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## SPAR: Sparse Projected Averaged Regression in R

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#### Abstract

**SPAR** is a package for building ensembles of predictive generalized linear models (GLMs) with high-dimensional (HD) predictors in R by making use of probabilistic variable screening and random projection tools. The package design is focused on extensibility, where the screening and random projections are implemented as classes with convenient constructor functions, allowing users to easily implement new procedures.

Keywords: random projection, variable screening, ensemble learning, R.

## 1. Introduction

SPAR is a new package designed for building predictive generalized linear models (GLMs) with high-dimensional (HD) predictors in R integrating probabilistic variable screening and random projection techniques of large predictors sets. The algorithm provides a computationally efficient procedure for high-dimensional regression for both discrete and continuous responses while the package design offers a flexible framework, allowing users to extend the implemented screening and projection techniques with their own procedures in a convenient way by using R's S3 classes. The adaptability of the algorithm and the extensibility of the package to combine different techniques enhances [SPAR{.pkg}'s suitability across a range of high-dimensional applications.

The algorithm builds an ensemble of GLMs in the spirit of Mukhopadhyay and Dunson (2020) and Parzer, Filzmoser, and Vana-Gür (2024) where in each model of the ensemble variable screening and random projections are used for dimensionality reduction of the predictors. Random projection is a computationally-efficient method which linearly maps a set of points in high dimensions into a much lower-dimensional space, but for very large p, it can suffer from noise accumulation, as too many irrelevant predictors are being considered for prediction purposes (Mukhopadhyay and Dunson 2020). Therefore, screening out irrelevant variables before performing the random projection is advisable in order to tackle this issue. The

screening can be performed in a probabilistic fashion, by randomly sampling covariates for inclusion in the model based on probabilities proportional to an importance measure (as opposed to random subspace sampling employed in e.g., random forests). Finally, in practice, the information from multiple such screening and projections can be combined by averaging, in order to reduce the variance introduced by the random sampling (of both projections and screening indicators) (Thanei, Heinze, and Meinshausen 2017).

While the package provides a first implementation of the described algorithm, there are several packages which provide functionality for random projections available R. Package RandPro (Aghila and Siddharth 2020; Siddharth and Aghila 2020) allows for four different random projection matrices to be applied to the predictor matrix before employing one of k-nearest neighbor, support vector machine or naive Bayes classifier. Package SPCAvRP (Gataric, Wang, and Samworth 2019) implements sparse principal component analysis, based on the aggregation of eigenvector information from "carefully-selected" axis-aligned random projections of the sample covariance matrix. Package RPEnsembleR (Cannings and Samworth 2021) implements the same idea of "carefully-selected" random projections when building an ensemble of classifiers. For Python van Rossum et al. (2011) the sklearn.random\_projection module implements two types of unstructured random matrix, namely Gaussian random matrix and sparse random matrix.

Related to screening, the users could seamlessly integrate different techniques for variable screening by writing they own procedure or leveraging the extensive landscape of packages implementing screening procedures in R. An incomplete overview of the packages available on the Comprehensive R Archive Network (CRAN) includes: package SIS (Saldana and Feng 2018), which implements the (iterative) sure independence screening procedure and extensions in Fan and Ly (2007), Fan and Song (2010), Fan, Feng, and Wu (2010), which also provides functionality for estimating a penalized generalized linear model or a cox regression model for the variables picked by the screening procedure; package VariableScreening (Li, Huang, and Dziak 2022) implements screening for iid data, varying-coefficient models, and longitudinal data using different screening methods such as sure independent ranking and screening – which ranks the predictors by their correlation with the rank-ordered response, or distance correlation sure independence screening – a non-parametric extension of the correlation coefficient. A collection of model-free screening techniques such as SIRS, DC-SIS, MV-SIS, the fused Kolmogorov filter (Mai and Zou 2015), the projection correlation method using knock-off features (Wanjun Liu and Li 2022), are provided in package MFSIS (Cheng, Wang, Zhu, Zhong, and Zhou 2024). Further packages are available which implement specific procedures: (Cho and Fryzlewicz 2016; Hu, Huang, Pan, Wang, Wen, Tian, Zhang, and Zhu 2024; Ma, Zhang, and Zhou 2015; Wu, Li, and Li 2022, Banerjee, Mukherjee, and Radchenko (2017)).

Packages which are similar in spirit to **SPAR**, which also build ensembles, but only for classification purposes, include package **RaSEn** (Tian and Feng 2021), which implements the RaSE algorithm for ensemble classification and classification problems, where random subspaces are generated and the optimal one is chosen to train a weak learner on the basis of some criterion, and package **RPEnsemble** (?), which implements the procedure in Cannings and Samworth (2017). **RaSEn** provides various choices of base classifiers but do not perform random projections while **RPEnsemble** implements only the random projection approach in the package and provides limited functionality for using different classifiers. Therefore, no other package

in R provides the functionality of **SPAR** for GLMs.

The package provides methods such plot, predict, coef, print, which allow user to more easily interact with the model output and analyze the results. The GLM framework, especially when combined with random projections which preserve information on the original coefficients (such as the one in Parzer et al. 2024), facilitates interpretability of the model out, allowing users to understanding variable effects.

The rest of the paper is organized as follows: Section 2 provides the methodological details of the implemented algorithm. The package is described in Section 3. Section 5 contains two examples of employing the package on real data sets. Finally, Section 6 concludes.

