optimization algorithms for sparse regression are extended to multi-model regression ensembles. In particular, we adapt optimization algorithms for \( \ell_0 \)-penalized problems to learn ensembles of sparse and diverse models. To generate an initial solution for our algorithm, we generalize forward stepwise regression to multi-model regression ensembles. The sparse and diverse models are learned jointly from the data and constitute alternative explanations for the relationship between the predictors and the response variable. Beyond the advantage of interpretability, in prediction tasks the ensembles are shown to outperform state-of-the-art competitors on both simulated and gene expression data. We study the effect of the number of models and show how the ensembles achieve excellent prediction accuracy by exploiting the accuracy-diversity tradeoff of ensembles. The optimization algorithms are implemented in publicly available R/C++ software packages.

Keywords: Ensemble methods; Sparse methods; Multi-model optimization; High-dimensional data; Model diversity.
1 Introduction

In modern data analysis tasks, a model with good prediction accuracy is typically not sufficient; in high-stakes data-driven decision making it is often necessary to obtain a model that is also interpretable. Recently, there have been a lot of influential articles advocating for the need of statistical procedures that retain a certain degree of interpretability despite their high prediction accuracy, see e.g. relevant discussions in Rudin (2019), Murdoch et al. (2019) and Rudin et al. (2022). The issue of interpretability is particularly important for the analysis of high-dimensional data where the number of predictors \( p \) is much greater than the number of samples \( n \) \((p \gg n)\), and parsimonious models where only a small subset \( t \ll p \) of the predictors are included are preferred. For example, in the analysis of deoxyribonucleic acid (DNA) microarrays, the expression levels for thousands of genes are collected. A valuable model would be one with high prediction accuracy, but also one in which only a small subset of genes are identified as relevant to predict the outcome of interest.

To address the problem of prediction accuracy and interpretability in the presence of high-dimensional data, sparse regularization methods have been developed over the last three decades. In essence, sparse regularization methods optimize the goodness-of-fit of a single model while penalizing its complexity, resulting in an interpretable model with good prediction accuracy. Many regularization methods have been developed for a large class of statistical models, see e.g. Hastie et al. (2019) for an extensive and modern treatment. While prediction has always been a subject of importance for sparse regularization methods, there is a much stronger emphasis on inference and uncovering the true mechanism of how the output is generated as a function of the predictor variables. A deep theoretical treatment of sparse regularization methods, in terms of estimation and variable selection, may be found in Bühlmann and Van De Geer (2011). While sparse regularization methods have well-established statistical theory and result in interpretable models, they are often outperformed in terms of prediction accuracy by ensemble methods.

Ensemble methods, where multiple diverse models are generated and aggregated, are some of the most popular “blackbox” algorithms for the analysis of high-dimensional data. They have led to a plethora of successful applications in genetics (see e.g. Dorani et al. (2018); Zahoor and Zafar (2020)), computer vision (see e.g. Rodriguez-Galiano et al. (2012); Yu and Zhang (2015)), speech recognition (see e.g. Krajewski et al. (2010); Rieger et al. (2014)), fraud detection (see e.g. Kim and Sohn (2012); Louzada and Ara (2012)), and many other fields. Diverse members are essential for the good predictive performance of ensembles (Brown et al., 2005). Current state-of-the-art methods rely on randomization or the sequential refitting of residuals to achieve diversity, which results in a large number of
uninterpretable models with poor individual prediction accuracy.

In this article, we introduce a unifying framework that combines the interpretability of sparse regularization methods with the high prediction accuracy of ensemble methods. In particular, we generalize sparse regression methods to multi-model regression ensembles. The proposed methodology results in ensembles comprised of a small number of sparse and diverse models, learned jointly from the data, that each have a high prediction accuracy. Thus each of the models in the ensembles provide a possible explanation for the relationship between the predictors and the response. Further, the ensembles achieve high prediction accuracy compared to state-of-the-art ensemble methods. To convey our ideas, we focus on regression ensembles.

The remaining of this article is organized as follows. In Section 2 we provide a literature review of sparse and ensemble methods. In Section 3 we introduce the unifying framework between sparse and ensemble methods. In Section 4, we generalize stepwise regression to multi-model ensembles, which will constitute the initialization procedure for the Algorithm of Section 5. In Section 5 we introduce a projected subsets gradient descent algorithm, adapting $\ell_0$ optimization approaches to multi-model regression ensembles. In Section 6 we perform an extensive simulation study to benchmark the proposed methodology against state-of-the-art methods. In Section 8 we benchmark the proposed methodology on a gene expression data application. Section 9 closes the article with a discussion.

2 Literature Review: Sparse and Ensemble Methods

We study the linear model with a dataset consisting of a response vector $y = (y_1, \ldots, y_n)^T \in \mathbb{R}^n$ and a design matrix $X \in \mathbb{R}^{n \times p}$ comprised of $n$ observations $x_i \in \mathbb{R}^p$ for $p$ predictors,

$$y_i = x_i' \beta_0 + \sigma \epsilon_i, \quad 1 \leq i \leq n,$$

where $\beta_0 \in \mathbb{R}^p$ and the elements of the noise vector $\epsilon = (\epsilon_1, \ldots, \epsilon_n)^T \in \mathbb{R}^n$ have variance 1. We are interested in the high-dimensional scenario where $p \gg n$ and the underlying model is sparse, i.e. only a small fraction of the available predictors are relevant for explaining the response. For simplicity, we omit the intercept term from the regression model. We assume that the response $y$ the entries of the design matrix, $x_{ij}, 1 \leq i \leq n$ and $1 \leq j \leq p$, are standardized so that

$$\frac{1}{n} \sum_{i=1}^{n} x_{ij} = 0, \quad \frac{1}{n} \sum_{i=1}^{n} x_{ij}^2 = 1, \quad 1 \leq j \leq p, \quad \frac{1}{n} \sum_{i=1}^{n} y_i = 0, \quad \frac{1}{n} \sum_{i=1}^{n} y_i^2 = 1.$$
2.1 Sparse Methods

Sparse regularization methods penalize model complexity. The purpose of such methods is to find the best sparse model that achieves good prediction accuracy. The most natural approach for sparse modeling is Best Subset Selection (BSS), first mentioned in the literature by Garside (1965), which solves the nonconvex problem

$$\min_{\beta \in \mathbb{R}^p} \|y - X\beta\|^2_2 \quad \text{subject to} \quad \|eta\|_0 \leq t.$$  \hspace{1cm} (1)

The largest number of nonzero coefficients $t \leq \min(n - 1, p)$ in the regression coefficients vector $\beta = (\beta_1, \beta_2, \ldots, \beta_p)^T$ is typically determined in a data-driven way, e.g. by cross-validation (CV). While BSS has been shown to have desirable variable selection and estimation properties (see e.g. Bunea et al. (2007); Shen et al. (2013)), it is an NP-hard problem (Welch, 1982). There are $\mathcal{K}(p, t) = \sum_{j=0}^{t} \binom{p}{j}$ possible subsets that must be evaluated to determine the exact solution. For example, $\mathcal{K}(15, 10) = 30,826$ which is already a large number of subsets, even in this setting with a small number of predictor variables. While many proposals have been made to determine the optimal subset based on the training data (see e.g. Mallows, 1973; Akaike, 1974; Schwarz, 1978), CV is often recommended (Hastie et al., 2009b) which makes the procedure even more computationally intensive. The branch-and-bound algorithm developed by Furnival and Wilson (1974) was initially the procedure of choice for BSS, but it did not scale well beyond $p > 30$. While an improved branch-and-bound algorithm was developed by Gatu and Kontoghiorghes (2006), the method still does not scale well beyond $p > 100$.

To address the computational infeasibility of BSS, stepwise algorithms were developed (see e.g. Jennrich and Sampson (1968); Pope and Webster (1972); Bendel and Afifi (1977)). At each step a variable is added (forward selection) and/or removed (backward elimination) from a subset of model predictors based on model goodness-of-fit until no further step can improve the model to a statistically significant extent. Stepwise algorithms have been heavily criticized and are regarded as a form of data dredging with poor model selection properties (see e.g. Rencher and Pun (1980); Wilkinson and Dallal (1981); Copas (1983); Hurvich and Tsai (1990); Roecker (1991)).

