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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 package for building predictive generalized linear models (GLMs) with high-dimensional (HD) predictors in R. In package **SPAR**, probabilistic variable screening and random projection of the predictors are performed to obtain an ensemble of GLMs, which are then averaged to obtain predictions in an high-dimensional regression setting.

Random projection is a computationally-efficient method which linearly maps a set of points in high dimensions into a much lower-dimensional space while approximately preserving pairwise distances. For very large p, random projection 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).

Several packages which provide functionality for random projections are available for 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.

On the other hand, there are a multitude of packages dealing with variable screening on the Comprehensive R Archive Network (CRAN). The (iterative) sure independence screening procedure and extensions in Fan and Lv (2007), Fan and Song (2010), Fan, Feng, and Wu (2010) are implemented in package **SIS** (Saldana and Feng 2018), 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: Sure Independent Ranking and Screening – which ranks the predictors by their correlation with the rank-ordered response (SIRS), Distance Correlation Sure Independence Screening – a non-parametric extension of the correlation coefficient (DC-SIS), MV Sure Independence Screening – using the mean conditional variance measure (MV-SIS).

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). Package **tilting** (Cho and Fryzlewicz 2016) implements an algorithm for variable selection in high-dimensional linear regression using tilted correlation, which takes into account high correlations among the variables in a data-driven way. Feature screening based on conditional distance correlation (Wang, Pan, Hu, Tian, and Zhang 2015) can be performed with the **cdcsis** package (Hu, Huang, Pan, Wang, Wen, Tian, Zhang, and Zhu 2024) while package **QCSIS** (Ma, Zhang, and Zhou 2015) implements screening based on (composite) quantile correlation.

Package **LqG** (Wu, Li, and Li 2022) provides a group screening procedure that is based on maximum Lq-likelihood estimation, to simultaneously account for the group structure and data contamination in variable screening.

Feature screening using an $L1$ fusion penalty can be performed with package **fusionclust** (Banerjee, Mukherjee, and Radchenko 2017). Package **SMLE** (Zang, Xu, and Burkett 2020) implements joint feature screening via sparse MLE (Xu and Chen 2014) in high-dimensional linear, logistic, and Poisson models. Package **TSGSIS** (Fang, Wang, and Hsiung 2017b) provides a high-dimensional grouped variable selection approach for detecting interactions that may not have marginal effects in high dimensional linear and logistic regression (Fang, Wang, and Hsiung 2017a).

Package **RaSEn** (Tian and Feng 2021) 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. Various choices of base classifiers are implemented, for instance, linear discriminant analysis, quadratic discriminant analysis, k-nearest neighbor, logistic or linear regression, decision trees, random forest, support vector machines. The selected percentages of variables can be employed for variable screening.

Package **Ball** (Zhu, Pan, Zheng, and Wang 2021) provides functionality for variable screening using ball statistics, which is appropriate for shape, directional, compositional and symmetric positive definite matrix data.

Package **BayesS5** (Shin and Tian 2020) implements Bayesian variable selection using simplified shotgun stochastic search algorithm with screening (Shin, Bhattacharya, and Johnson 2017) while package **bravo** (Li, Chakraborty, Dutta, and Roy 2024) implements the Bayesian iterative screening method proposed in (Wang, Dutta, and Roy 2021).

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

2.1. Variable screening

The general idea of variable screening is to select a (small) subset of variables, based on some marginal utility measure for the predictors, and disregard the rest for further analysis. In their seminal work on sure independence screening (SIS), Fan and Lv (2007) propose to use the vector of marginal empirical correlations $\hat{\alpha} = (\alpha_1, \dots, \alpha_p)' \in \mathbb{R}^p, \alpha_j = \text{Cor}(X_{.j}, y)$ for variable screening 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, where p grows exponentially with n, they show that this procedure has the *sure screening property*

$$\mathbb{P}(\mathcal{A} \subset \mathcal{A}_{\gamma_n}) \to 1 \text{ for } n \to \infty$$