## 2. Methods

The package implements a procedure for building an ensemble of GLMs where we employ screening and random projection to the predictor matrix pre-model estimation for the purpose of dimensionality reduction.

Throughout the section we assume to observe high-dimensional data  $\{(x_i, y_i)\}_{i=1}^n$ , where  $x_i \in \mathbb{R}^p$  is a predictor vector and  $y_i \in \mathbb{R}$  is the response, with  $p \gg n$ .

## 2.1. Variable screening

In this section we provide an overview of possible approaches to performing variable screening in a high-dimensional setting. In high-dimensional modeling, the goal of variable screening is to reduce the predictor set by selecting a small subset of variables with a strong *utility* to the response variable. This initial selection enables more efficient downstream analyses by discarding less relevant predictors early in the modeling process, thus reducing computational costs and potential noise accumulation stemming from irrelevant variables (see e.g., Mukhopadhyay and Dunson 2020).

Classic approaches sure independence screening (SIS), proposed by Fan and Lv (2007), use the vector of marginal empirical correlations  $\hat{\alpha}=(\alpha_1,\ldots,\alpha_p)'\in\mathbb{R}^p, \alpha_j=\operatorname{Cor}(X_{.j},y)$  to screen predictors in a linear regression setting by selecting the variable set  $\mathcal{A}_{\gamma}=\{j\in[p]:|w_j|>\gamma\}$  depending on a threshold  $\gamma>0$ , where  $[p]=\{1,\ldots,p\}$ . Under certain technical conditions, that this screening coefficient has the sure screening property  $\mathbb{P}(\mathcal{A}\subset\mathcal{A}_{\gamma_n})\to 1$  for  $n\to\infty$ . Extensions to SIS include modifications for GLMs (Fan and Song 2010), where screening is performed based on the log-likelihood or the slope coefficient of the GLM containing only  $X_j$  as a predictor:  $\hat{\alpha}_j=:\operatorname{argmin}_{\beta\in\mathbb{R}}\min_{\beta_0\in\mathbb{R}}\sum_{i=1}^n-\ell(\beta_j,\beta_0;y_i,x_{ij})$ . However, both approaches face limitations related to the required technical conditions which can rules out practically possible scenarios where an important variable is marginally uncorrelated to the response due to their multicollinearity. To tackle these issues, Fan, Samworth, and Wu (2009) propose to use an iterative procedure where SIS is applied subsequently on the residuals of the model estimated in a previous step.

To account for multicollinearity among the predictors, which can cause relevant predictors to be marginally uncorrelated with the response, various extensions have been proposed. In a linear regression setting, Wang and Leng (2016) propose employing the ridge estimator when the penalty term converges to zero while Cho and Fryzlewicz (2012) propose using the tilted correlation, i.e., the correlation of a tilted version of  $X_j$  with y. For discrete outcomes, joint feature screening Xu and Chen (2014) has been proposed.

In order to tackle potential model misspecification, a rich stream of literature focuses on developing semi- or non-parametric alternatives to SIS. For linear regression, approaches include using the ranked correlation (Zhu, Li, Li, and Zhu 2011), (conditional) distance correlation (Li, Zhong, and Zhu 2012; Wang, Pan, Hu, Tian, and Zhang 2015). or quantile correlation (Ma and Zhang 2016). For GLMs, Fan, Feng, and Song (2011) extend Fan and Song (2010) by fitting a generalized additive model with B-splines. Further extensions for discrete (or categorical) outcomes include the fused Kolmogorov filter (Mai and Zou 2013), using the mean conditional variance, i.e., the expectation in  $X_j$  of the variance in the response of the conditional cumulative distribution function  $P(X \le x|Y)$  (Cui, Li, and Zhong 2015). Ke (2023) propose a model free method where the contribution of each individual predictor is quantified marginally and conditionally in the presence of the control variables as well as the other candidates by reproducing-kernel-based  $R^2$  and partial  $R^2$  statistics.

**SPAR** allows the integration of various advanced screening techniques using a flexible framework, which in turn enables users to apply various screening methods tailored to their data characteristics in the algorithm generating the ensemble. This flexibility allows users to evaluate different strategies, ensuring that the most effective approach is chosen for the specific application at hand. Moreover, it incorporates probabilistic screening strategies, which can be particularly useful in ensembles, as they to enhance the diversity of predictors across ensemble models. Instead of relying on a fixed threshold or number of predictors to be screened, predictors are sampled with probabilities proportional to their screening score (see Mukhopadhyay and Dunson 2020; Parzer *et al.* 2024).

## 2.2. Random projection tools

The random projection method relies on the Johnson-Lindenstrauss (JL) lemma (Johnson and Lindenstrauss 1984), which asserts that there exists a random map  $\Phi \in \mathbb{R}^{m \times p}$  that embeds any set of points in p-dimensional Euclidean space collected in the rows of  $X \in \mathbb{R}^{n \times p}$  into a m-dimensional Euclidean space where pairwise distances are approximately preserved and it also gives a lower bound on the goal dimension m in order to preserve the distances between all pairs of points within a factor  $1 \pm \varepsilon$ :  $m > \frac{24 \log n}{3\varepsilon^2 - 2\varepsilon^3}$  for any  $0 < \varepsilon < 1$ . Computationally, an attractive feature of the method for high-dimensional settings is that the bound does not depend on p.

The random map  $\Phi$  that satisfies the JL lemma should be chosen such that it fulfills certain conditions (see Johnson and Lindenstrauss 1984) and the literature focuses on constructing such matrices either by sampling them from some "appropriate" distribution, by inducing sparsity in the matrix and/or by employing specific fast constructs which lead to efficient matrix-vector multiplications.