To address the shortcomings of stepwise procedures, sparse regularization methods were subsequently popularized first by basis pursuit denoising (Chen and Donoho, 1994) and then the closely related Lasso (Tibshirani, 1996), a convex relaxation of BSS which solves
problems of the form

\[
\min_{\beta \in \mathbb{R}^p} \| y - X \beta \|^2_2 \quad \text{subject to} \quad \| \beta \|_1 \leq t, \quad (3)
\]
or in its Lagragian form

\[
\min_{\beta \in \mathbb{R}^p} \| y - X \beta \|^2_2 + \lambda \| \beta \|_1. \quad (4)
\]

Many different sparse regularization methods have been proposed (see e.g. Zou and Hastie (2005); Candes and Tao (2007); Zhang (2010)). Efficient convex solvers have been developed for the Lasso (see e.g. Efron et al. (2004); Friedman et al. (2007)), however restrictive conditions on the covariance of the predictors must hold for the Lasso to have good variable selection properties (see e.g. Zhao and Yu (2006)) and good relative prediction error compared to BSS (see e.g. Zhang et al. (2014)).

Recent developments by Bertsimas et al. (2016) to study the BSS nonconvex problem (3) with a modern optimization lens has led to new research avenues in \( \ell_0 \)-penalized statistical procedures (see e.g. Bertsimas and Van Parys (2020); Takano and Miyashiro (2020); Kenney et al. (2021); Thompson (2022)). Bertsimas et al. (2016) first generate good local solutions with a projected gradient descent algorithm, and then use them as warm-starts for a MIO solver. Thompson (2022) adapted their approach approach to develop a robust version of BSS. Their approach scaled to problems of dimension \( p > 1,000 \), but even with the warm-starts the MIO solver may still take upwards of 30 minutes to compute. To reduce the need for a MIO solver, Hazimeh and Mazumder (2020) proposed a method that generates new candidate solutions to reduce the need for a MIO solver. Once a local (incumbent) solution has been obtained from a projected gradient descent algorithm, they apply small perturbations to the local solution to yield new starting points and apply the projected gradient descent algorithm to each one of them. If the best solution obtained from the new candidates improves on the incumbent solution, it is set as the new solution. This process is repeated until no significant difference occurs for the objective function. They showed empirical evidence that their proposal often recovers either the optimal or a near-optimal solution to BSS for \( p > 1,000 \) in a matter of seconds.

To explain the intuition for the potential reduction in prediction error of sparse regularization methods, consider an estimator \( \hat{f}(x) = \hat{\beta}^T x \) of the regression function \( f(x) = \beta_0^T x \). The mean squared prediction error (MSPE) of \( \hat{f} \) may be decomposed into its bias, variance and irreducible error,

\[
\text{MSPE} \left[ \hat{f} \right] = \mathbb{E}_x \left[ (f(x) - \hat{f}(x))^2 \right] + \sigma^2 = \text{Bias} \left[ \hat{f} \right]^2 + \text{Var} \left[ \hat{f} \right] + \sigma^2. \quad (5)
\]
Since least squares regression is the best linear unbiased estimator (BLUE), the rationale for regularized estimation is to exploit the bias-variance trade-off favorably, i.e. to incur a small increase in bias in exchange for a larger decrease in variance.

2.2 Ensemble Methods

To understand the competitive advantage of ensemble methods in terms of prediction accuracy, we first decompose their MSPE. For an ensemble comprised of $G$ regression functions, $\bar{f} = \sum_{g=1}^{G} \hat{f}_g / G$, then its MSPE can be decomposed as

$$\text{MSPE} [\bar{f}] = \text{Bias} [\bar{f}]^2 + \text{Var} [\bar{f}] + \sigma^2,$$

where

$$\text{Bias} [f] = \overline{\text{Bias}} \quad \text{and} \quad \text{Var} [f] = \frac{1}{G} \overline{\text{Var}} + \frac{G-1}{G} \overline{\text{Cov}},$$

and $\overline{\text{Bias}}, \overline{\text{Var}}$ and $\overline{\text{Cov}}$ are the average biases, variances and pairwise covariances of the $G$ regression functions in the ensemble (Ueda and Nakano, 1996). From (7) it is clear that an ensemble can successfully reduce its variance if the models in the ensemble are sufficiently diverse (uncorrelated), especially if the number of models is large.

The statistics and machine learning community have seen an increase in algorithmic approaches to generate ensembles over the last twenty years, with most proposals relying on randomization (see e.g. Breiman, 2001; Song et al., 2013) or boosting (see e.g. Friedman, 2001; Bühlmann and Yu, 2003; Schapire and Freund, 2012; Yu et al., 2020). Interpretability of such ensembles is typically unfeasible. However, several ad hoc methods have been developed to assess predictor importance (see e.g. Hastie et al., 2009a). In an attempt to bridge the gap between interpretability and ensemble methods, Bühlmann et al. (2006) introduced sparse boosting by minimizing some penalized $\ell_2$-loss function for better variable selection.

The purpose of these ensemble methods is to generate a collection of diverse models comprised of different subsets of predictors. For example, in Random Forests random sampling of the data (bagging) (Breiman, 1996a) and the random predictor subspace method (Amit and Geman, 1997; Ho, 1998; Dietterich, 2000) are combined to generate uncorrelated trees for the purpose of achieving a lower generalization error (Breiman, 2001). In gradient boosting, diverse members (typically decision trees) are generated by sequentially fitting the residuals of the previous fit.
2.3 A Unifying Methodology

The multiplicity of good models is a phenomenon that has long been acknowledged, see e.g. relevant discussions in McCullagh and Nelder (1989) and Mountain and Hsiao (1989). Different, yet equally good models can provide distinct explanations for the underlying relationship between predictors and response. However, based on the philosophy of Rudin (2019), current state-of-the-art ensemble methods lack interpretability as they typically consist of either a large number of models generated using random-based approaches or a (smaller) number of models indirectly generated by sequentially fitting residuals instead of the data. The models in the ensembles do not have high prediction accuracy on their own; they only work well when they are pooled together in the final ensemble fit. Thus each model is not insightful or reliable on its own. Hence, there is a gap between interpretable single model methods such as sparse regularization and algorithmic ensemble methods. We aim to fill this gap by developing a systematic approach to construct ensembles consisting of a relatively small number of interpretable sparse models with high individual prediction accuracy. Each of these models is learned directly from the data and provides a reliable relationship between the predictors and the response. Diversity between the models is imposed by restricting the sharing of predictors between different models.

3 Best Split Selection

We now formally introduce the unifying framework between sparse and ensemble methods. Suppose we wish to find a collection of \( G \geq 2 \) sparse and diverse models in an ensemble. Denote the matrix of model coefficients

\[
\beta_{1:G} = \begin{pmatrix} \beta_{11} & \beta_{12} & \ldots & \beta_{1G} \\ \beta_{21} & \beta_{22} & \ldots & \beta_{2G} \\ \vdots & \vdots & \ddots & \vdots \\ \beta_{p1} & \beta_{p2} & \ldots & \beta_{pG} \end{pmatrix},
\]

(8)

where \( \beta_{1:G} \in \mathbb{R}^{p \times G} \) and \( \beta_{gj} \) is the coefficient for predictor \( j \) of model \( g \), \( 1 \leq g \leq G \). For notational convenience let \( \beta^g = (\beta_{1g}, \beta_{2g}, \ldots, \beta_{pg})^T \in \mathbb{R}^p \) be the coefficients of model \( g \) and \( \beta_{j:} = (\beta_{j1}, \beta_{j2}, \ldots, \beta_{jG})^T \in \mathbb{R}^G \) the coefficients of predictor \( j \) across the \( G \) models. Then Best Split Selection (BSpS) solves, for a fixed number of sparse models \( G \), the nonconvex problem

\[
\min_{\beta_{1:} \ldots, \beta_{G:} \in \mathbb{R}^p} \sum_{g=1}^{G} (y - X\beta^g)^2 \quad \text{subject to} \quad \begin{cases} \|\beta^g\|_0 \leq t, & 1 \leq g \leq G, \\ \|\beta_{j:}\|_0 \leq u, & 1 \leq j \leq p. \end{cases}
\]

(9)
The parameter \( t \leq \min(n - 1, p) \) restricts the \( \ell_0 \)-norm of the columns of \( \beta_{1:G} \) and thus the number of nonzero coefficients in each model. The parameter \( u \leq G \) restricts the \( \ell_0 \)-norm of the rows of \( \beta_{1:G} \) and thus the number of models that share any given predictor. Note that if \( u = G \), then (9) is equivalent to BSS in (3) for the same value of \( t \) and there is no diversity among the models. Hence BSpS may be seen as a generalization of BSS to multiple groups. The tuning parameters may be chosen in a data-driven manner by using CV for instance.