with an explicit exponential rate of convergence, where $\mathcal{A} = \{j \in [p] : \beta_j \neq 0\}$ is the set of truly active variables. These conditions imply that $\mathcal{A}$ and $\mathcal{A}_{\gamma_n}$ contain less than n variables. One of the critical conditions is that on the population level for some fixed $i \in [n]$, $\min_{j\in\mathcal{A}} |\text{Cov}(y_i/\beta_j, x_{ij})| \geq c$ for some constant $c > 0$, which rules out practically possible scenarios where an important variable is marginally uncorrelated to the response. Fan and Song (2010) extend the approach to GLMs, where the screening is performed based on the log-likelihood of the GLM containing only X_j as a predictor: $\hat{\alpha}_j =: \min_{\beta_j\in\mathbb{R}} \sum_{i=1}^{n} -\ell(\beta; y_i, x_{ij})$.

A rich stream of literature focuses on developing semi- or non-parametric alternatives to SIS which should be more robust to model misspecification. For linear regression, approaches include using the ranked correlation (Zhu, Li, Li, and Zhu 2011), (conditional) distance correlation (Li, Zhong, and Zhu 2012; Wang *et al.* 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 $\mathsf{P}(X \leq x|Y)$ (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.

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.

2.2. Random projection

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 with $m < \mathcal{O}(\log n/\varepsilon^2)$ so that all pairwise distances are maintained within a factor of $1 \pm \varepsilon$, for any $0 < \varepsilon < 1$.

The random map Φ should be chosen such that it fulfills certain conditions (see Johnson and Lindenstrauss 1984). 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). Common choices are:

- Normal distribution.: $\Phi_{ij} \overset{iid}{\sim} N(0,1)$ (Frankl and Maehara 1988) or $\Phi_{ij} = \begin{cases} \sim N(0,1/\sqrt{\psi}) & \text{with prob. } \psi \\ 0 & \text{with prob. } 1-\psi \end{cases}$ (Matoušek 2008),
- Rademacher distribution (Achlioptas 2003; Li, Hastie, and Church 2006)

$$\Phi_{ij} = \begin{cases} \pm 1/\sqrt{\psi} & \text{with prob. } \psi/2 \\ 0 & \text{with prob. } 1-\psi, \quad 0 < \psi \leq 1, \end{cases},$$

  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.

Distributions which are not sub-Gaussian, such as standard Cauchy, have also been proposed in the literature to tackle scenarios where the data is high-dimensional, non-sparse, and heavy-tailed by preserving approximate ℓ_1 distances (see e.g., Li, Hastie, and Church 2007).

An orthonormalization is usually applied $(\Phi\Phi^\top)^{-1/2}\Phi$. Orthonormalization can constitute a computational bottleneck for the random projection method, however, in high-dimensions it can be omitted.

To speed computations, Ailon and Chazelle (2009) propose the fast Johnson- Lindenstrauss transform (FJLT), where the random projection matrix is given by $\Phi = PHD$ with P random and sparse, $P_{ij} \sim N(0, 1/q)$ with probability $1/q$ and 0 otherwise, H the normalized Hadamard (orthogonal) matrix $H_{ij} = p^{-1/2}(-1)^{\langle i-1,j-1\rangle}$, where $\langle i, j\rangle$ is the dot-product of the m-bit vectors i, j expressed in binary, and $D = \text{diag}(\pm 1)$ is a diagonal matrix with random elements D_{ii}.

Clarkson and Woodruff (2013) propose a sparse embedding matrix $\Phi = BD$, where $B \in \{0, 1\}^{m\times p}$ is random binary matrix and D is a $p \times p$ diagonal matrix with $(D_{ii} + 1)/2 \sim \text{Unif}\{0, 1\}$, and prove that the dimension m is bounded by a polynomial in $r\varepsilon^{-1}$ for $0 < \varepsilon < 1$ and r being the rank of X. While this is generally larger than that of FJLT, the sparse embedding matrix requires less time to compute ΦX compared to other subspace embeddings.