It turns out that the conditions are generally satisfied by nearly all sub-Gaussian distributions (Matoušek 2008). A common choice is the standard normal distribution  $\Phi_{ij} \stackrel{iid}{\sim} N(0,1)$  (Frankl and Maehara 1988) or a sparser version  $\Phi_{ij} \sim N(0,1/\sqrt{\psi})$  with probability  $\psi$  and 0 otherwise (Matoušek 2008). Another common choice which is computationally simpler to generate from

is the Rademacher distribution where  $\Phi_{ij}=\pm 1/\sqrt{\psi}$  with probability  $\psi/2$  and zero otherwise for  $0<\psi\leq 1$ . where Achlioptas (2003) shows results for  $\psi=1$  and  $\psi=1/3$  while Li, Hastie, and Church (2006) recommend using  $\psi=1/\sqrt{p}$  to obtain very sparse matrices. Further approaches include using Haar measure to generate random orthogonal matrices (Cannings and Samworth 2017) or distributions which are not sub-Gaussian, such as standard Cauchy for settings where the data is high-dimensional, non-sparse, and heavy-tailed by preserving approximate  $\ell_1$  distances (see e.g., Li, Hastie, and Church 2007). Instead of using sparse matrices, structured matrices, for which multiplication can more easily be performed have also been proposed (see e.g., Ailon and Chazelle 2009; Clarkson and Woodruff 2013a)

The conventional random projections mentioned above are data-agnostic. However, recent work has proposed incorporating information from the data either in choosing an appropriate random projection or directly in the random projection. For example, Cannings and Samworth (2017) build an ensemble classifier where they propose to choose the random projection matrix to be used in a model by selecting the one that minimizes the test error of the classification problem among a set of data-agnostic random projections. On the other hand, Parzer et al. (2024) propose to use a random projection matrix for GLMs which directly incorporates information about the relationship between the predictors and the response in the projection matrix, rather than a projection matrix which satisfies the JL lemma. More specifically, it constructs a matrix that where the vector of coefficients can be recovered after the projection, which is not the case for conventional random projections (Thanei et al. 2017) by using the sparse embedding matrix of Clarkson and Woodruff (2013a), where the random diagonal elements are replaced by a ridge coefficient with a minimal  $\lambda$  penalty. Another data-driven approach to random projection for regression has been proposed by Ryder, Karnin, and Liberty (2019), who propose a data-informed random projection using an asymmetric transformation of the predictor matrix without using information of the response.

**SPAR** has been designed in a way that allows the incorporation of different random projection techniques which allows users to tailor the employed procedure to their specific data needs.

#### 2.3. Generalized linear models

After we perform in each marginal model an initial screening step followed by a projection step, we assume that the reduced and projected set of predictors  $z_i$  together with the response arises from a GLM with the responses having conditional densities from a (reproductive) exponential dispersion family of the form

$$f(y_i|\theta_i,\phi) = \exp\Bigl\{\frac{y_i\theta_i - b(\theta_i)}{a(\phi)} + c(y_i,\phi)\Bigr\}, \quad g(\mathsf{E}[y_i|z_i]) = \gamma_0 + z_i'\gamma =: \eta_i, \tag{1}$$

where  $\theta_i$  is the natural parameter, a(.) > 0 and c(.) are specific real-valued functions determining different families,  $\phi$  is a dispersion parameter, and b(.) is the log-partition function normalizing the density to integrate to one. If  $\phi$  is known, we obtain densities in the natural exponential family for our responses. The responses are related to the m-dimensional reduced and projected predictors through the conditional mean, i.e., the conditional mean of  $y_i$  given  $z_i$  depends on a linear combination of the predictors through a (invertible) link function g(.), where  $\gamma_0 \in \mathbb{R}$  is the intercept and  $\gamma \in \mathbb{R}^m$  is a vector of regression coefficients for the m projected predictors.

Given that m, the goal dimension of the projection need not necessarily be small in comparison to n (we recommend using a dimension of around n/2), we observe that adding a small  $L_2$  penalty in the marginal models, especially for the binomial family, can make estimation more stable as it alleviates problems related to separation. The marginal models we estimate therefore involve minimizing the following function:

$$\mathrm{argmin}_{\gamma \in \mathbb{R}^m} \min_{\gamma_0 \in \mathbb{R}} \sum_{i=1}^n -\ell(\beta; y_i, z_i) + \frac{\varepsilon}{2} \sum_{j=1}^m \gamma_j^2, \, \varepsilon > 0$$

We will employ function glmnet() of package glmnet (Tay, Narasimhan, and Hastie 2023) in the estimation of the marginal models.

## 2.4. Algorithm

We present the general algorithm implemented in package SPAR.

