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# spar: Sparse Projected Averaged Regression in R

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#### Abstract

Package spar for R builds ensembles of predictive generalized linear models with high-dimensional predictors. It employs an algorithm utilizing variable screening and random projection tools to efficiently handle the computational challenges associated with large sets of predictors. The package is designed with a strong focus on extensibility. Screening and random projection techniques are implemented as S3 classes with user-friendly constructor functions, enabling users to easily integrate and develop new procedures. This design enhances the package's adaptability and makes it a powerful tool for a variety of high-dimensional applications.

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

#### 1. Introduction

The spar package for R (R Core Team 2024) offers functionality for estimating generalized linear models (GLMs) in high-dimensional settings, where the number of predictors p significantly exceeds the number of observations n i.e., p > n or even  $p \gg n$ . To address the challenges of high dimensionality, the package implements an algorithm which integrates variable screening methods with random projection techniques to effectively reduce the predictor space.

Random projection is a computationally-efficient method which linearly maps a set of points in high dimensions into a much lower-dimensional space. Several packages in R provide functionality for random projections. For instance, package **RandPro** (Aghila and Siddharth 2020; Siddharth and Aghila 2020) allows a Gaussian random matrix, a sparse matrix (Achlioptas

2003; Li, Hastie, and Church 2006) or a matrix generated using the equal probability distribution with the elements  $\{-1,1\}$  to be applied to the predictor matrix before employing one of k nearest neighbor, support vector machine or naive Bayes classifier on the projected features. 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. Additionally, package **RPEnsembleR** (Cannings and Samworth 2021) implements a similar idea when building the ensemble of classifiers: for each classifier in the ensemble, a collection of (Gaussian, axis-aligned projections, or Haar) random projection matrices is generated, and the one that minimizes a risk measure for classification on a test set is selected. For Python (van Rossum et al. 2011) the **sklearn.random\_projection** module (Pedregosa, Varoquaux, Gramfort, Michel, Thirion, Grisel, Blondel, Prettenhofer, Weiss, Dubourg et al. 2011) implements two types of unstructured random matrices, namely Gaussian random matrix and sparse random matrix.

Random projection can suffer from noise accumulation for very large p, 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). The R landscape for variable screening techniques is very rich. An overview of some notable packages on the Comprehensive R Archive Network (CRAN) includes the following packages. Package SIS (Saldana and Feng 2018), which implements the (iterative) sure independence screening procedure and its extensions, as detailed in Fan and Ly (2007), Fan and Song (2010), Fan, Feng, and Wu (2010). This package also provides functionality for estimating a penalized generalized linear model or a cox regression model for the variables selected by the screening procedure. Package VariableScreening (Li, Huang, and Dziak 2022) offers screening methods for independent and identically distributed (iid) data, varying-coefficient models, and longitudinal data and includes techniques such as sure independent ranking and screening (SIRS), which ranks the predictors by their correlation with the rank-ordered response, or distance correlation sure independence screening (DC-SIS), a non-parametric extension of the correlation coefficient. Package MFSIS (Cheng, Wang, Zhu, Zhong, and Zhou 2024) provides a collection of model-free screening techniques including SIRS, DC-SIS, the fused Kolmogorov filter (Mai and Zou 2015) the projection correlation method using knock-off features (Wanjun Liu and Li 2022), among others. Additional packages implement specific procedures but their review is beyond the scope of the current paper.

Although combining variable screening with random projection effectively reduces the predictor set and computational costs, the variability introduced by random sampling – both in projections and screening indices – can be mitigated by averaging the results from multiple iterations (Thanei, Heinze, and Meinshausen 2017). To address these points, **spar** builds an ensemble of GLMs in the spirit of Mukhopadhyay and Dunson (2020) and Parzer, Filzmoser, and Vana-Gür (2024a) where, in each model of the ensemble, i) variables are first screened based on a screening coefficient, ii) the selected variables are then projected to a lower dimensional space, iii) a GLM is estimated using the projected predictors. Finally, additional sparsity in the coefficients of the original variables can be introduced through a thresholding parameter, which together with the number of models in the ensemble can be chosen using

a validation set or via cross-validation. The final coefficients are then obtained by averaging over the marginal models in the ensemble. This algorithm performs sparse projected averaged regression (SPAR) for both discrete and continuous data in the GLM framework in a computationally efficient way. Different variants of the algorithm have been shown to perform well in terms of prediction power on a variety of datasets (see Mukhopadhyay and Dunson 2020). In particular, Parzer et al. (2024a) show that when paired with a carefully constructed data-driven random projection the algorithm performs superiorly in terms of predictions and variable ranking in settings exhibiting different degrees of sparsity in the coefficients.

A variety of screening coefficients are provided as well as several procedures for generating random projection matrices. These procedures can be classified into data-agnostic and data-driven, where the former, unlike the latter, does not incorporate information from the data in the construction of the matrices. However, the package is designed with flexibility in mind, providing users with a versatile framework to extend the implemented screening and projection techniques with their own custom procedures. This is facilitated by leveraging R's S3 classes, making the process convenient and user-friendly. Therefore, users can seamlessly integrate various techniques by either writing their own procedures or leveraging the existing R packages.