BSpS thus aims to find \( G \) sparse models, in such a way that each model explains well the response and the different models do not have much overlap. In this way, the models complement each other well in an ensemble. While there are many proposals in the literature to obtain an optimal ensembling function (see e.g. Breiman (1996b)), for simplicity in this article the ensemble fit corresponding to the \( G \) models selected by (9) is given by

\[
\bar{\beta} = \frac{1}{G} \sum_{g=1}^{G} \tilde{\beta}^g.
\]  

(10)

Hence, in contrast to algorithmic ensemble methods, but similarly to regularization methods, the ensemble model is an interpretable, sparse linear model. The ensemble model combines the information of the \( G \) individual models, which individually provide an explanation for the relationship between a subset of the predictors and the response.

### 3.1 Split Combinatorics

The total number of possible splits of \( p \) variables into \( G \) groups, for \( p \geq G \), was derived by Christidis et al. (2020). We extend their combinatorics result to the BSpS optimization problem (9) for the case without overlap between the models \( (u = 1) \). Note that the computational problem for BSpS is even larger if predictors are allowed to be shared between groups \( (u > 1) \). Let \( p_g \) be the number of variables in group \( g \), \( 1 \leq g \leq G \), and let \( q = \sum_{g=1}^{G} p_g \). Also let \( h_i(p_1, \ldots, p_G) \) be the number of elements in the sequence \( p_1, \ldots, p_G \) that are equal to \( i \), \( 1 \leq i \leq t \). The number of possible splits of \( p \) features into \( G \) groups comprised of at most \( t \) variables is given by

\[
T(p, G, t) = \sum_{p_1 \leq \cdots \leq p_G \leq t} \binom{p}{q} \left[ \frac{q!}{p_1! \cdots p_G!} \prod_{i=1}^{t} \frac{1}{h_i(p_1, \ldots, p_G)!} \right].
\]  

(11)

For example, \( T(15, 3, 10) = 171,761,941 \). Thus, even for a relatively small number of predictor variables, the issue of computational infeasibility of BSpS becomes apparent and will be magnified further if \( t \) and \( u \) in (9) are chosen by CV. The BSS optimization problem in (3) can always make use of MIO to generate global solutions using locally optimal
solutions as initial candidates (see e.g. Bertsimas et al. (2016); Thompson (2022)). The computational infeasibility of BSpS, as seen from the combinatorics in (11), eliminates this approach for (9).

3.2 Related Work

In related work, Christidis et al. (2020) recently introduced the Split Regularized Regression (SplitReg) method which can be seen as a computationally more attractive, multi-convex relaxation of BSpS. While hard thresholds are used in BSpS in (9), soft thresholds are used in SplitReg which can be incorporated in the objective function more easily.

In detail, SplitReg is a minimizer $\beta_{1:G} = (\beta^1, \ldots, \beta^G) \in \mathbb{R}^{p \times G}$ of an objective function of the form

$$ J(y, X, \beta^1, \ldots, \beta^G) = \sum_{g=1}^{G} \left\{ \frac{1}{2n} \|y - X\beta^g\|_2^2 + \lambda_s P_s(\beta^g) + \frac{\lambda_d}{2} \sum_{g \neq h} P_d(\beta^h, \beta^g) \right\} $$

(12)

where $P_s$ and $P_d$ are sparsity and diversity penalty functions, and the constants $\lambda_s, \lambda_d > 0$, which may be chosen e.g. by CV, control the magnitude of the effect of the sparsity and diversity penalties. Christidis et al. (2020) propose to use as sparsity and diversity penalties

$$ P_s(\beta) = \|\beta\|_1 \quad \text{and} \quad P_d(\beta^g, \beta^h) = \sum_{j=1}^{p} |\beta^g_j||\beta^h_j| $$

(13)

Hence, $P_s(\beta)$ is the Lasso penalty while the diversity penalty $P_d(\beta^g, \beta^h)$ is an $\ell_1$-norm relaxation of the hard threshold in (9). Note that for $\lambda_d = 0$, SplitReg in (12) is equivalent to sparse estimation with the penalty $P_s$, irrespective of the number of groups $G$.

The ensemble fit corresponding to the solution of (12) is again given by (10). Christidis et al. (2020) showed that with the penalties in (13) the ensemble estimator yields consistent predictions and has a fast rate of convergence. Moreover, the general framework (12) allows the diversity penalty to be combined with alternative sparsity penalties such as the group Lasso (Yuan and Lin, 2006) for categorical variables or the fused Lasso (Tibshirani et al., 2005) for data containing spatial or temporal structures. The SplitReg objective function is multi-convex and can be solved efficiently via a block coordinate descent algorithm.

Unlike the parameters $t$ and $u$ in BSpS, the parameters $\lambda_s$ and $\lambda_d$ do not directly control the number of predictors in each model and the number of models that can share any given predictor. There is theoretical and empirical evidence that such sparse regularization methods can negatively affect variable selection (see e.g. Van De Geer and Bühlmann (2009); Hazimeh and Mazumder (2020)). Further, the penalties (13) in SplitReg induce shrinkage of the coefficients, and empirical studies and it has been suggested that shrinkage may
have a negative effect on prediction in high signal-to-noise scenarios (see e.g. Hastie et al. (2020)). We develop computational tools to directly optimize BSpS in (9) and alleviate the issues associated with shrinkage-inducing methods. In Section 4 we generalize forward stepwise regression to optimize BSpS in (9) for the special case \( u = 1 \), which constitutes an initial starting point for our main algorithm. In Section 5 we develop a computing algorithm capable of handling any \( u \in \{1, \ldots, G\} \).

4 Stepwise Split (Regularized) Regression

In this section, we generalize forward stepwise regression to multi-model regression ensembles. Our aim is to develop a fast algorithm that generate solutions for BSpS in (9) in the particular case that \( u = 1 \) (i.e. when models are fully disjoint), which will constitute the initial starting point for our main algorithm in Section 5.

For notational convenience, for any subset \( S \subseteq \{1, \ldots, p\} \) we denote \(|S|\) the cardinality of the set \( S \), \( \beta_S \in \mathbb{R}^{|S|} \) the subvector of \( \beta \in \mathbb{R}^p \) with element indices \( S \), and \( X_S \in \mathbb{R}^{n \times |S|} \) the submatrix of \( X \) with column indices \( S \). We denote by \( I_n \in \mathbb{R}^{n \times n} \) the identity matrix of order \( n \) and \( F_{(d_1,d_2)}^{-1}(t) \) the quantile function of the \( F \)-distribution with \( d_1 \) and \( d_2 \) degrees of freedom, respectively.

The stepwise split (regularized) regression algorithm is described in detail in Algorithm 1. Initially, each model is comprised of no predictor variables. At each iteration of step 1, the candidate predictor that provides the largest improvement in goodness-of-fit to each unsaturated model is identified. The unsaturated model with the most statistically significant possible goodness-of-fit improvement based on an \( F \)-test (at some level \( \gamma \in [0,1] \)) is updated by adding its optimal candidate predictor to its set of model predictors. Once a predictor is included in a set of model predictors, it is removed from the set of candidate predictors and can no longer be used in another model. A model is declared saturated if there are no remaining candidate predictors providing any statistically significant improvement to the goodness-of-fit, or if it contains \( n - 1 \) predictors. This process is repeated until all \( G \) models are saturated.

The least squares or Lasso fit is applied to each model in step 2. If the Lasso is the fitting method of choice, each model is shrunk by a custom parameter \( \lambda^{(g)} \) chosen by CV. For completeness we include the stepwise procedure in Algorithm 1, which we refer as Step-SplitReg, in the simulation study and real data applications of Sections 6 and 8 respectively. Based on our numerical experiments, a Lasso fit to each model in step 2 produces an ensemble with better prediction accuracy and better variable selection compared to using a least squares fit, and so Step-SplitReg results are reported for the case where a Lasso fit is used for each model.
Algorithm 1 Stepwise Split (Regularized) Regression

**Input:** Design matrix $X \in \mathbb{R}^{n \times p}$, response vector $y \in \mathbb{R}^n$, number of models $G \geq 2$, and significance threshold $\gamma \in [0, 1]$.