- Choose family with corresponding log-likelihood  $\ell(.)$  and link
- Standardize predictors  $X: n \times p$  by subtracting the sample column mean and dividing the sample standard deviation.
- Calculate screening coefficients  $\hat{\alpha}$  e.g.,
- For  $k = 1, \dots, M$  models:
  - screen 2n predictors based on the screening coefficient  $\hat{\alpha}_j$  yielding screening index set  $I_k = \{j_1^k, \dots, j_{2n}^k\} \subset [p]$ ; if probabilistic screening should be employed draw the predictors without replacements using an initial vector of probabilities  $p_j \propto |\hat{\alpha}_j|$ . Otherwise, select the 2n variables with the highest  $|\hat{\alpha}_j|$ .
  - project screened variables to a random dimension  $m_k \sim \text{Unif}\{\log(p), \dots, n/2\}$  using **projection matrix**  $\Phi_k$  to obtain  $Z_k = X_{\cdot I_k} \Phi_k^{\top} \in \mathbb{R}^{n \times m_k}$ :
  - fit a **GLM** of y against  $Z_k$  (with small  $L_2$ -penalty Tay et~al.~(2023)) to obtain estimated coefficients  $\gamma^k \in \mathbb{R}^{m_k}$  and  $\hat{\beta}^k_{I_k} = \Phi'_k \gamma^k,~\hat{\beta}^k_{\bar{I}_k} = 0$ .
- for a given threshold  $\nu > 0$ , set all  $\hat{\beta}_j^k$  with  $|\hat{\beta}_j^k| < \nu$  to 0 for all j, k
- choose M and  $\lambda$  via a validation set or cross-validation by repeating steps 1 to 4 and evaluating a prediction performance measure on the withheld fold; and choose

$$(M_{\text{best}}, \lambda_{\text{best}}) = \operatorname{argmin}_{M, \lambda} \text{Dev}(M, \lambda)$$
 (2)

- combine via the coefficients simple average  $\hat{\beta} = \sum_{k=1}^{M} \hat{\beta}^k/M$
- output the estimated coefficients and predictions for the chosen M and  $\lambda$ .

## 3. Software

The package be installed from GitHub

```
R> devtools::install_github("RomanParzer/SPAR")
and loaded by:
R> library("SPAR")
In this section we rely for illustration purposes on an example data set from the package:
R> data("example_data", package = "SPAR")
R> str(example_data)
```

#### 3.1. Main functions and their arguments

The two main functions for fitting the SPAR algorithm are:

```
R> spar(x, y, family = gaussian("identity"), rp = NULL, screencoef = NULL,
+ xval = NULL, yval = NULL, nnu = 20, nus = NULL, nummods = c(20),
+ measure = c("deviance", "mse", "mae", "class", "1-auc"),
+ inds = NULL, RPMs = NULL, ...)
```

which implements the algorithm in Section 2.4 without cross-validation and returns an object of class "spar", and

```
R> spar.cv(x, y, family = gaussian("identity"), rp = NULL, screencoef = NULL,
+ nfolds = 10, nnu = 20, nus = NULL, nummods = c(20),
+ measure = c("deviance", "mse", "mae", "class", "1-auc"), ...)
```

which implements the cross-validated procedure and returns an object of class "spar.cv".

The common arguments of these functions are:

- x is an  $n \times p$  numeric matrix of predictor variables.
- y numeric response vector of length n.
- family object from stats::family().
- rp an object of class 'randomprojection'
- screencoef an object of class 'screencoef'
- nnu is the number of threshold values  $\nu$  which should be considered for thresholding; defaults to 20
- nus is an optional vector of  $\nu$  values to be considered for thresholding. If it is not provided, is defaults to a grid of nnu values. This grid is generated by including zero and nnu-1 equally spaced quantiles of the absolute values of the estimated coefficients from the marginal models.
- nummods is the number of models to be considered in the ensemble; defaults to 20. If a vector is provided, all combinations of nus and nummods are considered when choosing the optimal  $\nu_{\rm best}$  and  $M_{\rm best}$ .
- measure gives the measure based on which the thresholding value  $\nu_{\rm opt}$  and the number of models M should be chosen on the validation set (for spar()) or in each of the folds (in

spar.cv()). Defaults to "deviance", which is available for all families. Other options
are "mse" or "mae" (between responses and predicted means, for all families), "class"
(misclassification error) and "1-auc" (one minus area under the ROC curve) both just
for binomial family.

Furthermore, spar() has the specific arguments:

- xval and yval which are used as validation sets for choosing  $\nu_{\text{best}}$  and  $M_{\text{best}}$ . If not provided, x and y will be employed.
- inds is an optional list of length max(nummods) containing column index-vectors corresponding to variables that should be kept after screening for each marginal model; dimensions need to fit those of the dimensions of the provided matrices in RPM.
- RPMs is an optional list of length max(nummods) which contains projection matrices to be used in each marginal model.

Function spar.cv() has the specific argument nfolds which is the number of folds to be used for cross-validation. It relies on spar() as a workhorse, which is called for each fold. The random projections for each model are held fixed throughout the cross-validation to reduce the computational burden. This is possible by calling spar() in each fold with a predefined inds and RPMs argument.

## 3.2. Screening coefficients

The objects for creating screening coefficients are implemented as S3 classes 'screencoef'. These objects are created by several screen\_\* functions, which take . . . and a list of controls control as arguments. These functions return an object of class 'screencoef' which in turn is a list with three elements:

- name.
- generate\_fun an R function for generating the screening coefficient. This function should have the following arguments:
  - a 'screencoef' object which has as attributes all the information passed through
     ...,
  - data, which should be a list of x the matrix of standardized predictors and y the vector of (standardized in the Gaussian case) responses. It returns a vector of screening coefficients of length p.
- control, which is the control list in screen\_\*. These controls are arguments which are needed in generate\_fun in order to generate the desired screening coefficients.