Parzer, Vana-Gür, and Filzmoser (2023) propose employing $D_{ii} = \hat{\alpha}$ in the sparse embedding matrix of Clarkson and Woodruff (2013), $\hat{\alpha}$ is a screening coefficient in the regression such as the ridge or the HOLP coefficients, and show that the proposed projection increases the predictive performance in a linear regression setting.

2.3. Algorithm

- choose family with corresponding log-likelihood $\ell(.)$ and link
- standardize predictors $X : n \times p$
- calculate screening coefficients $\hat{\alpha}$ e.g.,
  - ridge: $\hat{\alpha} =: \text{argmin}_{\beta\in\mathbb{R}^p} \sum_{i=1}^n -\ell(\beta; y_i, x_i) + \frac{\varepsilon}{2}\sum_{j=1}^p \beta_j^2$, $\varepsilon > 0$
  - marginal likelihood: $\hat{\alpha}_j =: \min_{\beta_j\in\mathbb{R}} \sum_{i=1}^n -\ell(\beta; y_i, x_{ij})$
- For $k = 1, \dots, M$ models:
  - draw $2n$ predictors with probabilities $p_j \propto |\hat{\alpha}_j|$ yielding screening index set $I_k = \{j_1^k, \dots, j_{2n}^k\} \subset [p]$
  - project remaining variables to dim. $m_k \sim \text{Unif}\{\log(p), \dots, n/2\}$ using **projection matrix** Φ_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, Narasimhan, and Hastie (2023)) to obtain estimated coefficients $\gamma^k \in \mathbb{R}^{m_k}$ and $\hat{\beta}_{I_k}^k = \Phi_k'\gamma^k$, $\hat{\beta}_{\bar{I}_k}^k = 0$.
- for a given threshold $\lambda > 0$, set all $\hat{\beta}_j^k$ with $|\hat{\beta}_j^k| < \lambda$ to 0 for all j, k
- *Optional:* choose M and λ via cross-validation by repeating steps 1 to 4 for each fold and evaluating a prediction performance measure on the withheld fold; and choose

$$(M_{\text{best}}, \lambda_{\text{best}}) = \text{argmin}_{M,\lambda}\text{Dev}(M, \lambda) \tag{1}$$

- combine via **simple average** $\hat{\beta} = \sum_{k=1}^M \hat{\beta}^k/M$

-
- output the estimated coefficients and predictions for the chosen M and λ

3. Software

The package be installed from GitHub

```
devtools::install_github("RomanParzer/SPAR")
```

and loaded by:

```
library("SPAR")
```

In this section we rely for illustration purposes on an example data set from the package:

```
data("example_data", package = "SPAR")
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
```

3.1. Main functions and their arguments

The two main functions for fitting the SPAR algorithm are:

```
spar(x, y, family = gaussian("identity"), rp = NULL, scrcoef = 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 2.3 without cross-validation and returns an object of class "`spar`", and

```
spar.cv(x, y, family = gaussian("identity"), rp = NULL, scrcoef = 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 type '`randomprojection`'
- `scrcoef` an object of type '`screeningcoef`'
- `nnu` is the number of threshold values ν which should be considered for thresholding; defaults to 20
- `nus` is an optional vector of ν 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 ν_{best} and M_{best}.
- `measure` gives the measure based on which the thresholding value ν_{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 ν_{best} and M_{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 "`screeningcoef`". 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 "`screeningcoef`" which in turn is a list with three elements:

- `name`,
- `generate_scrcoef` – an R function for generating the screening coefficient. This function should have the following arguments:

  - `scrcoef`, which is a "`screeningcoef`" 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_scrcoef` 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. It allows to pass a list of controls through the `control` argument to `stats::glm` such as weights, family, offsets.
- `screen_corr()` - 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_ridge()` - computes by default the ridge coefficient where the penalty λ is very small (see Parzer, Filzmoser, and Vana-Gür 2024, for motivation). 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`.