The package provides methods such as plot, predict, coef, print, which allow users 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. 2024a), facilitates interpretability of the model output, allowing users to understand variable effects.

While **spar** offers the first implementation of the described algorithm and, to the best of our knowledge, no other package offers the same functionality for GLMs, few other R packages focus on building ensembles of *classifiers* where the dimensionality of the predictors is reduced. Most notably, package **RPEnsemble** (Cannings and Samworth 2021) implements the procedure in Cannings and Samworth (2017) where "carefully-selected" random projections are used for projecting the predictors before they are employed in a classifier such as k-nearest neighbor, linear or quadratic discriminant analysis. On the other hand, package **RaSEn** (Tian and Feng 2021) implements the RaSE algorithm for ensemble classification and regression problems, where random subspaces are generated and the optimal one is chosen to train a weak learner on the basis of some criterion.

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 and Section 4 exemplifies how a new screening coefficient and a new random projection can be integrated in the package. 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  $p \gg n$ . The predictor vectors are collected in the rows of the predictor matrix  $X \in \mathbb{R}^{n \times p}$ .

## 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 such as sure independence screening (SIS), proposed by Fan and Lv (2007), use the vector of marginal empirical correlations  $\hat{\omega} = (\omega_1, \dots, \omega_p)^{\top} \in \mathbb{R}^p, \omega_j = \operatorname{Cor}(X_j, y)$ , where y is the  $(n \times 1)$  vector of responses and  $X_j$  is the j-th column of the matrix of predictors, 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  $[p] = \{1, \dots, p\}$ . Under certain technical conditions, this screening coefficient has the sure screening property  $\mathsf{P}(\mathcal{A} \subset \mathcal{A}_{\gamma_n}) \to 1$  for  $n \to \infty$ , where  $\mathcal{A} = \{j \in [p] : \beta_j \neq 0\}$  is the set of truly active variables. Extensions to SIS include modifications for GLMs (Fan and Song 2010), where screening is performed based on the log-likelihood  $\ell(.)$  or the slope coefficient of the GLM containing only  $X_j$  as a predictor:  $\hat{\omega}_j =: \operatorname{argmin}_{\beta \in \mathbb{R}} \min_{\beta_0 \in \mathbb{R}} \sum_{i=1}^n -\ell(\beta_j, \beta_0; y_i, x_{ij})$ , where  $x_{ij}$  is the j-th entry of the vector  $x_i$ .

However, both mentioned approaches face limitations related to the required technical conditions which can rule 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. Additionally, 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 where the effect of other variables is reduced. 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), 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 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. 2024a).

#### 2.2. Random projection tools

spar has been designed to allow the incorporation of various random projection techniques, enabling users to tailor the procedure to their specific data needs. Below, we provide background information on random projection techniques and an overview of possible choices for building such random projection matrices.

The random projection method relies on the Johnson-Lindenstrauss (JL) lemma (Johnson and Lindenstrauss 1984), which asserts that for each set of points in p-dimensional Euclidean space collected in the rows of  $X \in \mathbb{R}^{n \times p}$  there exists a linear map  $\Phi \in \mathbb{R}^{m \times p}$  such that all pairwise distances are approximately preserved within a factor of  $(1 \pm \epsilon)$  for  $m \ge m_0 = \mathcal{O}(\epsilon^{-2} \log(n))$ . 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 with high probability should be chosen such that it fulfills certain technical conditions 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 where  $\Phi_{ij} \stackrel{iid}{\sim} N(0,1/\sqrt{\psi})$  with probability  $\psi$  and 0 otherwise (Matoušek 2008). Another computationally simpler option is the Rademacher distribution where  $\Phi_{ij} = \pm 1/\sqrt{\psi}$  with probability  $\psi/2$  and zero otherwise for  $0 < \psi \le 1$ , where Achlioptas (2003) shows results for  $\psi = 1$  and  $\psi = 1/3$  while Li et al. (2006) recommend using  $\psi = 1/\sqrt{p}$  to obtain very sparse matrices.

Further approaches include using the Haar measure to generate random orthogonal matrices (Cannings and Samworth 2017) or a non-sub-Gaussian distribution like the standard Cauchy, proposed by Li *et al.* (2006) for preserving approximate  $\ell_1$  distances in settings where the data is high-dimensional, non-sparse, and heavy-tailed. Structured matrices, which allow for more efficient multiplication, have also been proposed (see e.g., Ailon and Chazelle 2009; Clarkson and Woodruff 2013).

The conventional random projections mentioned above are data-agnostic. However, recent work has proposed incorporating information from the data either to select the "best" random projection or to directly inform the random projection procedure. For example, Cannings and Samworth (2017) build an ensemble classifier where the random projection matrix is chosen 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. (2024a) 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. Parzer, Filzmoser, and Vana-Gür (2024b) also provide in the linear regression a theoretical bound on the expected gain in prediction error in using a projection which incorporates information about the true  $\beta$  coefficients compared to a conventional random projection. Motivated by this result, they propose to construct a projection matrix using the sparse embedding matrix of Clarkson and Woodruff (2013), where the random diagonal elements are replaced in practice by a ridge coefficient with a minimal  $\lambda$  penalty. This method has the advantage of allowing the regression coefficients to be recovered after the projection, which is in general not possible with conventional random projections (Thanei et al. 2017).