**Initialize:** The set of candidate predictors $J = \{1, \ldots, p\}$. For each model $(1 \leq g \leq G)$ the set of predictors $J^{(g)} = \emptyset$, the model saturation indicator $T^{(g)} = \text{false}$ and the hat matrix $H^{(g)} = 0 \in \mathbb{R}^{n \times n}$.

1: Repeat the following steps until $\gamma^* \geq \gamma$ or $T^{(g)} = \text{true}$ for all $1 \leq g \leq G$:

1.1: For each model $g$ satisfying $T^{(g)} = \text{false}$:

1.1.1: Identify candidate predictor maximizing decrease in residuals sum of squares,

$$ j^{(g)} = \arg \max_{j \in J} \tau_j^{(g)}, \quad \tau_j^{(g)} = \frac{y^T (I_n - H^{(g)}) x_j}{x_j^T (I_n - H^{(g)}) x_j}. $$

1.1.2: Calculate the $p$-value $\gamma^{(g)}$ of predictor $j^{(g)}$ in the enlarged model,

$$ \gamma^{(g)} = 1 - F^{-1}_{(1, |J^{(g)}|+1)} \left( \frac{(|J^{(g)}|+1) \tau_j^{(g)}}{(y - H^{(g)} X_{J^{(g)}})^T (y - H^{(g)} X_{J^{(g)}}) - \tau_j^{(g)}} \right). $$

1.1.3: If $\gamma^{(g)} \geq \gamma$ set $T^{(g)} = \text{true}$.

1.2: Identify the unsaturated model $g^*$ with the smallest $p$-value $\gamma^{(g^*)}$.

1.3: If $\gamma^{(g^*)} < \gamma$:

1.3.1: Update the candidates $J = J \setminus \{j^{(g^*)}\}$ and the set of model predictors $J^{(g^*)} = J^{(g^*)} \cup \{j^{(g^*)}\}$.

1.3.2: If $|J^{(g^*)}| = n - 1$, set $T^{(g^*)} = \text{true}$. Otherwise, update the model hat matrix

$$ H^{(g^*)} = X_{J^{(g^*)}} \left( X_{J^{(g^*)}}^T X_{J^{(g^*)}} \right)^{-1} X_{J^{(g^*)}}^T. $$

2: For each model $g$ $(1 \leq g \leq G)$, set $\hat{\beta}^g = 0_p \in \mathbb{R}^p$ and if (custom) regularization is applied,

$$ \hat{\beta}^g_{|J^{(g)|}} = \arg \min_{\beta \in \mathbb{R}^{|J^{(g^*)}|}} \|y - X_{J^{(g)}} \beta\|^2 + \lambda^{(g)} \|\beta\|_1, $$

where $\lambda^{(g)}$ is chosen by CV. Otherwise,

$$ \hat{\beta}^g_{|J^{(g)|}} = X_{J^{(g)}} \left( X_{J^{(g)}}^T X_{J^{(g)}} \right)^{-1} y. $$

3: Return the sets of model predictors $J^{(g)}$ and their coefficients $\hat{\beta}^g$, $1 \leq g \leq G$.

An R/C++ library implementing Algorithm 1 is available on CRAN (R Core Team, 2022)
under the name stepSplitReg (Christidis et al., 2022b). Many more features than those described in Algorithm 1 are available, including different model saturation criteria and different regularization procedures for the final sets of model predictors. While the stacking procedure of Breiman (1996b) is available in the package, in this article we focus on the simple case where each model is weighted equally using (10). A reference manual with the complete details of the package is available at https://CRAN.R-project.org/package=stepSplitReg.

5 Projected Subsets Gradient Descent

We adapt ideas from $\ell_0$-penalized optimization to the BSpS problem in (3), and develop an algorithm that is perfectly suited for the cross-validation of the diversity tuning parameter $u$ in (9) and minimizes the need for a time-consuming local combinatorial search. For notational convenience, denote the loss function

$$L (\beta|\mathbf{y}, \mathbf{X}) = \sum_{g=1}^{G} (\mathbf{y} - \mathbf{X}\beta^g)^2,$$  \hspace{1cm} (14)

where the gradient of the loss is given by

$$\nabla_\beta L (\beta|\mathbf{y}, \mathbf{X}) = \mathbf{X}^T (\mathbf{X}\beta - \mathbf{y}).$$  \hspace{1cm} (15)

We note that (15) is Lipschitz continuous with Lipschitz constant $L_\beta = \|\mathbf{X}^T\mathbf{X}\|_2$ the spectral norm of $\mathbf{X}^T\mathbf{X}$, i.e.

$$\|\nabla_\beta L (\beta|\mathbf{y}, \mathbf{X}) - \nabla_\beta L (\tilde{\beta}|\mathbf{y}, \mathbf{X})\|_2 \leq L_\beta \|\beta - \tilde{\beta}\|_2 \quad \forall \beta, \tilde{\beta} \in \mathbb{R}^p.$$

The loss function (14) is bounded from above by its quadratic approximation with Lipschitz constant $L_\beta$,

$$L (\tilde{\beta}|\mathbf{y}, \mathbf{X}) \leq L_Q (\tilde{\beta}|\mathbf{y}, \mathbf{X}) = L (\beta|\mathbf{y}, \mathbf{X}) + \nabla_\beta L (\beta|\mathbf{y}, \mathbf{X})^T (\tilde{\beta} - \beta) + \frac{1}{2} L_\beta \|\tilde{\beta} - \beta\|_2^2.$$

We define $S^{(g)} \subseteq J$ the subsets of predictors that are used in at most $u - 1$ models excluding model $g$, i.e.

$$S^{(g)} = \left\{ j \in J : \sum_{\substack{h=1 \\text{to} \ G \ \text{with} \ h \neq g}}^{G} \mathbb{I}(j \in J^{(h)}) \leq u - 1 \right\},$$  \hspace{1cm} (16)

where $J^{(g)} = \{ j \in J : \beta^g_j \neq 0 \}, 1 \leq g \leq G$, as defined in Section 4. Central to our algorithm
is the projected subset operator, which we define for any vector $v \in \mathbb{R}^p$ and some subset $S \subseteq J$ as

$$
P(v; S, t) \in \arg \min_{w \in \mathbb{R}^p} \|w - v\|_2^2.
$$

The operator $P(v; S, t)$ retains the $t$ largest elements in absolute value of the vector $v$ that belong to the set $S$. It is a set-valued map since more than one possible permutation of the indices $\{j \in J : j \in S\}$ may exist.

The projected subsets gradient descent (PSGD) algorithm is given in Algorithm 2. The algorithm assumes initial solutions $\tilde{\beta}^1, \ldots, \tilde{\beta}^G$ are provided. In step 1 of the computing algorithm, the projected subset gradient descent algorithm is applied to each model once cyclically until convergence. In particular the update for model $g$ of the projected subset gradient descent algorithm using subset $S^{(g)}$ and model size $t$ can be written as

$$
\hat{\beta}^g \in \arg \min_{\beta^g \in \mathbb{R}^p} \mathcal{L}_Q \left( \tilde{\beta} | y, X \right)
$$

$$
= \arg \min_{\beta^g \in \mathbb{R}^p} \left\| \tilde{\beta}^g - \left( \beta^g - \frac{1}{L_\beta} \nabla_\beta \mathcal{L} \left( \beta^g | y, X \right) \right) \right\|_2^2
$$

$$
= \mathcal{P} \left( \beta^g - \frac{1}{L_\beta} \nabla_\beta \mathcal{L} \left( \beta^g | y, X \right); S^{(g)}, t \right).
$$

We note that for each model the iterative algorithm produces a sequence of converging solutions (Bertsimas et al., 2016, Proposition 6). After convergence is reached, its set of predictor variables $J^{(g)} = \{j \in J : \hat{\beta}^g_j \neq 0\}$ is updated and the final model coefficient is computed.

In the optional step 2 of Algorithm 2, local combinatorial searches using random permutations of the groups are performed to improve on the solution from step 1. Based on our numerical experiments, a poor initial solution in step 1 increases the need for step 2 to yield better solutions which come with a high computational cost. However, a carefully designed algorithm that generates good initial solutions for Algorithm 2 alleviates the need for the random permutations of models cyclic update in step 2.