Further arguments related to screening can be passed through `...`, which will then be saved as attributes of the "`screeningcoef`" 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`, boolean which indicates whether 1/4 of the data should be used for computing the screening coefficient and the rest 3/4 for estimating the SPAR algorithm; defaults to `FALSE`
- `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.

```
unclass(screen_marglik())
#> $name
#> [1] "screen_marglik"
#>
#> $generate_scrcoef
#> function(scrcoef, data) {
#>   y <- data$y
#>   x <- data$x
#>   if (is.null(scrcoef$control$family)) {
#>     scrcoef$control$family <- attr(scrcoef, "family")
#>   }
#>   coefs <- apply(x, 2, function(xj){
#>     glm_res <- do.call(function(...) glm(y ~ xj,  ...),
#>                        scrcoef$control)
#>     glm_res$coefficients[2]
#>   })
#>   coefs
#> }
#> <environment: namespace:SPAR>
#>
#> $control
#> list()
#>
#> attr(,"split_data")
#> [1] FALSE
#> attr(,"type")
#> [1] "prob"
```

Function `generate_scrcoef_marglik` defines the generation of the screening coefficient. It considers the controls in `scrcoef$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 `screeningcoef` object. In `generate_scrcoef_marglik`, we employ `family` attribute of the "`screeningcoef`" object if the control list argument does not contain any particular family.

For convenience, a constructor function `constructor_screeningcoef()` is provided, which can be used to create new `screen_*` functions.

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 which take `...` and a list of controls `control` as arguments.

These functions return an object of class "`randomprojection`" which in turn is a list with three elements:

- `name`,
- `generate_rp_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 with `m` rows and `length(included_vector)` columns.

- `update_data_rp` function with attributes relying with information from the data. This is relevant for the data driven random projections. This function should have with arguments `rp`, which is a randomprojection object and `data`, which is a list containing `x` (the matrix of predictors used as input in `spar()` and `spar.cv`) and `y` the vector of responses.
- `update_rpm_w_data` function for updating the random projection matrix with data. This can be used for the case where a list of random projection matrices is provided by argument `RPMs`. In this case, the random structure is kept fixed, but the data-dependent part gets updated with the provided data. Defaults to NULL. If not provided, the values of the provided RPMs do not change.
- `control`, which is the control list in `screen_*`. These controls are arguments which are needed in `generate_scrcoef` in order to generate the desired screening coefficients.

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 are employed for all in "`randomprojection`" objects in function `spar()`:

- `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 $(1 \pm \epsilon)$: $m > \frac{24}{3\epsilon^2 - 2\epsilon^3} \log n$.

For illustration purposes, consider the implemented function `rp_gaussian`, which is a random projection with entries draws from the standard normal distribution.

```
rp_gaussian()
#> $name
#> [1] "rp_gaussian"
#>
#> $generate_rp_fun
#> function(rp, m, included_vector) {
#>   p <- length(included_vector)
#>   vals <- rnorm(m * p)
#>   RM <- matrix(vals, nrow = m, ncol = p)
#>   RM <- Matrix(RM, sparse = TRUE)
#>   return(RM)
#> }
#> <environment: namespace:SPAR>
#>
#> $update_data_fun
#> NULL
#>
#> $control
#> list()
#>
#> attr(,"use_data")
#> [1] FALSE
#> attr(,"class")
#> [1] "randomprojection"
```

Name	Random projection method
`gaussian`	Standard Gaussian
`sparse`	Rademacher
`cw`	sparse embedding matrix
`cwdatadriven`	data driven sparse embedding matrix

Table 1: Overview of implemented random projection matrices.

3.4. Methods

```
data("example_data")
spar_res <- spar(example_data$x, example_data$y,
                 xval = example_data$xtest,
                 yval = example_data$ytest,
                 nummods=c(5,10,15,20,25,30))
spar_res
#> SPAR object:
#> Smallest Validation Measure reached for nummod=30,
#>              nu=1.36e-02 leading to 1098 / 2000 active predictors.
#> Summary of those non-zero coefficients:
#>     Min.  1st Qu.   Median     Mean  3rd Qu.     Max.
#> -0.84883 -0.06693  0.01612  0.02765  0.12026  1.06543
```

Methods `print`, `plot`, `coef`, `predict` are available for both “`spar`” and “`spar.cv`” classes.