Moreover, 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.

#### 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 response having conditional density from a (reproductive) exponential dispersion family of the form

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

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:

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

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

## 2.4. SPAR algorithm

We present the general algorithm for sparse projected averaged regression (SPAR) implemented in package **spar**.

- 1. Choose family with corresponding log-likelihood  $\ell(.)$  and link.
- 2. Standardize the  $(n \times p)$  matrix of predictors X for all families and the vector of responses y for the Gaussian family by subtracting the sample column mean and dividing by the sample standard deviation.
- 3. Calculate screening coefficients  $\hat{\omega}$ .
- 4. For  $k=1,\ldots,M$  models: a. If p>2n, screen 2n predictors based on the screening coefficient  $\hat{\omega}$ , which yields for model k the screening index set  $I_k=\{j_1^k,\ldots,j_{2n}^k\}\subset [p];$  if probabilistic screening should be employed draw the predictors sequentially without replacement using an initial vector of probabilities  $p_j\propto |\hat{\omega}_j|$ . Otherwise, select the 2n variables with the highest  $|\hat{\omega}_j|$ . If p<2n, perform no screening and  $I_k=\{1,\ldots,p\}$ . b. project screened variables to a random dimension  $m_k\sim \text{Unif}\{\log(p),\ldots,n/2\}$  using **projection matrix**  $\Phi_k$  to obtain  $Z_k=X_{\cdot I_k}\Phi_k^{\top}\in\mathbb{R}^{n\times m_k}$ , where  $X_{\cdot I_k}$  contains the columns in X having a column index in  $I_k$ . c. fit a  $(L_2$  penalized) **GLM** of y on  $Z_k$  to obtain estimated coefficients  $\hat{\gamma}^k\in\mathbb{R}^{m_k}$  and  $\hat{\beta}_{I_k}^k=\Phi_k^{\top}\hat{\gamma}^k,\,\hat{\beta}_{\bar{I}_k}^k=0$ .
- 5. For a given threshold  $\nu > 0$ , set all  $\hat{\beta}_j^k$  with  $|\hat{\beta}_j^k| < \nu$  to 0 for all j, k.
- 6. Choose M and  $\nu$  via a validation set or cross-validation by repeating steps 1 to 4 and employing a loss function on the test set  $K(M, \nu)$

$$(M_{\mathrm{best}},\nu_{\mathrm{best}}) = \mathrm{argmin}_{M,\nu} K(M,\nu)$$

- 7. Combine models of the ensembles via the coefficients using **simple average**  $\hat{\beta} = \sum_{k=1}^{M} \hat{\beta}^k / M$ .
- 8. Output the estimated coefficients and predictions for the chosen M and  $\nu$ .

## 3. Software

The package can 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 the example data set from the package which contains n=200 observations of a continuous response y and p=2000 predictors x which can be used as a training data set and n=100 observations to be used as a test set.

```
R> data("example_data", package = "spar")
R> str(example_data)
```

```
#> List of 7
#> $ x     : num [1:200, 1:2000] 1.8302 -0.4251 -1.3893 -0.0947 0.4304 ...
#> $ y     : num [1:200] -5.64 -23.63 -17.09 13.18 20.91 ...
#> $ xtest : num [1:100, 1:2000] -0.166 -0.3729 0.0379 0.6774 0.2174 ...
#> $ ytest : num [1:100] 10.61 -34.1 29.3 35.53 8.67 ...
#> $ mu     : num 1
#> $ beta : num [1:2000] 1 -2 3 2 1 -3 2 3 1 -2 ...
#> $ sigma2: num 83
```

This data set has been simulated from a linear regression model with  $\sigma^2 = 83$ , an intercept  $\mu = 1$  and  $\beta$  coefficients with 100 non-zero entries, where the non-zero entries are uniformly sampled from  $\{-3, -2, -1, 1, 2, 3\}$ .

## 3.1. Main functions and their arguments

The two main functions for fitting the SPAR algorithm are:

```
spar(x, y, family = gaussian("identity"), model = spar_glmnet(),
  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

```
spar.cv(x, y, family = gaussian("identity"), model = spar_glmnet(), rp = NULL, screencoef
  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:

- $\mathbf{x}$  an  $n \times p$  numeric matrix of predictor variables,
- y numeric response vector of length n,
- family object from stats::family(); defaults to gaussian();
- model an object of class 'sparmodel' which specifies the model employed for each element of the ensemble, defaults to a penalized GLM using spar\_glmnet();
- rp an object of class 'randomprojection', defaults to rp\_cw(data=TRUE);
- screencoef an object of class 'screencoef', defaults to screen\_glmnet();
- 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 quantiles of the absolute values of the estimated coefficients from the marginal models, chosen to be equally spaced on the probability scale.

- 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()). The default value for measure is "deviance", which is available for all families. Other options are mean squared error "mse" or mean absolute error "mae" (between responses and predicted conditional 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  $\nu_{\rm best}$  and  $M_{\rm best}$ . 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, which are generated by first calling spar() on the whole dataset, before starting the cross-validation procedure. However, it is possible to specify whether the data associated with the random projection (relevant for data-driven random projections) should be updated in each fold iteration with the corresponding training data. This is achieved by modifying elements of the 'randomprojection' object, which we will exemplify in Section 4.