The following screening coefficients are implemented in **SPAR**:

• screen\_marglik() - computes the screening coefficients by the coefficient of  $x_j$  in a univariate GLM using the stats::glm() function.

$$\hat{\alpha}_j =: \mathrm{argmin}_{\beta_j \in \mathbb{R}} \mathrm{min}_{\beta_0 \in \mathbb{R}} \sum_{i=1}^n -\ell(\beta_0, \beta; y_i, x_{ij})$$

It allows to pass a list of controls through the control argument to stats::glm such as weights, family, offsets.

- screen\_cor() computes the screening coefficients by the correlation between y and  $x_j$  using the function stats::cor(). It allows to pass a list of controls through the control argument to stats::cor.
- screen\_glmnet() computes by default the ridge coefficient where the penalty  $\lambda$  is very small (see Parzer *et al.* 2024, for motivation).

$$\hat{\alpha} =: \operatorname{argmin}_{\beta \in \mathbb{R}^p} \sum_{i=1}^n -\ell(\beta; y_i, x_i) + \frac{\varepsilon}{2} \sum_{j=1}^p \beta_j^2, \, \varepsilon > 0$$

The function relies on glmnet::glmnet() and, while it assumes by default  $\alpha=0$  and a small penalty, it allows to pass a list of controls through the control argument to glmnet::glmnet() such as alpha = 1. Used as default if screencoef = NULL in function call of spar() or spar.cv().

Further arguments related to screening can be passed through ..., which will be saved as attributes of the 'screencoef' object. More specifically, the following are employed in function spar():

- nscreen integer giving the number of variables to be retained after screening; defaults to 2n
- split\_data\_prop, double between 0 and 1 which indicates the proportion of the data that should be used for computing the screening coefficient. The remaining data will be used for estimating the SPAR algorithm; defaults to NULL. In this case the whole data will be used for estimating the screening coefficient and the SPAR algorithm.
- type character either "prob" (indicating that probabilistic screening should be employed) or "fixed" (indicating that a fixed set of nscreen variables should be employed across the ensemble; defaults to type = "prob".

For illustration purposes, consider the implemented function screen\_marglik(), which is used to define a screening procedure based on the coefficients of univariate marginal GLMs between each predictor and the response.

A user-friendly print of the 'screencoef' is provided:

#### R> obj

The structure of the object is the following:

#### R> unclass(obj)

Function generate\_scrcoef\_marglik defines the generation of the screening coefficient. It considers the controls in object\$control when calling the stats::glm() function. Given that the proposed framework estimates GLMs for the marginal models, the spar() function assigns by default its family argument as an attribute for the screencoef object. In generate\_scrcoef\_marglik, we employ family attribute of the 'screencoef' object if the control list argument does not contain any particular family.

For convenience, a constructor function constructor\_screencoef() is provided, which can be used to create new screen\_\* functions. An example is presented in Section 4.1

#### 3.3. Random projections

Similar to the screening procedure, the objects for creating random projections are implemented as S3 classes 'randomprojection' and are created by functions rp\_\*(..., control = list()), which take ... and a list of controls control as arguments.

These functions return an object of class 'randomprojection' which is a list with three elements:

- name,
- generate\_fun function for generating the random projection matrix. This function should have with arguments rp, which is a 'randomprojection' object, m, the target dimension and a vector of indexes included\_vector which shows the column index of the original variables in the x matrix to be projected using the random projection. This is needed due to the fact that screening can be employed pre-projection. It returns a sparse random projection matrix of class "dgCMatrix" of the Matrix with m rows and length(included\_vector) columns.
- update\_data\_rp optional function with attributes relying with information from the data which should only be computed once, before the start of the SPAR algorithm. This function should have with arguments rp, which is a 'randomprojection' object and data, which should be a list of x the matrix of standardized predictors and y the vector of (standardized in the Gaussian case) responses. This function is relevant for data driven random projections, because to keep computational costs low, all data-dependent computations which do not need to be computed in each random projection will be computed once before the start of the algorithm. All computed quantities which will be used in the generate\_fun function should be saved as attributes to the randomprojection object, which is what this function returns.
- update\_rpm\_w\_data optional function for updating the random projection matrices provided in the argument RPMs of functions spar and spar.cv with data-dependent parameters. If argument RPMs is provided, the random structure is kept fixed, but the data-dependent part gets updated with the provided data set. Defaults to NULL. If not provided, the values of the provided RPMs do not change. This is particularly relevant in the cross-validation procedure.
- control, which is the control list in rp\_\*. These controls are arguments which are needed ingenerate\_fun' in order to generate the desired random projection.

Further arguments related to the random projection can be passed through ..., which will then be saved as attributes of the 'randomprojection' object.

More specifically, the following attributes are relevant in the SPAR algorithm:

• mslow: integer giving the minimum dimension to which the predictors should be projected; defaults to  $\log(p)$ 

- msup: integer giving the maximum dimension to which the predictors should be projected; defaults to n/2
- use data: boolean indicating whether the random projection is data driven.

Note that for random projection matrices which satisfy the JL lemma, mslow can be determined by employing the result of the JL lemma, which gives a lower bound on the goal dimension in order to preserve the distances between all pairs of points within a factor  $(1 \pm \epsilon)$ :  $m > \frac{24}{3\epsilon^2 - 2\epsilon^3} \log n$ .

The following random projections are implemented in **SPAR**:

- rp\_gaussian() random projection object where the generated matrix will have entries from a normal distribution (defaults to standard normal entries)
- rp\_sparse() random projection object where the generated matrix will be the one in (Achlioptas 2003) with psi=1 by default.
- rp\_cw() sparse embedding random projection in (Clarkson and Woodruff 2013b) for rp\_cw(data = FALSE). Defaults to rp\_cw(data=TRUE), which replaces the random elements on the diagonal by the ridge coefficients with a small penalty, as introduced in Parzer et al. (2024).