To generate good initial solutions for Algorithm 2, in Algorithm 3 we decrement the diversity of the models progressively until $u = G$ in (9). Initial sets of model predictors and their coefficients are generated using Algorithm 1. Then Algorithm 2 is applied for
Algorithm 2 Projected Subsets Gradient Descent (PSGD)

**Input:** Design matrix $X \in \mathbb{R}^{n \times p}$, response vector $y \in \mathbb{R}^n$, current solutions $\tilde{\beta}^1, \ldots, \tilde{\beta}^G$, Lipschitz constant $L_\beta$, sparsity and diversity tuning parameters $t$ and $u$, and tolerance parameter $\epsilon > 0$, (optional) number of cycling iterations $C$.

**Initialize:** The current model predictors $J^{(g)} = \{j \in J : \tilde{\beta}^g_j \neq 0\}$, $1 \leq g \leq G$.

1: Repeat the following steps for each model $g$, $1 \leq g \leq G$:

1.1: Update the allowed predictors $S^{(g)} = \{j \in J : \sum_{h=1 \atop h \neq g}^G I(j \in J^{(h)}) \leq u - 1\}$.

1.2: Update $\tilde{\beta}^g$ as

$$\tilde{\beta}^g \in \mathcal{P} \left( \tilde{\beta}^g - \frac{1}{L_\beta} \nabla_\beta \mathcal{L} \left( \tilde{\beta}^g | y, X \right) ; S^{(g)} , t \right)$$

until $\mathcal{L}(\tilde{\beta}^g | y, X) - \mathcal{L}(\tilde{\hat{\beta}}^g | y, X) \leq \epsilon$.

1.3: Update the model predictors $J^{(g)} = \{j \in J : \tilde{\beta}^g_j \neq 0\}$.

1.4: Compute the final model coefficients

$$\hat{\beta}^g = \arg \min_{\beta \in \mathbb{R}^p} \mathcal{L}(\beta | y, X)$$

$$\beta^g_j = 0, j \notin J^{(g)}$$

2: (Optional) Repeat the following steps $C$ times:

2.1: Draw a random permutation $(\omega(1), \ldots, \omega(G))$ of $(1, \ldots, G)$.

2.2: Repeat step 1 using the new order $(\omega(1), \ldots, \omega(G))$ and the current solutions as initial values.

2.3: If $\sum_{g=1}^G \mathcal{L}(\tilde{\hat{\beta}}^g | y, X) < \sum_{g=1}^G \mathcal{L}(\tilde{\beta}^g | y, X)$, retain new solutions. Otherwise keep the old solutions $J^{(g)} = \{j \in J : \tilde{\hat{\beta}}^g_j \neq 0\}$ and $\tilde{\beta}^g = \tilde{\beta}^g$, $1 \leq g \leq G$.

3: Return the sets of model predictors $J^{(g)}$ and their coefficients $\hat{\beta}^g$, $1 \leq g \leq G$.

$u = 1, 2, \ldots, G$. Based on our numerical experiments, Algorithm 3 produces competitive solutions in terms of minimizing the objective function of BSpS in (9) compared to the local combinatorial searches of Algorithm 2. For the purpose of running large experiments on simulated and real data, in the remaining of this article we use Algorithm 3 without the local combinatorial search in Algorithm 2.

The sparsity and diversity tuning parameters in (9), $t$ and $u$ respectively, need to be determined from the training data. We use 5-fold CV for the grids of candidates $t$ and $u$, looking to minimize the CV MSPE. For a fixed sparsity level $t$, Algorithm 3 is perfectly suited to generate solutions for a grid of candidates for $u$. This process is repeated for every
candidate $t$.

**Algorithm 3 Decrementing Diversity PSGD**

**Input:** Design matrix $X \in \mathbb{R}^{n \times p}$, response vector $y \in \mathbb{R}^n$, Lipschitz constant $L_\beta$, maximum model size $t$, and tolerance parameter $\epsilon > 0$.

**Initialize:** Using Algorithm 1 initialize the sets of model predictors and their coefficients for $u = 1$, $J^{(g)}(1)$ and $\hat{\beta}^{(g)}(1)$, $1 \leq g \leq G$.

1: Using Algorithm 2 update $J^{(g)}(1)$ and $\hat{\beta}^{(g)}(1)$ with the current solutions as initial solutions.

2: For $u = 2, \ldots, G$ repeat the following step:

2.1: Compute $J^{(g)}(u)$ and $\hat{\beta}^{(g)}(u)$ using Algorithm 2 with initial solutions $J^{(g)}(u - 1)$ and $\hat{\beta}^{(g)}(u - 1)$, $1 \leq g \leq G$.

3: Return the sets of model predictors $J^{(g)}(u)$ and their coefficients $\hat{\beta}^{(g)}(u)$, $1 \leq u, g \leq G$.

An R/C++ library implementing the PSGD Algorithms 2, 3 and the CV procedure is available on CRAN under the name PSGD (Christidis et al., 2022a). Multithreading is available in the library with OpenMP (Chandra et al., 2001) to reduce the computational cost of the method. The computational cost of the method (using a single thread) as function of the number of models $G$ is explored in Section 7. A reference manual with the complete details of the package is available at https://CRAN.R-project.org/package=PSGD.

6 Simulation Study

For each Monte Carlo replication, we generate data from the linear model

$$y_i = x_i^t \beta_0 + \sigma \epsilon_i, \quad 1 \leq i \leq n,$$

where the $x_i \in \mathbb{R}^p$ are multivariate normal with zero mean and correlation matrix $\Sigma \in \mathbb{R}^{p \times p}$ and the $\epsilon_i$ are standard normal. We consider two combinations of $p$ and $n$, namely $(p, n) = (500, 50)$ and $(p, n) = (150, 50)$. For each $p$, we consider the proportion of active variables $\zeta = 0.1, 0.2$ and 0.4.

The $p_0 = \lfloor p \zeta \rfloor$ nonzero elements of the $p$-dimensional vectors $\beta_0$ are randomly generated as described in Fan and Lv (2008), i.e. nonzero coefficients are set to $(-1)^u(a + |z|)$, where $a = 5 \log n / \sqrt{n}$, $u$ is drawn from a Bernoulli distribution with parameter 0.2 and $z$ is drawn from the standard Gaussian distribution. For $(p, n) = (500, 50)$, the $\ell_2$-norms $\|\beta_0\|$ range from 21.01 to 43.22 for all proportions sparsity levels $1 - \zeta$ considered. For
$(p, n) = (150, 75)$, the $\ell_2$-norms $\|\beta_0\|$ range from 11.30 to 22.80. We consider two different scenarios for $\Sigma$.

**Scenario 1:**

$$
\Sigma_{i,j} = \begin{cases} 
1 & \text{if } i = j \\
\rho & \text{if } i \neq j \\
0 & \text{otherwise}.
\end{cases}
$$

**Scenario 2:**

$$
\Sigma_{i,j} = \begin{cases} 
1 & \text{if } i = j \\
\rho & \text{if } 1 \leq i, j \leq p_0, i \neq j \\
0 & \text{otherwise}.
\end{cases}
$$

In Scenario 1, all the predictors are correlated among each other. In Scenario 2, the active variables are only correlated with each other. For both scenarios we consider the values $\rho \in \{0.2, 0.5, 0.8\}$. Then $\sigma$ is chosen to give a desired signal to noise ratio (SNR), defined as $\text{SNR} = \beta_0' \Sigma \beta_0 / \sigma^2$. We consider SNRs of 1, 3 and 5. We report results for all scenarios across all considered sparsity levels, correlations, SNRs and the two combinations of $p$ and $n$.

### 6.1 Methods

We ran a simulation study comparing the prediction accuracy of eleven methods. In particular we consider four sparse regression methods, their analogous split regression methods, and three “blackbox” regression ensemble methods. All computations were carried out in R with their default settings.

1. **Stepwise** forward regression, computed using the lars package (Hastie and Efron, 2013).

2. **Fast-BSS**, computed using the L0Learn package (Hazimeh et al., 2021) with the $\ell_0$-$\ell_1$ penalty option.

3. **Lasso**, computed using the glmnet package (Friedman et al., 2010).

4. Elastic Net (**EN**) with $\alpha = 3/4$ for the $\ell_1$-$\ell_2$ mixing parameter, computed using the glmnet package (Friedman et al., 2010).