#### 3.2. Screening coefficients

The objects for creating screening coefficients are implemented as S3 classes 'screencoef'. These objects are created by several implemented screen\_\* functions, which take ... and a list of controls control as arguments.

Consider as an example function screen\_marglik which implements a screening procedure based on the coefficients of univariate GLMs:

```
R> screen_marglik
#> function(..., control = list()) {
#> out <- list(name = name,
#> generate_fun = generate_fun,
#> control = control)
```

```
#>
       attr <- list2(...)</pre>
       attributes(out) <- c(attributes(out), attr)</pre>
#>
       if (is.null(attr(out, "type"))) {
#>
         attr(out, "type") <- "prob"
#>
       } else {
#>
         stopifnot(
#>
            "'type' must be either 'prob' or 'fixed'." =
#>
              (attr(out, "type") == "prob" | attr(out, "type") == "fixed")
#>
          )
#>
       }
#>
       class(out) <- c("screencoef")</pre>
#>
#>
       return(out)
#>
     }
#> <bytecode: 0x11c7acd68>
#> <environment: 0x11c7a4cf8>
```

Arguments related to the screening procedure can be passed through ..., and will be saved as attributes of the 'screencoef' object. More specifically, the following attributes are relevant for 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 marginal models in the SPAR algorithm; defaults to NULL. In this case the whole data will be used for estimating the screening coefficient and the marginal models.
- 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".

The control argument, on the other hand, is a list containing extra parameters to be passed to the main function computing the screening coefficients.

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

• screen\_marglik() - computes the screening coefficients by the coefficient of  $x_j$  for  $j=1,\ldots,p$  in a univariate GLM using the stats::glm() function.

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

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.* 2024a, for clarification).

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

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. This screening coefficient is used as a default if screencoef=NULL in function call of spar() or spar.cv().

All implemented screen\_\* functions return an object of class 'screencoef' which in turn is a list with three elements:

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

For illustration purposes, consider the object created by calling screen marglik():

```
R> obj <- screen_marglik()</pre>
```

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

```
R> obj
#> Name: screen marglik
#> Main attributes:
#> * proportion of data used for screening: 1
#> * number of screened variables: not provided, will default to 2n
#> * type: probabilistic screening
#> * screening coefficients: not yet computed from the data.
The structure of the object is the following:
R> unclass(obj)
#> $name
#> [1] "screen_marglik"
#>
#> $generate_fun
#> function(y, x, object) {
     if (is.null(object$control$family)) {
#>
       object$control$family <- attr(object, "family")</pre>
#>
#>
     coefs <- apply(x, 2, function(xj){</pre>
#>
```

```
#>
       glm_res <- do.call(function(...) glm(y ~ xj, ...),</pre>
#>
                            object$control)
#>
       glm_res$coefficients[2]
#>
     })
#>
     coefs
#> }
#> <environment: namespace:spar>
#>
#> $control
#> list()
#>
#> attr(,"type")
#> [1] "prob"
```

Function generate\_fun() defines the generation of the screening coefficient. Note that it considers the controls in object\$control when calling the stats::glm() function (unless it is provided, the family argument in stats::glm() will be set to the "global" family of the SPAR algorithm which is assigned inside the spar() function an attribute for the screencoef object).

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.

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.
- 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 existing results which give a lower bound on the goal dimension in order to preserve the distances between all pairs of points within a factor  $(1 \pm \epsilon)$ . For example, Achlioptas (2003) show  $m_0 = \log n(4 + 2\tau)/(\epsilon^2/2 - \epsilon^3/3)$  for probability  $1 - n^{-\tau}$ .

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

• rp\_gaussian() - random projection object where the generated matrix will have iid 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 2013) 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. (2024a).

The rp\_\* 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 arguments rp, which is itself a 'randomprojection' object, m, the target dimension and a vector of indices included\_vector which indicates 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 can return a matrix or a sparse matrix of class "dgCMatrix" of the Matrix with m rows and length(included\_vector) columns.
- update\_data\_rp optional function used for data-driven random projections, which updates the 'randomprojection' object with data information which is relevant for the random projection. The updating happens only once, before the start of the SPAR algorithm, where appropriate attributes are added to the 'randomprojection' object. All relevant quantities are to be used in the generate\_fun() function. This function should have arguments rp, which is a 'randomprojection' object to be updated, x the matrix of standardized predictors and y the vector of (standardized in the Gaussian case) responses. Returns a randomprojection object.
- 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. While update\_data\_rp is employed only once at the start of the algorithm, update\_rpm\_w\_data specifies how to modify each random projection provided in RPMs. This is particularly relevant for the cross-validation procedure, which employs the random projection matrices generated by calling the spar() function on the whole dataset before starting the cross-validation exercise. For example, in our implementation of the data-driven rp\_cw(), we only update RPMs by adjusting with the vector of screening coefficients computed on the current training data in each fold, but do not modify the random elements in each fold, to reduce the computational burden. Defaults to NULL. If not provided, the values of the provided RPMs do not change.
- control, which is the control list in rp\_\*. These controls are arguments needed in generate\_fun() in order to generate the desired random projection.