For illustration purposes, consider the implemented function rp\_gaussian, which is a random projection with entries drawn from the normal distribution.

```
R> rp_gaussian()
```

The generate\_fun returns a sparse matrix object of class "dgCMatrix" by using the Matrix::Matrix function. Note that included\_vector gives the indexes of the variables which have been selected by the screening procedure. In this case, where the random projection does not use any data information, we are only interested in the length of this vector.

The elements update\_data\_fun and update\_rpm\_w\_data of the object are NULL, as this conventional random projection is data agnostic.

#### 3.4. Methods

Methods print, plot, coef, predict are available for both "spar" and "spar.cv" classes.

print

The print method returns information on  $\nu_{\text{best}}$   $M_{\text{best}}$ , the number of active predictors (i.e., predictors which have at least a nonzero coefficient across the marginal models) and a five-point summary of the non-zero coefficients.

coef

```
+ nummods = c(5,10,15,20,25,30))
R> spar_res
R> spar_cv
```

Method coef takes as inputs a spar or spar.cv object, together with further arguments:

- nummod number of models used to compute the averaged coefficients; value of nummod with minimal
   measure is used if not provided.
- nu threshold level used to compute the averaged coefficients; value with minimal measure is used if not provided.

```
R> str(coef(spar_res))
```

It returns a list with the intercept, vector of beta coefficients and the nummod and nu employed in the calculation.

Additionally for "spar.cv", the coef method also has argument opt\_par which is one of c("1se","best") and chooses whether to select the best pair of nus and nummods according to cross-validation measure, or the solution within one standard deviation of that optimal cross-validation measure. This argument is ignored when nummod and nu are given.

#### predict

Functionality for computing predictions is provided through the method predict which takes a spar or spar.cv object, together with

- xnew matrix of new predictor variables; must have same number of columns as x.
- type the type of required predictions; either on "response" level (default) or on "link" level
- avg\_type type of averaging used across the marginal models; either on "link" (default) or on "response" level
- nummod number of models used to compute the averaged coefficients; value of nummod with minimal measure is used if not provided.
- nu threshold level used to compute the averaged coefficients; value with minimal measure is used if not provided.
- coef optional vector of coefficients to be used directly in the prediction.

Additionally, for class "spar.cv", argument opt\_par is available and used in the computation of the coefficients to be used for prediction (see above description of method coef).

plot

Plotting functionality is provided through method plot which allows for the following arguments:

- x an object of class "spar" or "spar.cv"
- plot\_type one of:
  - "Val\_Measure" plots the (cross-)validation measure for either a grid of nu values for a fixed number of models nummod or viceversa.
  - "Val\_numAct" plots the number of active variables for either a grid of nu values for a fixed number of models nummod or viceversa.
  - "res-vs-fitted" produces a residuals-vs-fitted plot. The residuals are computed as  $y \hat{y}$ , where  $\hat{y}$  is the prediction computed on response level.
  - "coefs" produces a plot of the value of the standardized coefficients for each predictor in each marginal model (before thresholding). For each predictor, the values of the coefficients are sorted from largest to smallest across the marginal models and then represented in the plot.
- plot\_along, one of c("nu", "nummod"); indicates whether the (cross-)validation ignored when plot\_type="res-vs-fitted" or plot\_type="coefs".
- nummod fixed value for number of models when plot\_along = "nu" for plot\_type
   "Val\_Measure" or "Val\_numAct"; if plot\_type="res-vs-fitted", it is used in the predict method, as described above.
- nu- fixed value for ν when plot\_along = "nummod" for plot\_type = "Val\_Measure" or "Val\_numAct"; if plot\_type="res-vs-fitted", it is used in the predict method, as described above.
- xfit if plot\_type = "res-vs-fitted", it is the matrix of predictors used in computing the fitted values. Must provided for this plot, as the spar or spar.cv objects do not store the original data.
- yfit if plot\_type = "res-vs-fitted", vector of responses used in computing the residuals. Must provided for this plot, as the spar or spar.cv objects do not store the original data.
- prange, optional vector of length 2 in case plot\_type = "coefs" which gives the limits of the predictors' plot range; defaults to c(1, p).
- coef\_order optional index vector of length p in case plot\_type = "coefs" to give the order of the predictors; defaults to 1 : p.

For class "spar.cv" there is the extra argument opt\_par = c("best", "1-se") which, for plot\_type = "res-vs-fitted" indicates whether the predictions should be based on coefficients using the best  $(\nu, M)$  combination or on the one which delivers the largest error within 1-standard-deviation from the minimum.

The plot methods return objects of class "ggplot" Wickham (2016).

## 4. Extensibility

The user can implement their own screening and random projections.

## 4.1. Screening coefficients

We exemplify how new screening coefficients implemented in package **VariableScreening** can easily be used in the framework of **SPAR**.