The `print` method return information on

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**.

```
generate_scr_sirs <- function(scrcoef, data) {
  res_screen <- do.call(function(...)
    VariableScreening::screenIID(data$x, data$y, ...),
    scrcoef$control)
  coefs <- res_screen$measurement
  coefs
}
```

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_screeningcoef`:

```
screen_sirs <- constructor_screeningcoef(
  "screen_sirs",
  generate_scrcoef = generate_scr_sirs)
```

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.

```
set.seed(123)
spar_example <- spar(example_data$x, example_data$y,
                     scrcoef = screen_sirs(type = "fixed",
                                           control=list(method = "SIRS")),
                     measure = "mse")
print(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.       Max.
#> -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 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,

```
update_data_cannings <- function(rp, data) {
  attr(rp, "data") <- data
  rp
}
generate_cannings <- function(rp, m, included_vector) {
  p <- length(included_vector)
  if (is.null(rp$control$B2)) rp$control$B2 <- 50
  x <- attr(rp, "data")$x[, included_vector]
  y <- attr(rp, "data")$y

  ## Sample for all B2 cases
  B2 <- rp$control$B2
  n <- nrow(x)
  id_test <- sample(n, size = n %/% 4)
  xtrain <- x[-id_test, ]
  xtest <- x[id_test,]
  ytrain <- y[-id_test]
  ytest <- y[id_test]
  ## Update with family argument of SPAR if not available
  if (is.null(rp$control$family)) {
    rp$control$family <- attr(rp, "family")
  }
  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){
    R0 <- matrix(1/sqrt(p) * rnorm(p * m), nrow = p, ncol = m)
    RM <- qr.Q(qr(R0))[, seq_len(m)]
    RM <- Matrix(t(RM), sparse = TRUE)
    xrp <- tcrossprod(xtrain, RM)
    mod <- do.call(function(...)
      glm.fit(x =  cbind(1, xrp), y = ytrain, ...), control_glm)
    eta_test <- drop(cbind(1, tcrossprod(xtest, RM)) %*% mod$coefficients)
    pred <- family$linkinv(eta_test)
    if (family$family == "binomial") {
      pred <- (pred > 0.5) + 0
      out <- mean(pred != ytest)
    } else {
      out <- mean((pred - ytest)^2)
    }
    list(RM, out)
  })
  id_best <- which.min(sapply(error_all, "[[", 2))
  RM <- error_all[[id_best]][[1]]
  return(RM)
}
```

```
rp_cannings <- constructor_randomprojection(
  "rp_cannings",
  generate_fun = generate_cannings,
  update_data_fun = update_data_cannings
)
```

We can now estimate SPAR

```
set.seed(123)
ystar <- ( example_data$y > 0 ) + 0
ystarval <- ( example_data$ytest > 0 ) + 0
spar_example_1 <- spar(
  x=example_data$x, y=ystar,
  xval = example_data$xtest, yval = ystarval,
  family = binomial(),
  nummods = 100,
  scrcoef = screen_marglik(type = "fixed"),
  rp = rp_cannings(control = list(B2 = 50))
)

spar_example_2 <- spar(x = example_data$x, y = ystar,
  family = binomial(),
  scrcoef = screen_marglik(type = "fixed"),
  rp = rp_cw(data = TRUE),
  nummods = 100,
  xval = example_data$xtest, yval = ystarval
)
spar_example_1$val_res
spar_example_2$val_res
```

5. Illustrations

5.1. Face image data

We illustrate the package on a data set containing $n = 698$ black and white face images of size $p = 64 \times 64 = 4096$ and the faces' horizontal looking direction angle as the response variable. The Isomap face data can be found online on https://web.archive.org/web/20160913051505/http://isomap. stanford.edu/datasets.html

```
library("R.matlab")
temp <- tempdir()
download.file("https://web.archive.org/web/20150922051706/http://isomap.stanford.edu/face_
system(sprintf('uncompress %s', paste0(temp, "/face_data.mat.Z")))
facedata <- readMat(file.path(temp, "face_data.mat"))

x <- t(facedata$images)
```

```
y <- facedata$poses[1,]
```

We can visualize e.g., the first observation in this data set by:

```
library(ggplot2)
i <- 1
ggplot(data.frame(X = rep(1:64,each=64),Y = rep(64:1,64),
                  Z = facedata$images[,i]),
       aes(X, Y, fill = Z)) +
  geom_tile() +
  theme_void() +
  ggtitle(paste0("y = ",round(facedata$poses[1,i],1))) +
  theme(legend.position = "none",
        plot.title = element_text(hjust = 0.5))
```

We can split the data into training vs test sample:

```
set.seed(1234)
ntot <- length(y)
ntest <- ntot * 0.25
testind <- sample(1:ntot, ntest, replace=FALSE)
xtrain <- as.matrix(x[-testind, ])
ytrain <- y[-testind]
xtest <- as.matrix(x[testind, ])
ytest <- y[testind]
```

We can now estimate the model on the training data:

```
library(SPAR)
spar_faces <- spar.cv(xtrain, ytrain,
                      family = gaussian(),
                      nummods = c(5, 10, 20, 50),
                      type.measure = "mse")
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 λ values, where the number of models is fixed to the value found to perform best in cross-validation exercise:

```
plot(spar_faces)
```

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

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

The coefficients from each of the marginal models (before averaging) can be plotted using the `plot(..., plot_type = "coefs")`

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

The `predict()` function can be applied to the '`spar.cv`' object:

```
ynew <- predict(spar_faces, xnew = xtest)
```

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:

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

Additionally, for this data set, one can visualize the effect of each pixel $\hat{\beta}_j x^{\text{new}}_{i,j}$ in predicting the face orientation in a given image e.g., 9th in the test set:

```
i <- 9
plot4 <- ggplot(data.frame(X = rep(1:64, each = 64),
                           Y = rep(64:1, 64),
                           effect = xtest[i,] * face_coef$beta),
                aes(X, Y, fill= effect)) +
  geom_tile() +
  theme_void() +
  scale_fill_gradient2() +
  ggtitle(bquote(hat(y) == .(round(ynew[i])))) +
  theme(plot.title = element_text(hjust = 0.5))
plot4
```

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 ($n = 174$).

The data set can be downloaded from https://archive.ics.uci.edu/dataset/732/darwin:

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

Before proceeding with the analysis, the data is screened for multivariate outliers using the DDC algorithm in package **cellWise**.

```
darwin_orig <- list(
  x = as.matrix(darwin_tmp[, !(colnames(darwin_tmp) %in% c("ID", "class"))]),
  y = as.numeric(darwin_tmp$class) - 1)

tmp <- cellWise::DDC(darwin_orig$x,
                     list(returnBigXimp = TRUE,
                          tolProb = 0.999,
                          silent = TRUE))
darwin <- list(x = tmp$Ximp,
               y = darwin_orig$y)
```

We estimate the spar model with binomial family and logit link and use 1—area under the ROC curve as the cross-validation measure:

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

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 λ values, where the number of models is fixed to the value found to perform best in cross-validation exercise:

```
plot(spar_darwin)
```

The plot of the coefficients can be interpreted nicely in this example:

```
ntasks <- 25
nfeat <- 18
reorder_ind <- c(outer((seq_len(ntasks) - 1) * nfeat, seq_len(nfeat), "+"))
feat_names <- sapply(colnames(darwin$x)[seq_len(nfeat)],
                     function(name) substr(name, 1, nchar(name) - 1))

plot(spar_darwin,"coefs",coef_order = reorder_ind) +
  geom_vline(xintercept = 0.5 + seq_len(ntasks - 1) * ntasks,
             alpha = 0.2, linetype = 2) +
  annotate("text",x = (seq_len(nfeat) - 1) * ntasks + 12,
           y = 45,label=feat_names, angle = 90,
           size = 3)
```

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** provides an implementation for estimating an ensemble of GLMs after performing probabilistic screening and random projection in a high-dimensional setting.

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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