For illustration purposes, consider the implemented function rp\_gaussian, which is a random projection with entries drawn from the normal distribution. The print method returns key information about the random projection procedure.

```
R> obj <- rp_gaussian()
R> obj
```

```
#> Name: rp_gaussian
#> Main attributes:
#> * Data-dependent: FALSE
#> * Lower bound on goal dimension m: not provided, will default to log(p).
* * Upper bound on goal dimension m: not provided, will default to n/2.
We turn to looking at the structure of the object:
R> unclass(obj)
#> $name
#> [1] "rp_gaussian"
#>
#> $generate_fun
#> function(rp, m, included_vector) {
     p <- length(included_vector)</pre>
#>
     control_rnorm <-</pre>
#>
#>
       rp$control[names(rp$control) %in% names(formals(rnorm))]
     vals <- do.call(function(...)</pre>
#>
       rnorm(m * p, ...), control_rnorm)
#>
#>
     RM <- matrix(vals, nrow = m, ncol = p)
#>
     return(RM)
#> }
#> <environment: namespace:spar>
#>
#> $update_data_fun
#> NULL
#>
#> $update_rpm_w_data
#> NULL
#>
#> $control
#> list()
#> attr(,"data")
#> [1] FALSE
```

The generate\_fun() function returns a matrix with m rows and length(included\_vector) columns. Note that included\_vector gives the indices 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 element update\_data\_fun and update\_rpm\_w\_data are NULL as this conventional random projection is data-agnostic.

#### 3.4. Marginal models

The package provides a class 'sparmodel' for the marginal model to be fitted for each element of the ensemble. The framework currently assumes that the linear predictor is a linear

combination of the projected variables.

Similar to the objects for random projection and screening coefficients, the functions which create these objects have ... (to be saved as attributes) and control (to be used in the main function for building the model).

The two functions implemented are spar\_glmnet, which allows regularized GLMs as marginal models (by default using a ridge penalty with the minimal penalty provided by function glmnet::glmnet()), and spar\_glm() which estimates unregularized GLMs using stats::glm.fit().

An object of class 'sparmodel' is a list with elements:

- name.
- model\_fun a function which takes y (the vector of standardized responses), z (the matrix of reduced predictors) and a further argument which is the object of class 'sparmodel' itself.
- update\_model an optional function which can add further attributes to the 'sparmodel' object which is called at the beginning of the SPAR algorithm. In the case of spar\_glmnet() this function manipulates the 'family' object in a way which is convenient for glmnet::glmnet().

#### 3.5. Methods

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

print

The print method returns information on  $\nu_{\rm best}$   $M_{\rm best}$ , 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.

```
R> spar_res <- spar(example_data$x, example_data$y,</pre>
                  xval = example_data$xtest,
                  yval = example_data$ytest,
                  nummods = c(5,10,15,20,25,30))
R> spar_cv <- spar.cv(example_data$x, example_data$y,
                    nummods = c(5,10,15,20,25,30))
R> spar_res
#> spar object:
#> Smallest Validation Measure reached for nummod=30,
#>
                 nu=1.70e-02 leading to 956 / 2000 active predictors.
#> Summary of those non-zero coefficients:
       Min.
             1st Qu.
                       Median
                                   Mean 3rd Qu.
                                                     Max.
#> -1.00560 -0.06818
                      0.02037
                                0.02954 0.11796
```

<sup>&</sup>lt;sup>1</sup>In the case of families Gaussian, binomial and Poisson with canonical link, the family object is replaced by a string containing the name of the family. This leads to [glmnet].pkg using the specialized algorithm rather than the general algorithm implemented for all [family].class objects.

```
R> spar_cv
#> spar.cv object:
#> Smallest CV-Meas 2238.8 reached for nummod=15,
                 nu=0.00e+00 leading to 1656 / 2000 active predictors.
#> Summary of those non-zero coefficients:
       Min. 1st Qu.
#>
                       Median
                                  Mean 3rd Qu.
                                                    Max.
#> -0.66958 -0.04925 0.00890 0.02044 0.07815 0.97138
#>
#> Sparsest coefficient within one standard error of best CV-Meas
#>
                 reached for nummod=5, nu=8.09e-03
#> leading to 882 / 2000 active
#>
                 predictors with CV-Meas 2807.5.
#> Summary of those non-zero coefficients:
#>
       Min. 1st Qu.
                       Median
                                  Mean 3rd Qu.
                                                    Max
#> -0.99769 -0.11765  0.06234  0.03665  0.17299  1.09612
```

## coef

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))
#> List of 4
#> $ intercept: num 2.78
#> $ beta : num [1:2000] 0 0 0.418 0 0 ...
#> $ nummod : num 30
#> $ nu : num 0.017
```

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 yielding sparsest vector of coefficients 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 the plot method, which takes a spar or spar.cv object, together with further arguments:

- 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"); for plot\_type = "Val\_Measure" or plot\_type = "Val\_numAct" it indicates whether the values of the cross-validation measure or number of active variables, respectively, should be shown for a grid of  $\nu$  values while keeping the number of models nummod fixed or viceversa. This argument is 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  $\nu$  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. This argument must be provided for the plot of residuals and fitted values, 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. This argument must be provided for the plot of residuals and fitted values, 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", "1se") 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 combination which delivers the sparsest  $\beta$  having validation measure within one standard deviation from the minimum

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

## 4. Extensibility

#### 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(y, x, object) {
+ res_screen <- do.call(function(...)
+ VariableScreening::screenIID(x, 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 the helper 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 the 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.