5. **Step-SplitReg**, computed using the stepSplitReg package with a custom Lasso fit for each model.

6. **Fast-BSpS**, computed using the PSGD package.
7. **SplitReg-Lasso**, computed using the SplitReg package (Christidis et al., 2020).

8. **SplitReg-EN** with $\alpha = 3/4$ for the $\ell_1$-$\ell_2$ mixing parameter, computed using the SplitReg package.

9. Random GLM (RGLM) (Song et al., 2013), computed using the RGLM package (Song and Langfelder, 2013).

10. Random Forest (RF), computed using the randomForest package (Liaw and Wiener, 2002).

11. Extreme Gradient Boosting (XGBoost) (Chen and Guestrin, 2016), computed using the xgboost package (Chen et al., 2020).

For a fast computation of BSS, we use the state-of-the-art method of Hazimeh and Mazumder (2020). In their implementations, Hazimeh et al. (2021) recommend to combine $\ell_0$ regularization with shrinkage-inducing penalties to avoid overfitting and improve predictive performance, and thus we use the $\ell_0$-$\ell_2$ combination of penalties. For the four split regression methods, we use $G = 5$ models, a potentially suboptimal number of models. For RGLM and RF we use $G = 5$ and their default number of models, $G = 100$ and $G = 500$ respectively. To reduce the computational burden of the PSGD algorithm in our large simulation study, we use the grids $u \in \{1, 2, 3, 4, 5\}$ and $t \in \{0.3n, 0.4n, 0.5n\} = \{15, 20, 25\}$ in the CV procedure of BSpS. The finer grids $t \in \{1, \ldots, n - 1\}$ and $u \in \{1, \ldots, 5\}$ may be used for optimal predictive performance, however at a higher computational cost.

### 6.2 Performance Measures

For each configuration, we randomly generate $N = 50$ training and test sets and for each of the methods measure average performance on the test sets. In each replication of a particular configuration, a training set is generated to fit the procedures, and a large independent test set of size $m = 2,000$ is used to compute the MSPE. The MSPEs reported are relative to the irreducible error $\sigma^2$, hence the best possible result is 1. We also report the recall (RC) and precision (PR), defined for each parametric method as

$$
RC = \frac{\sum_{j=1}^{p} I(\beta_j \neq 0, \hat{\beta}_j \neq 0)}{\sum_{j=1}^{p} I(\beta_j \neq 0)}, \quad PR = \frac{\sum_{j=1}^{p} I(\beta_j \neq 0, \hat{\beta}_j \neq 0)}{\sum_{j=1}^{p} I(\hat{\beta}_j \neq 0)},
$$

where $\beta$ and $\hat{\beta}$ are the true and estimated regression coefficients, respectively. For the split regression methods and RGLM, the average of the models (10) is the vector of coefficients used to compute the recall and the precision. For the tree-based ensemble methods RF and XGBoost, the RC and PR are computed by identifying the predictors used in the trees of
the ensembles. We do not report the RC and PR of RGLM and RF when their default number of models are used since their recall is always 1 and precision the proportion of active variables $\zeta$. Note that large values of RC and PR are desirable.

### 6.3 Results

In Table 1 we report the average rank for each performance measure across all simulations settings. The best two ranks for each performance measure are in bold. The detailed results of the simulation study are available in the supplementary material. Fast-BSpS had the best average rank in terms of MSPE for both cases $p = 500$ and $p = 150$, whereas SplitReg-EN had the second best performance in both cases. RGLM-100 had the best average performance out of the “blackbox” methods, however its performance deteriorated to the worst average rank when $G = 5$, the same number of models as Fast-BSpS. In Section 7, we investigate this phenomenon in greater details by studying the effect of the number of groups on Fast-BSpS and RGLM. Step-SplitReg was not competitive in terms of MSPE compared to Fast-BSpS or the SplitReg methods, however it did outperform its single-model stepwise method consistently.

In terms of RC, Fast-BSpS had the second best rank overall, only beaten slightly by RGLM-5. However, RGLM-5 had the third worst overall rank in PR, whereas Fast-BSpS had the best PR rank for $p = 500$ and the best overall PR rank out of all ensemble methods.

An investigation of the full simulation results in the supplementary material reveals that Fast-BSpS had its best performances relative to the competitors across all performance measures in Scenario 2, which is more realistic than Scenario 1 where it is hard to distinguish active from inactive predictors due to the correlation induced between them.

### 7 The Number of Models

For an ensemble comprised of a relatively small number of models, a balance of individual model prediction accuracy and diversity between the models is necessary for overall ensemble prediction accuracy. To achieve diversity, individual model accuracy must typically take a hit (Brown et al., 2005). The BSpS framework searches for $G$ diverse models that have a small loss in the objective function (9). Thus each model in BSpS is learned directly from the data, sparse, and achieves a high prediction accuracy. Thus in a sense Fast-BSpS controls the accuracy-diversity tradeoff directly.

In RGLM, bagging and the random subspace method are used to create $G$ bags comprised of different samples and predictors. Then, a subset of predictors in each bag are retained based on a measure of correlation with the response, and forward selection is applied to this subset. RGLM thus resorts to randomization to generate a collection of diverse
Table 1: Average rank of the methods over the scenarios, correlations, SNRs and sparsity levels for \((p, n) = (500, 50)\) and \((p, n) = (150, 50)\). The last column contains the overall rank over both combinations of \((p, n)\).

| Method          | \(p = 500\) | \(p = 150\) | Overall Rank |
|-----------------|--------------|--------------|--------------|
|                 | MSPE | RC | PR | MSPE | RC | PR | MSPE | RC | PR |
| Stepwise        | 12.06 | 11.00 | **3.87** | 11.17 | 11.00 | **3.07** | 11.62 | 11.00 | **3.47** |
| Fast-BSS        | 4.81 | 6.89 | 6.02 | 5.50 | 6.77 | 4.91 | 5.15 | 6.83 | 5.46 |
| Lasso           | 7.20 | 9.81 | 4.22 | 6.50 | 9.78 | **3.65** | 6.85 | 9.80 | **3.93** |
| EN              | 6.15 | 8.81 | 4.19 | 5.89 | 8.72 | 4.30 | 6.02 | 8.77 | 4.25 |
| Step-SplitReg   | 9.07 | **1.85** | 10.26 | 6.96 | 5.21 | 8.98 | 8.02 | 3.53 | 9.62 |
| Fast-BSpS       | **2.67** | 3.70 | **3.02** | **2.26** | **2.24** | 5.81 | **2.46** | **2.97** | 4.42 |
| SplitReg-Lasso  | 3.56 | 5.00 | 6.15 | 3.31 | 5.58 | 5.00 | 3.44 | 5.29 | 5.58 |
| SplitReg-EN     | **2.85** | 3.85 | 5.59 | **2.65** | 4.60 | 5.41 | **2.75** | 4.22 | 5.50 |
| RGLM-5          | 12.24 | **3.24** | 8.46 | 12.69 | **1.46** | 9.50 | 12.46 | **2.35** | 8.98 |
| RGLM-100        | 3.57 | – | – | 6.50 | – | – | 5.04 | – | – |
| RF-5            | 10.02 | 7.63 | 10.15 | 10.30 | 6.13 | 10.67 | 10.16 | 6.88 | 10.41 |
| RF-500          | 5.67 | – | – | 5.83 | – | – | 5.75 | – | – |
| XGBoost         | 11.13 | 4.20 | 4.07 | 11.44 | 4.50 | 4.70 | 11.29 | 4.35 | 4.38 |

models, resulting in models that are individually weak and not built to achieve the optimal accuracy-diversity balance given the number of models \(G\) used. By the bias-variance-covariance decomposition of regression ensembles in (6) and (7), if individual models are weak, a large number of them would be required for the covariance term to dominate the variance term of the ensemble and thus for the ensemble to achieve a good prediction accuracy.

### 7.1 Accuracy-Diversity Empirical Study

We conduct a simulation to study the effect of the number of models on Fast-BSpS and RGLM with \(G = 2, 3, 4, 5\), as well as \(G = 100\) (the default) for RGLM. We use \(N = 50\) replications of Scenario 2 in the simulation study of Section 6 with \(p = 500\), \(\rho = 0.5\), and a SNR of 3. For each replication, Fast-BSpS and RGLM are applied to a training set of size \(n = 50\) and then a test set of size \(m = 2,000\) is used to compute the ensemble MSPE, the average mean squared prediction error \(\overline{\text{MSPE}}\) of the individual models as well as their average pairwise correlations \(\overline{\text{Cor}}\). The mean squared prediction errors reported are relative to the irreducible error \(\sigma^2\), hence the best possible result is 1. The computation is repeated for various values of the proportion of active variables, namely \(\zeta \in \{0.1, 0.2, 0.4\}\). The
results are reported in Table 2.

