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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" axisaligned 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 4 contains two examples of employing the package on real data sets. Finally, Section 5 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 $\hat{\alpha} = (\alpha_1, \dots, \alpha_p)' \in \mathbb{R}^p, \alpha_j = \operatorname{Cor}(X_{.j}, y)$ 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

$$\mathbb{P}(\mathcal{A}\subset\mathcal{A}_{\gamma_n})\to 1$$
 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}_{γ_n} contain less than n variables. One of the critical conditions is that on the population level for some fixed $i\in[n]$, $\min_{j\in\mathcal{A}}|\mathrm{Cov}(y_i/\beta_j,x_{ij})|\geq c$ 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: $\hat{\alpha}_j=:\min_{\beta_i\in\mathbb{R}}\sum_{i=1}^n -\ell(\beta;y_i,x_{ij})$.

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, @wang2015conditional). or quantile correlation (Ma and Zhang 2016). For GLMs, Fan, Feng, and Song (2011) extend Fan and Song (2010) by fitting a generalized additive model with B-splines. Further extensions for discrete (or categorical) outcomes include the fused Kolmogorov filter (Mai and Zou 2013), using the mean conditional variance, i.e., the expectation in X_j of the variance in the response of the conditional cumulative distribution function $P(X \leq x|Y)$ (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.: $\Phi_{ij} \stackrel{iid}{\sim} N(0,1)$ (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 $D=\mathrm{diag}(\pm 1)$ 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: $\hat{\alpha} =: \mathrm{argmin}_{\beta \in \mathbb{R}^p} \sum_{i=1}^n -\ell(\beta; y_i, x_i) + \frac{\varepsilon}{2} \sum_{j=1}^p \beta_j^2, \, \varepsilon > 0$ 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. $m_k \sim \mathrm{Unif}\{\log(p), \dots, n/2\}$ using **projection** matrix Φ_k to obtain $Z_k = X_{I_k} \Phi_k^{\top} \in \mathbb{R}^{n \times m_k}$:
 - 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 $\hat{\beta}^k_{I_k} = \Phi'_k \gamma^k$, $\hat{\beta}^k_{\bar{I}_k} = 0$.
- for a given threshold $\lambda > 0$, set all $\hat{\beta}_i^k$ with $|\hat{\beta}_i^k| < \lambda$ 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

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

• 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

3.1. Functionality

The two main functions in the package are:

```
spar(x, y, family = gaussian(), ...)
and
spar.cv(x, y, family = gaussian(), nfolds = 10L, ...)
```

Most important arguments:

- $\mathbf{x} \ n \times p$ numeric matrix of predictor variables.
- y numeric response vector of length n.
- family object from stats::family().
- type.rpm type of random projection matrix to be employed; one of "cwdatadriven", "cw" Clarkson and Woodruff (2013), "gaussian", "sparse".
- nscreen max number of variables kept after screening in each marginal model; defaults to 2n.
- type.screening measure by which the coefficients are screened; "ridge" performs screening based on ridge regression, "marglik" marginal likelihood of fitting a GLM for each predictor, "corr" correlation of the response with each predictor.
- type.measure loss to use for choosing λ and M; defaults to "deviance" (available for all families). Other options are "mse" or "mae" (for all families), "class" and "1-auc" for "binomial".
- nlambda number of λ values to be considered for thresholding and optionally lambdas, a vector of values.
- nummods vector containing the size of the different ensembles M to consider for the prediction.

Methods print, plot, coef, predict are available.

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.

3.2. Extensibility

The user can implement their own screening and random projections. We exemplify how a new screening coefficients based on

4. Illustrations

4.1. 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()</pre>
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"))</pre>
x <- t(facedata$images)</pre>
y <- facedata$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)</pre>
ntest <- ntot * 0.25
testind <- sample(1:ntot, ntest, replace=FALSE)</pre>
```

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)</pre>
```

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)</pre>
```

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</pre>
```

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

plot4

4.2. 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)</pre>
```

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

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

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:

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).

5. 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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