We start by defining the function for generating the screening coefficients using the screenIID() function in VariableScreening.

```
R> generate_scr_sirs <- function(object, data) {
+ res_screen <- do.call(function(...)
+ VariableScreening::screenIID(data$x, data$y, ...),
+ object$control)
+ coefs <- res_screen$measurement
+ coefs
+}</pre>
```

Note that screenIID() also takes method as an argument. To allow for flexibility, we do not fix the method in generate\_scr\_sirs but rather allow the user to pass a method through the control argument in the screen\_\* function. This function is created using constructor\_screencoef:

```
R> screen_sirs <- constructor_screencoef(
+ "screen_sirs",
+ generate_fun = generate_scr_sirs)</pre>
```

We now call the spar() function with the newly created screening procedure. We consider method SIRS of Zhu et al. (2011), which ranks the predictors by their correlation with the rank-ordered response and we do not perform probabilistic variable screening but employ the top 2n variables in each marginal model.

## 4.2. Random projections

We exemplify how new random projections can be implemented in the framework of **SPAR**.

We implement the random projection of Cannings and Samworth (2017), who propose using the Haar measure for generating the random projections. They simulate matrices from Haar measure by independently drawing each entry of a matrix Q from a standard normal distribution, and then to take the projection matrix to be the transpose of the matrix of

left singular vectors in the singular value decomposition of Q. Moreover, they suggest using "good" random projections, in the sense that they deliver the best out-of-sample prediction. The proposed approach employs  $B_1$  models in an ensemble of classifiers and for each model k,  $B_2$  data independent random projections are generated and the one with the lowest error on a test set is the one chosen to project the variables in model k.

We can implement such a random projection in **SPAR** by the following building block:

```
R> update_data_cannings <- function(rp, data) {
+ attr(rp, "data") <- data
+ rp
+}</pre>
```

This the function which adds data information to the random projection object. Here, the whole data can be added as information for the M random projection (alternatively, one could only pass sufficient statistics for computing the desired measures).

While the  $B_2$  random projections are data agnostic, the generate\_fun element of the random projection will need the data information in order to evaluate which method performs best in terms of an error measure. We will in the following define the function for the generation of the random projection matrix to be used in a model k.

This helper simulates  $m \times p$  matrices from the Haar measure:

```
R> simulate_haar <- function(m, p) {
+ RO <- matrix(1/sqrt(p) * rnorm(p * m), nrow = p, ncol = m)
+ RM <- qr.Q(qr(RO))[, seq_len(m)]
+ RM <- Matrix(t(RM), sparse = TRUE)
+}</pre>
```

The function that generates the random projection matrix for model k used 25% of the data as a test set for choosing the best among  $B_2$  random projections in terms of minimizing misclassification error for the binomial family and MSE for all other families:

```
error_all <- lapply(seq_len(B2), FUN = function(s){</pre>
     RM <- simulate_haar(m, p)</pre>
     xrp <- tcrossprod(xtrain, RM)</pre>
     mod <- do.call(function(...)</pre>
       glm.fit(x = cbind(1, xrp), y = ytrain, ...), control_glm)
     eta_test <- drop(cbind(1, tcrossprod(xtest, RM)) %*% mod$coefficients)</pre>
     pred <- family$linkinv(eta_test)</pre>
     out <- ifelse(family$family == "binomial",</pre>
                     mean(((pred > 0.5) + 0) != ytest),
                     mean((pred - ytest)^2))
     list(RM, out)
  })
+ id_best <- which.min(sapply(error_all, "[[", 2))
+ RM <- error_all[[id_best]][[1]]
+ return(RM)
+}
```

In the cross-validation procedure, sample new random projection matrices and pick the best one for the current iteration. Given that we do not wish to keep the random structure of the matrices fixed, we do not specify a function update\_rpm\_w\_data.

Putting it all together, we get:

```
R> rp_cannings <- constructor_randomprojection(
+ "rp_cannings",
+ generate_fun = generate_cannings,
+ update_data_fun = update_data_cannings
+)</pre>
```

We can now estimate SPAR for a binomial model, where we transform the response to a binary variable.

```
R> ystar <- (example_data$y > 0) + 0
R> ystarval <- (example_data$ytest > 0) + 0
```

We use 100 models (which is in line to recommendations for  $B_1$  in Cannings and Samworth (2017)), and no screening procedure. If no screening is desired, nscreen can be set to p in the screen\_\* function:

```
R>
R> spar_example_2 <- spar(x = example_data$x, y = ystar,</pre>
+ family = binomial(),
+ screencoef = screen_marglik(nscreen = ncol(example_data$x)),
+ rp = rp cw(data = TRUE),
+ nummods = 100,
+ xval = example_data$xtest, yval = ystarval,
+ measure = "class"
+)
We can extract the measures on the validation set by:
R> head(spar_example_1$val_res)
We can compare the two approaches by looking at the minimum Meas achieved:
R> min_val_1 <- min(spar_example_1$val_res$Meas)</pre>
R> id_best_1 <- max(which(spar_example_1$val_res$Meas == min_val_1))</pre>
R> min_val_2 <- min(spar_example_2$val_res$Meas)</pre>
R> id_best_2 <- max(which(spar_example_2$val_res$Meas == min_val_2))</pre>
R.>
R> spar_example_1$val_res[id_best_1, ]
R> spar_example_2$val_res[id_best_2, ]
```

## 5. Illustrations

#### 5.1. Face image data

We illustrate the functionality of **SPAR** on the Isomap data set containing n = 698 black and white face images of size  $p = 64 \times 64 = 4096$  together with the faces' horizontal looking direction angle as the response variable.<sup>1</sup>

```
R> url <- "https://web.archive.org/web/20150922051706/http://isomap.stanford.edu/face_data
R> download.file(url, file.path("face_data.mat.Z"))
R> system('uncompress face_data.mat.Z')
The .mat file format can be read using R.matlab (Bengtsson 2022)
R> library("R.matlab")
R> facedata <- readMat(file.path("face_data.mat"))
R> x <- t(facedata$images)
R> y <- facedata$poses[1,]
We can visualize e.g., the first observation in this data set in Figure ??:
R> library(ggplot2)
R> i <- 1</pre>
```