```
R> set.seed(123)
R> spar_example <- spar(example_data$x, example_data$y,</pre>
     screencoef = screen_sirs(type = "fixed",
       control=list(method = "SIRS")),
                    measure = "mse")
R> spar_example
#> spar object:
#> Smallest Validation Measure reached for nummod=20,
#>
                 nu=1.75e-03 leading to 396 / 2000 active predictors.
#> Summary of those non-zero coefficients:
#>
         Min.
                 1st Qu.
                              Median
                                           Mean
                                                    3rd Qu.
#> -0.6918230 -0.0928444 0.0009116 0.0943062
                                                 0.1777889
                                                            2.0089709
```

## 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 the 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, x, y) {
+ attr(rp, "data") <- list(x, y)
+ rp
+}</pre>
```

This is 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 <code>generate\_fun</code> 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) {
+ R0 <- matrix(1/sqrt(p) * rnorm(p * m), nrow = p, ncol = m)</pre>
```

```
+ RM <- qr.Q(qr(R0))[, seq_len(m)]
+ RM <- Matrix::Matrix(t(RM), sparse = TRUE)
+}</pre>
```

The function that generates the random projection matrix for model k uses 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:

```
R> generate_cannings <- function(rp, m, included_vector) {</pre>
     p <- length(included_vector)</pre>
     if (is.null(rp$control$B2)) rp$control$B2 <- 50</pre>
     x <- attr(rp, "data")$x[, included_vector]</pre>
     y <- attr(rp, "data")$y
     B2 <- rp$control$B2
     n \leftarrow nrow(x)
     id_{test} \leftarrow sample(n, size = n \%/\% 4)
     xtrain <- x[-id_test, ]; xtest <- x[id_test,]</pre>
     ytrain <- y[-id_test]; ytest <- y[id_test]</pre>
     if (is.null(rp$control$family)) rp$control$family <- attr(rp, "family")</pre>
     family <- rp$control$family
     control_glm <-
        rp$control[names(rp$control) %in% names(formals(glm.fit))]
     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 <- (cbind(1, tcrossprod(xtest, RM)) %*% mod$coefficients)
       pred <- family$linkinv(as.vector(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))</pre>
    RM <- error_all[[id_best]][[1]]</pre>
    return(RM)
+}
```

In the cross-validation procedure, we do not generate new matrices for each step to keep computational costs low, so we do not specify a function update\_rpm\_w\_data.

Putting it all together, we get:

```
R> rp_cannings <- constructor_randomprojection(</pre>
```

```
+ "rp_cannings",
+ generate_fun = generate_cannings,
+ update_data_fun = update_data_cannings
+)
We can now estimate SPAR for a binomial model.
```

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> set.seed(123)
R> spar_example_1 <- spar(</pre>
+ x = example_data$x, y=ystar,
+ xval = example_data$xtest, yval = ystarval,
+ family = binomial(),
+ nummods = 100,
+ screencoef = screen_marglik(nscreen = ncol(example_data$x)),
+ rp = rp_cannings(control = list(B2 = 50)),
+ measure = "class"
+)
Using the data-driven rp_cw():
R> set.seed(123)
R> spar_example_2 <- spar(x = example_data$x, y = ystar,
+ 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)
#>
                 nu nummod numAct Meas
    nnu
      1 0.000000000
                       100
                             2000 0.19
#> 1
#> 2
     2 0.002514423
                       100
                             2000 0.19
100
                             2000 0.19
100
                             2000 0.19
#> 5
                       100
                             2000 0.19
      5 0.010181484
#> 6
      6 0.012843941
                     100
                             2000 0.20
```

We can compare the two approaches by looking at the minimum measure Meas achieved on the validation set:

```
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))
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> spar example 1$val res[id best 1, ]
                 nu nummod numAct Meas
#>
     nnu
#> 9
       9 0.02132582
                        100
                              2000 0.18
R> spar_example_2$val_res[id_best_2, ]
                 nu nummod numAct Meas
#> 8
       8 0.01035825
                        100
                              1718 0.16
```

## 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>2</sup>

We can visualize one observation in this data set in Figure 1 (code for reproducing the figure is provided in the supplementary materials).

This data set has the issue of many columns being almost constant, which can make estimation unstable. Given that <code>spar()</code> and <code>spar.cv()</code> ignore constant columns, we can alleviate this issue by setting all columns which have a low standard deviation to zero.

```
R> x[, apply(x, 2, sd) < 0.01] <- 0
```

We split the data into training vs test sample

```
R> set.seed(123)
R> ntot <- length(y); ntest <- ntot * 0.25
R> testind <- sample(ntot, ntest, replace = FALSE)
R> xtrain <- as.matrix(x[-testind, ]); ytrain <- y[-testind]</pre>
```

 $<sup>^2{\</sup>rm The~Isomap}$  face data can be found online on https://web.archive.org/web/20160913051505/http://isomap.stanford.edu/datasets.html.