Table 2: MSPE, MSPE and Cor of Fast-BSpS and RGLM as a function of the number of models under Scenario 2 with \( \rho = 0.5 \) and SNR= 3.

| Method    | \( \zeta = 0.1 \) | \( \zeta = 0.2 \) | \( \zeta = 0.4 \) |
|-----------|-------------------|-------------------|-------------------|
|           | MSPE  | MSPE  | Cor  | MSPE  | MSPE  | Cor  | MSPE  | MSPE  | Cor  |
| Fast-BSpS-2 | 1.29  | 1.57  | 0.85 | 1.31  | 1.55  | 0.87 | 1.27  | 1.53  | 0.85 |
| Fast-BSpS-3 | 1.21  | 1.62  | 0.83 | 1.22  | 1.62  | 0.85 | 1.21  | 1.56  | 0.85 |
| Fast-BSpS-4 | 1.20  | 1.75  | 0.80 | 1.21  | 1.73  | 0.83 | 1.18  | 1.61  | 0.84 |
| Fast-BSpS-5 | 1.19  | 1.76  | 0.80 | 1.16  | 1.75  | 0.82 | 1.16  | 1.63  | 0.83 |
| RGLM-2     | 4.34  | 7.37  | 0.25 | 4.38  | 7.51  | 0.27 | 3.50  | 5.95  | 0.34 |
| RGLM-3     | 3.38  | 7.69  | 0.22 | 3.17  | 7.15  | 0.29 | 2.75  | 6.00  | 0.34 |
| RGLM-4     | 2.86  | 7.74  | 0.22 | 2.63  | 6.95  | 0.30 | 2.37  | 6.07  | 0.33 |
| RGLM-5     | 2.47  | 7.50  | 0.23 | 2.30  | 6.69  | 0.31 | 2.12  | 6.13  | 0.34 |
| RGLM-100   | 1.36  | 7.70  | 0.23 | 1.25  | 7.03  | 0.29 | 1.17  | 6.64  | 0.33 |

For Fast-BSpS, it can be seen that for all sparsity levels MSPE increases with the number of models, while MSPE and Cor decrease. As the number of models increases, the average accuracy of the individual models has less impact on the ensemble MSPE compared to Cor and Fast-BSpS achieves the proper balance for this tradeoff, resulting in high accuracy for the ensemble.

For RGLM, the individual models are extremely weak, with the MSPE of the individual models being between seven to eight times the variance of the noise. The individual strength of the models are not controlled or learned for the number of models in the ensemble, they are equally weak regardless of the number of models. However, Cor is much lower than RGLM for all number of models. When the number of models is increased, the average pairwise correlation between the models are becoming more important, and only when \( G = 100 \) does RGLM achieve an adequate ensemble MSPE, although still higher than Fast-BSpS with \( G = 2 \) for all sparsity levels. Thus RGLM relies on a large number of weak decorrelated models to achieve a low ensemble MSPE.

In applied research, investigation of the individual models of Fast-BSpS could therefore reveal insightful information for the relationship between the predictors and the response, while RGLM (or other random/indirect methods) do not enjoy this property. Indeed beyond the high prediction accuracy of the individual models of Fast-BSpS, they learn the models directly from the data and enjoy good variable selection as do sparse methods. In Table 3 we report the RC and PR of Fast-BSpS and RGLM as function of the number of models. It can be seen that Fast-BSpS enjoys near-perfect PR and a high RC relative to RGLM. RGLM has poor PR inherently due to the random nature of its methodology, and only
achieves high RC when a lot of models are used. For \( G = 100 \), RGLM naturally achieves a RC of 1 and a PR of \( \zeta \).

Table 3: RC and PR of Fast-BSpS and RGLM as a function of the number of models under Scenario 2 with \( \rho = 0.5 \) and SNR = 3.

| Method       | \( \zeta = 0.1 \) | \( \zeta = 0.2 \) | \( \zeta = 0.4 \) |
|--------------|-------------------|-------------------|-------------------|
|\( \zeta = 0.1 \) | RC  | PR  | RC  | PR  | RC  | PR  |
| Fast-BSpS-2  | 0.56 | 1.00 | 0.29 | 1.00 | 0.16 | 1.00 |
| Fast-BSpS-3  | 0.79 | 0.99 | 0.44 | 1.00 | 0.20 | 1.00 |
| Fast-BSpS-4  | 0.81 | 0.89 | 0.55 | 1.00 | 0.29 | 1.00 |
| Fast-BSpS-5  | 0.82 | 0.87 | 0.69 | 1.00 | 0.33 | 1.00 |
| RGLM-2       | 0.26 | 0.22 | 0.25 | 0.43 | 0.22 | 0.77 |
| RGLM-3       | 0.33 | 0.20 | 0.33 | 0.40 | 0.30 | 0.74 |
| RGLM-4       | 0.40 | 0.19 | 0.42 | 0.40 | 0.39 | 0.76 |
| RGLM-5       | 0.47 | 0.19 | 0.49 | 0.39 | 0.46 | 0.77 |
| RGLM-100     | 1.00 | 0.10 | 1.00 | 0.20 | 1.00 | 0.40 |

7.2 Computational Cost

While Fast-BSpS shows great promise in terms of prediction accuracy, it comes at a high cost. The computational cost (in seconds) of the CV procedure of Fast-BSpS in Scenario 2 of Section 6, across all sparsity levels \( \zeta \in \{0.1, 0.2, 0.4\} \), is provided in Table 4 as a function of the number of models. We include for comparison the computational cost of the multi-convex relaxation of BSpS as described in Section 3.2 using the SplitReg package (Christidis et al., 2020) as well as step-SplitReg as described in Section 4 using the stepSplitReg package.

The step-SplitReg method has by far the smallest computational cost. The CPU seconds for the \( R \) function calls of Fast-BSpS are significantly higher and more sensitive to the number of models compared to the multi-convex relaxation. We note that no local combinatorial search is performed in the execution of Algorithm 2 which may increase the cost further. The computational cost can also increase substantially if a fine grid for the sparsity parameter \( t \) is used. However, given the difficulty in optimizing \( \ell_0 \)-penalized problems, it is expected that the cost of Fast-BSpS will be higher.
Table 4: Computation time of R function calls for the SplitReg, stepSplitReg and PSGD packages in CPU seconds for varying number of models. CPU seconds are on a 2.7 GHz Intel Xeon processor in a machine running Linux 7.8 with 125 GB of RAM.

| Package     | Number of Models |
|-------------|------------------|
|             | 2    | 3    | 4    | 5    |
| SplitReg    | 2.23 | 6.56 | 10.41| 14.91|
| stepSplitReg| 0.25 | 0.69 | 1.05 | 1.17 |
| PSGD        | 4.67 | 19.38| 31.43| 55.92|

8 Bardet-Biedl Syndrome Gene Expression Data

We benchmark Fast-BSpS and the competitor methods of Section 6 on the Bardet-Biedl syndrome (BBS) gene expression dataset in Li et al. (2020). In Scheetz et al. (2006) mutation and functional studies were performed and identified TRIM32 (tripartite motif-containing protein 32) as a gene with high correlation with BBS. The purpose of this study is to perform predict the gene expression level of TRIM32 using the expression levels of \( p = 200 \) genes from mammalian-eye tissue samples identified as relevant in Scheetz et al. (2006).

The dataset contains 120 mammalian-eye tissue samples. To mimic a high-dimensional scenario, in each of the \( N = 50 \) replications we randomly split the data into a training set of size \( n = 30 \) and a test set with the remaining \( m = 90 \) samples. For Fast-BSpS we use \( u \in \{1, 2, 3, 4, 5\} \) and \( t \in \{0.3n, 0.4n, 0.5n\} = \{9, 12, 15\} \). The other methods are computed using their default settings as in Section 6. We report the MSPE for all the methods and \( \overline{\text{MSPE}} \) for the ensemble methods.