 $<sup>^1{\</sup>rm The~Isomap}$  face data can be found online on https://web.archive.org/web/20160913051505/http://isomap.stanford.edu/datasets.html.

and estimate on the training data the SPAR algorithm with cross-validation. We employ a Gaussian random projection where entries are generated from a normal distribution with mean zero and standard deviation 1/p and with screening based on the ridge coefficients:

```
R> library(SPAR)
R> p <- ncol(xtrain)
R> spar_faces <- spar.cv(
+ xtrain, ytrain,
+ rp = rp_gaussian(control = list(c(mean = 0, sd = 1/p))),
+ screencoef = screen_cor(method = "kendall"),
+ nummods = c(5, 10, 20, 50),
+ measure = "mse")
R> spar_faces
```

The plot method for 'spar.cv' objects displays by default the measure employed in the cross-validation (in this case MSE) for a grid of  $\nu$  values, where the number of models is fixed to the value found to perform best in cross-validation exercise:

```
R> plot(spar_faces)
```

The coefficients of the different variables (in this example pixels) obtained by averaging over the coefficients the marginal models (for optimal  $\lambda$  and number of models) are given by:

```
R> face_coef <- coef(spar_faces, opt_par = "best")
R> str(face_coef)
```

For a sparser solution we can compute the coefficients using opt\_par = "1se" which leads to more sparsity and a lowe number of models.

```
R> face_coef_1se <- coef(spar_faces, opt_par = "1se")
R> str(face_coef_1se)
```

The standardized coefficients from each of max(nummods) models (before averaging and before thresholding) can be plotted by:

```
R> plot(spar_faces, "coefs")
```

The predict() function can be applied to the 'spar.cv' object. We will employ the sparser solution chosen by the opt\_par = "1se" rule:

```
R> ynew <- predict(spar_faces, xnew = xtest, coef = face_coef_1se)
```

In the high-dimensional setting it is interesting to look at the relative mean square prediction error which compares the MSE to the MSE of a model containing only an intercept:

```
R> rMSPEconst <- mean((ytest - mean(y))^2)
R> mean((ynew-ytest)^2)/rMSPEconst
```

Additionally, for this data set, one can visualize the effect of each pixel  $\hat{\beta}_j x_{i,j}^{\text{new}}$  in predicting the face orientation in a given image e.g., the 10th one in the test set:

#### 5.2. Darwin data set

The Darwin dataset (Cilia, De Gregorio, De Stefano, Fontanella, Marcelli, and Parziale 2022) contains a binary response for Alzheimer's disease (AD) together with extracted features from 25 handwriting tests (18 features per task) for 89 AD patients and 85 healthy people (n=174).<sup>2</sup>

Before proceeding with the analysis, the data is screened for multivariate outliers using the DDC algorithm in package **cellWise** (Raymaekers and Rousseeuw 2023).

```
R> darwin_orig <- list(
+ x = darwin_tmp[, !(colnames(darwin_tmp) %in% c("ID", "class"))],
+ y = as.numeric(darwin_tmp$class) - 1)
R> tmp <- cellWise::DDC(
+ as.matrix(darwin_orig$x),
+ list(returnBigXimp = TRUE,
+ tolProb = 0.999,</pre>
```

<sup>&</sup>lt;sup>2</sup>The data set can be downloaded from https://archive.ics.uci.edu/dataset/732/darwin

```
+ silent = TRUE))
R> darwin <- list(x = tmp$Ximp, y = darwin_orig$y)</pre>
```

The structure of the data is:

```
R> str(darwin)
```

We estimate the SPAR algorithm with the screening and random projection introduced in Parzer *et al.* (2024) for binomial family and logit link, using 1—area under the ROC curve as the cross-validation measure,

```
R> spar_darwin <- spar.cv(darwin$x, darwin$y,
+ family = binomial(logit),
+ nummods = c(5, 10, 20, 50),
+ measure = "1-auc")</pre>
```

We can look at the average number of active variables for a grid of  $\nu$  where the number of models is fixed to the value found to perform best in cross-validation exercise by using the plot method for "spar.cv" (see Figure ??).

```
R> plot(spar_darwin, plot_type = "Val_numAct")
```

The predictors are ordered by task, where the first 18 covariates represent different features measured for the first task. Given that there is clear grouping in the variables in this example, we can reorder the coefficients plot by grouping them by feature, rather than task. We can achieve this by using reordering argument coef\_order in method plot with plot\_type = "coefs" (see Figure ??).

In general we observe that the different features measures across different tasks have the same impact on the probability of AD (observable by the blocks of blue or red lines).

## 6. Conclusion

Package **SPAR** can be employed for modeling data in a high-dimensional setting, where the number of predictors is much higher than the number of observations. The package provides

an implementation of the SPAR algorithm, which combines variable screening and random projection in an ensemble of GLMs. The package provides flexible classes for i) specifying the screening coefficient based on which screening should be performed (both in a classical or probabilistic fashion), ii) generating the random projection to be employed in each marginal model.

## Computational details

The results in this paper were obtained using R 4.4.0.

R itself and all packages used are available from the Comprehensive R Archive Network (CRAN) at https://CRAN.R-project.org/.

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