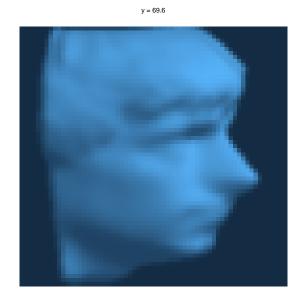


Figure 1: Image corresponding to one observation in the *Isomap faces* data set.

#### R> xtest <- as.matrix(x[testind, ]); ytest <- y[testind]</pre>

and estimate on the training data the SPAR algorithm with cross-validation. We employ the data-driven random projection proposed in Parzer *et al.* (2024b) with screening based on the ridge coefficients. To ensure convergence of the **glmnet** algorithm, we set the lambda.min.ratio parameter to 0.001.

```
R> library("spar")
R> set.seed(123)
R> spar_faces <- spar.cv(</pre>
  xtrain, ytrain,
   screencoef = screen_glmnet(control = list(lambda.min.ratio = 0.001)),
   rp = rp_cw(data = TRUE,
              control = list(lambda.min.ratio = 0.001)),
  nummods = c(5, 10, 20, 50),
  measure = "mse")
R> spar_faces
#> spar.cv object:
#> Smallest CV-Meas 12.9 reached for nummod=20,
#>
                 nu=0.00e+00 leading to 3421 / 4096 active predictors.
#> Summary of those non-zero coefficients:
#>
         Min.
                 1st Qu.
                              Median
                                           Mean
                                                   3rd Qu.
                                                                  Max.
#> -21.200344 -0.110813
                           0.000345
                                                  0.116550 11.707854
                                       0.028759
#>
#> Sparsest coefficient within one standard error of best CV-Meas
                 reached for nummod=5, nu=5.08e-03
#> leading to 1413 / 4096 active
                 predictors with CV-Meas 18.5.
#>
```

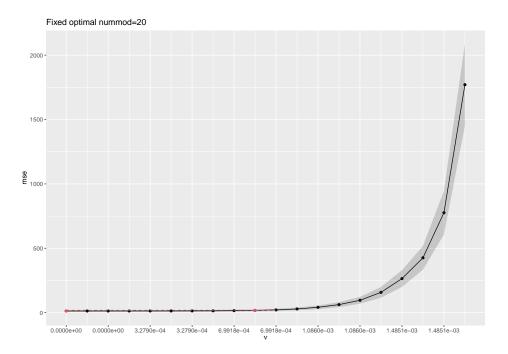


Figure 2: Plot of mean squared error over a grid of threshold values  $\nu$  for fixed number of optimal models M=20 for the *Isomap faces* data set. The red points correspond to the threshold which achieves the lowest cross-validation measure and the one with the largest cross-validation measure within one standard deviation away from minimum. Confidence bands represent one standard deviation in the measures across the number of folds.

```
#> Summary of those non-zero coefficients:
#> Min. 1st Qu. Median Mean 3rd Qu. Max.
#> -20.35394 -0.46454 -0.06084 0.06864 0.51548 17.15842
```

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 (see Figure 2).

#### R> plot(spar\_faces)

We observe that no thresholding delivers the lowest MSE but that using thresholds between 7e-4 and 1.1e-3 does not cause a large increase in MSE. The 1-standard-error rule would suggest picking  $\nu=0.00508$ .

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)
#> List of 4
#> $ intercept: num -23.7
#> $ beta : num [1:4096] 0 0.1369 0.1401 -0.0157 -1.3096 ...
#> $ nummod : num 20
#> $ nu : num 0
```

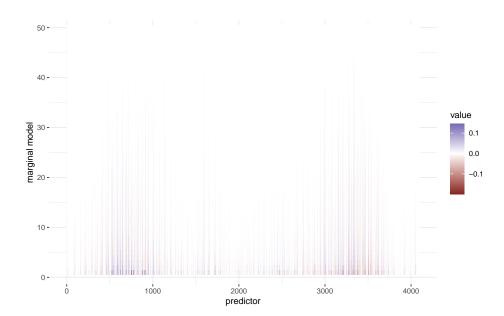


Figure 3: Coefficient plot for all variables and all M = 50 models in the SPAR ensemble for the *Isomap faces* data set. The coefficients are standardized, before thresholding.

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

```
R> face_coef_1se <- coef(spar_faces, opt_par = "1se")
R> str(face_coef_1se)
#> List of 4
#> $ intercept: num -23.7
#> $ beta : num [1:4096] 0 0 0 0 -1.9 ...
#> $ nummod : num 5
#> $ nu : num 0.00508
```

The standardized coefficients from each of max(nummods) models (before averaging and before thresholding) can be plotted by setting plot\_type = "coefs" (see resulting plot in Figure~3).

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

We observe that pixels close to each other have more correlation than pixels further apart.

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
#> [1] 0.02048181
```

Additionally, for this data set, one can visualize the effect of each pixel  $\hat{\beta}_j^{\text{1se}} x_{i,j}^{\text{new}}$  in predicting

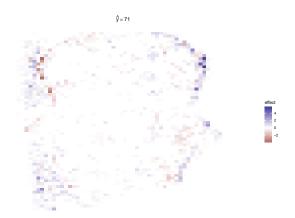


Figure 4: The effect of each pixel  $\hat{\beta}_j^{\text{1se}} x_{i,j}^{\text{new}}$  in predicting the face orientation in Figure 1.

the face orientation in a given image e.g., the 11th one in the test set. The contribution of each pixel can be visualized in Figure 4.