The results are reported in Table 5, where in each column the two best performances are in bold. For the ensemble MSPE, RGLM-100 and Fast-BSpS had the best two performances, with RGLM-100 edging out Fast-BSpS slightly. While RGLM-100 had a slightly lower MSPE than Fast-BSpS, the individual \( \overline{\text{MSPE}} \) of RGLM-5 or RGLM-100 were the worst out of all the methods, being nearly three times the \( \overline{\text{MSPE}} \) of Fast-BSpS or either of the SplitReg methods. On the other hand, Fast-BSpS achieved the second best individual \( \overline{\text{MSPE}} \) slightly behind SplitReg-EN, matching the MSPE of its base sparse estimator BSS or the Lasso. Fast-BSpS thus achieved to not only produce a competitive ensemble prediction accuracy with only \( G = 5 \) models, but each models is on average as reliable and accurate as standard sparse estimators.

As it was seen in Section 7, the individual models of Fast-BSpS not only have good prediction accuracy, but they also tend to use the relevant predictors with high precision, whereas RGLM relies on randomness to create diverse models which results in models with
Table 5: MSPE and MSPE over the \( N = 50 \) random splits into training and testing sets for the BBS gene expression dataset.

| Method          | MSPE | MSPE |
|-----------------|------|------|
| Stepwise        | 0.82 | -    |
| Fast-BSS        | 0.65 | -    |
| Lasso           | 0.65 | -    |
| EN              | 0.63 | -    |
| Step-SplitReg   | 0.57 | 0.93 |
| Fast-BSpS       | 0.49 | 0.65 |
| SplitReg-Lasso  | 0.65 | 0.67 |
| SplitReg-EN     | 0.62 | 0.63 |
| RGLM-5          | 0.69 | 1.71 |
| RGLM-100        | 0.45 | 1.67 |
| RF-5            | 0.73 | 1.02 |
| RF-500          | 0.67 | 1.03 |
| XGBoost         | 0.84 | 1.04 |

poor variable selection. Since the models in Fast-BSpS are learned directly from the data, each predictor included in a model was included for its relevance in minimizing the error term of the models in (9). Taking this one step further, we can use the models in Fast-BSpS to rank the gene sets in order of importance. Defining the sets

\[
\mathcal{A}_k = \left\{ j : \sum_{g=1}^{G} \mathbb{1}\left( j \in S^{(g)} \right) \geq k \right\}, \quad 1 \leq k \leq G,
\]

where \( \mathcal{A}_G \subseteq \mathcal{A}_{G-1} \subseteq \cdots \subseteq \mathcal{A}_1 \), we can study the distribution of the genes across the different models. These sets identify genes related to TRIM32 in order of importance, since these genes appear in more than one model if there are no surrogate genes that may be used to reduce the loss function of BSpS in (9). Applying Fast-BSpS to the BBS dataset, \(|\mathcal{A}_3 = 18|\), \(|\mathcal{A}_2 = 28|\) and \(|\mathcal{A}_1 = 29|\). Genes shared by more than a single model had the same sign across all the models, re-enforcing the understanding of their relationship with the gene expression level of TRIM32.

To illustrate that Fast-BSpS can identify important genes that may be missed by sparse regression methods, let us consider \( \mathcal{A}_3 \). This set contains 18 genes that appear in at least half of the 5 Fast-BSpS individual models and thus yield an important contribution to the ensemble. Interestingly, none of these genes appears in the Fast-BSS and thus would be considered irrelevant for the prediction of the gene expression level of TRIM32.

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9 Discussion and Future Directions

We introduced a new data-driven ensemble framework that generates a collection of sparse and diverse models learned directly from the data. In particular we introduced BSpS, a generalization of BSS to multiple groups. In BSpS the objective is to find the best possible split of predictors in a collection of models such that the sum of their individual losses is minimized. The split of predictors must satisfy the sparsity constraint, i.e. the maximum size of each model, and the diversity constraint, i.e. the maximum number of models that can share any given predictor. Each model has a prediction accuracy that is competitive with its base sparse estimator BSS, and thus presents a possible explanation for the relationship between the predictors and the response.

An investigation of the intractable combinatorial problem posed by BSpS reveals the need for computational tools to generate approximate solutions. Related work in Christidis et al. (2020) to minimize an objective function with a sparsity and diversity penalty may be viewed as a multi-convex relaxation of BSpS, which does not allow to directly control the maximal model size and the number of models that may share predictors, and may have poorer prediction and variable selection performance compared to the direct optimization of BSpS. In this article we generalized forward stepwise regression to multiple groups to generate an initial solution to BSpS in the fully diverse \((u = 1)\) case, and a projected subsets gradient descent algorithm to generate approximate solutions to BSpS for any \(u\) in (9) that is perfectly suited for the CV procedure of the tuning parameters. Our empirical investigations via our simulation study and real data application reveal that our approach to optimize BSpS directly yields and ensemble with competitive prediction accuracy and variable selection properties compared to the multi-convex relaxation of BSpS and “blackbox” regression ensemble methods.

We showed that the proposed methodology is efficient in exploiting the accuracy-diversity tradeoff of regression ensembles, such that the optimal balance of individual model accuracy and diversity is achieved by our proposed algorithm. Contrary to other “blackbox” regression ensemble methods such as RGLM, our methodology results in ensembles that do not rely on a large number of weak models to achieve a high prediction accuracy. Rather it relies on the search for strong individual models that have a certain degree of diversity to reduce the variance of the ensemble. This allows for the usefulness of the sets \(\mathcal{A}_k, 1 \leq k \leq G\), in (18) to rank the predictors in order of importance to predict the outcome accurately. This is particularly important in gene expression data where interpretability and the identification of the relevant genes is just as important as prediction accuracy.

For applied scientists, problem-specific knowledge can be incorporated into the BSpS framework very easily. For example, if certain predictors (e.g. genes) are known to be
particularly important or relevant in the prediction of the outcome, it may be easily incorporated by generalizing BSpS in (9) to

$$\min_{\beta^1, \ldots, \beta^G \in \mathbb{R}^p} \sum_{g=1}^{G} (y - X\beta^g)^2 \quad \text{subject to} \quad \begin{cases} \|\beta^g\|_0 \leq t, & 1 \leq g \leq G, \\
\|\beta_j\|_0 \leq u_j, & 1 \leq j \leq p. \end{cases}$$

(19)

where $u_j$ is the maximum number of models that may share predictor $j$, $1 \leq j \leq p$.

The PSGD algorithm we proposed is an efficient way to generate solutions for the BSpS nonconvex problem in (9). However, compared to Step-SplitReg and SplitReg, it suffers from a slower computation time, particularly as the number of groups or the dimension of the data are increased. A future area of research is to develop alternative computing procedures for BSpS. One possible improvement on the current algorithm is to apply the general idea of accelerated proximal gradient descent of Beck and Teboulle (2009) to projected gradients and incorporate it in our algorithm. Perhaps a better initialization procedure than the Step-SplitReg may be developed, or an efficient way to apply local combinatorics to search for better solutions to BSpS.

We hope our new data-driven ensemble framework will motivate new and exciting research on this new paradigm for ensemble modeling. For example, BSpS in (9) may be easily generalized to GLMs or other models with some general loss, i.e.

$$\min_{\beta^1, \ldots, \beta^G \in \mathbb{R}^p} \sum_{g=1}^{G} \mathcal{L}(\beta^g|y, X) \quad \text{subject to} \quad \begin{cases} \|\beta^g\|_0 \leq t, & 1 \leq g \leq G, \\
\|\beta_j\|_0 \leq u_j, & 1 \leq j \leq p. \end{cases}$$

(20)

In the analysis of high-dimensional data, sparse modeling was the main focus in the literature for many years, with the overwhelming majority of proposals being different alternative approaches to the NP-hard BSS problem. Our proposal is a generalization of the sparse modeling framework, generating more not one single interpretable model with good prediction accuracy but multiple such models. We hope our introduction to split modeling will be the central focus for new developments for the analysis of high-dimensional data.

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Conflict of Interests

The authors declare no potential conflict of interests.

Data Availability Statement

The R packages stepSplitReg and PSGD created for this article are publicly available on CRAN together with their respective reference manuals. The data and scripts to replicate the numerical experiments are available at https://doi.org/10.5281/zenodo.6450556.

Supplementary Material

The supplementary material contains the full results of our simulations and real data experiments.

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