#### 5.2. Darwin data set

The structure of the data is:

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>3</sup>

```
R> download.file("https://archive.ics.uci.edu/static/public/732/darwin.zip",
+ "darwin.zip")
R> darwin_tmp <- read.csv(unzip("darwin.zip", "data.csv"),
+ stringsAsFactors = TRUE)</pre>
```

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,
+ silent = TRUE))
#>
#> The final data set we will analyze has 174 rows and 446 columns.
#>
R> darwin <- list(x = tmp$Ximp, y = darwin_orig$y)</pre>
```

<sup>&</sup>lt;sup>3</sup>The data set can be downloaded from https://archive.ics.uci.edu/dataset/732/darwin

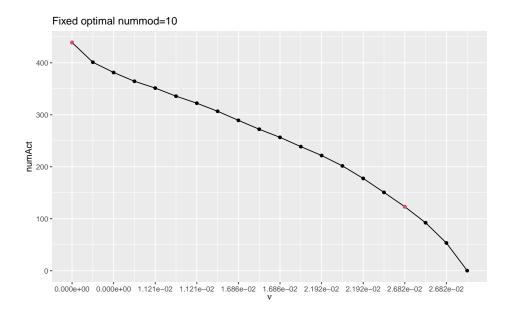


Figure 5: Average number of active variables for the grid of thresholding values  $\nu$  and M=10 models for the *Darwin* data set. The red points correspond to the average number of active variables for the model with the lowest cross-validation measures and to the one chosen by the 1-standard-error rule.

```
R> str(darwin)
#> List of 2
#> $ x: num [1:174, 1:450] 5160 3721 2600 2130 2310 ...
#> ... attr(*, "dimnames")=List of 2
#> ... $: NULL
#> ... $: chr [1:450] "air_time1" "disp_index1" "gmrt_in_air1" "gmrt_on_paper1" ...
#> $ y: num [1:174] 1 1 1 1 1 1 1 1 1 1 ...
```

We estimate the SPAR algorithm with the screening and random projection introduced in Parzer *et al.* (2024a) 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 5). We observe again that no thresholding achieves the best measure and translates to almost all variables being active (some variables can be inactive at  $\nu=0$  as they may never be screened). The 1-standard-error rule would however indicate that more sparsity can be introduced without too much increase in the cross-validation measure.

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

The coefficients of the predictors across the maximum number of considered marginal models

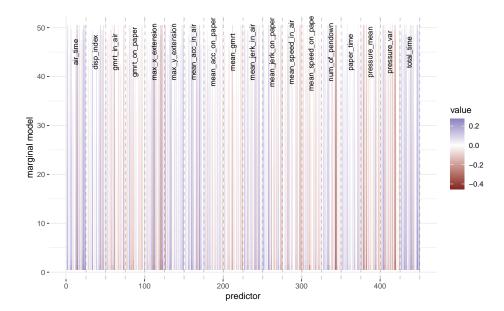


Figure 6: Coefficient plot for all variables and all considered M = 50 models in the SPAR ensemble *Darwin* data set. The coefficients are standardized, before thresholding.

(in this case M=50) can be visualized with plot. In the dataset, 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 for plotting by grouping them by feature, rather than task. This allows to assess how the different features (e.g., time it takes to complete a certain task) relate to the likelihood of having AD and how stable the sign and magnitude of the coefficient is across the models in the ensemble. We can achieve this by using reordering argument coef\_order in method plot\_type = "coefs" (see Figure 6 which can be reproduced with code in the supplementary materials).

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 an algorithm for sparse projected and average regression (SPAR) proposed in Parzer et al. (2024a) which combines variable screening and random projection in an ensemble of GLMs. The package provides flexible classes for i) specifying the coefficient based on which screening should be performed (both in a classical fashion, where the predictors with the highest screening coefficient are selected for subsequent or in a probabilistic fashion, where variables are sampled for inclusion with probabilities proportional to their screening coefficient), ii) generating the random projection to be employed in each marginal model. Screening coefficients based on marginal correlation between the predictors and the response, marginal coefficients from a GLM or ridge coefficients are provided in the package. Moreover,

several random projections are implemented: the Gaussian and sparse matrices which are data-agnostic and satisfy the JL lemma and the data-driven projection proposed in Parzer et al. (2024b) for linear regression and extended to GLMs in Parzer et al. (2024a). This data-driven random projection has the advantage of allowing the regression coefficients to be recovered after the projection, which is in general not possible with conventional random projections (Thanei et al. 2017). Methodologically, the SPAR algorithm particularly when paired with the data-driven random projection in Parzer et al. (2024a) has been demonstrated to perform effectively across different degrees of sparsity of the coefficient vector and to offer competitive predictions and variable ranking in both sparse and dense settings.

The flexibility and adaptability of the **spar** package make it an attractive choice for practitioners and researchers. It encourages exploration of new methods for variable screening and random projections or the combination of existing approaches to tailor solutions to specific data requirements.

## Computational details

The results in this paper were obtained using R 4.4.0.

R itself and all packages used are available from CRAN at https://CRAN.R-project.org/.

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