

# Package ‘SMMA’

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**Type** Package

**Title** Soft Maximin Estimation for Large Scale Array-Tensor Models

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**Description**

Efficient design matrix free procedure for solving a soft maximin problem for large scale array-tensor structured models. Currently Lasso and SCAD penalized estimation is implemented.

**License** GPL (>= 2)

**Imports** Rcpp (>= 0.12.12)

**LinkingTo** Rcpp, RcppArmadillo

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## R topics documented:

|                        |   |
|------------------------|---|
| predict.SMMA . . . . . | 2 |
| print.SMMA . . . . .   | 3 |
| RH . . . . .           | 4 |
| SMMA . . . . .         | 5 |

**Index**

**10**

predict.SMMA

*Make Prediction From a SMMA Object***Description**

Given new covariate data this function computes the linear predictors based on the estimated model coefficients in an object produced by the function `softmaximin`. Note that the data can be supplied in two different formats: i) as a  $n' \times p$  matrix ( $p$  is the number of model coefficients and  $n'$  is the number of new data points) or ii) as a list of two or three matrices each of size  $n'_i \times p_i, i = 1, 2, 3$  ( $n'_i$  is the number of new marginal data points in the  $i$ th dimension).

**Usage**

```
## S3 method for class 'SMMA'
predict(object, x = NULL, X = NULL, ...)
```

**Arguments**

|                     |   |
|---------------------|---|
| <code>object</code> | An object of class SMMA, produced with <code>softmaximin</code>   |
| <code>x</code>      | a matrix of size $n' \times p$ with $n'$ is the number of new data points.  |
| <code>X</code>      | a list containing the data matrices each of size $n'_i \times p_i$ , where $n'_i$ is the number of new data points in the $i$ th dimension. |
| <code>...</code>    | ignored   |

**Value**

A list of length `nlambda` containing the linear predictors for each model. If new covariate data is supplied in one  $n' \times p$  matrix `x` each item is a vector of length  $n'$ . If the data is supplied as a list of matrices each of size  $n'_i \times p_i$ , each item is an array of size  $n'_1 \times \dots \times n'_d$ , with  $d \in \{1, 2, 3\}$ .

**Author(s)**

Adam Lund

**Examples**

```
##size of example
n1 <- 65; n2 <- 26; n3 <- 13; p1 <- 13; p2 <- 5; p3 <- 4

##marginal design matrices (Kronecker components)
X1 <- matrix(rnorm(n1 * p1, 0, 0.5), n1, p1)
X2 <- matrix(rnorm(n2 * p2, 0, 0.5), n2, p2)
X3 <- matrix(rnorm(n3 * p3, 0, 0.5), n3, p3)
X <- list(X1, X2, X3)

component <- rbinom(p1 * p2 * p3, 1, 0.1)
Beta1 <- array(rnorm(p1 * p2 * p3, 0, .1) + component, c(p1, p2, p3))
```

```

Beta2 <- array(rnorm(p1 * p2 * p3, 0, .1) + component, c(p1 , p2, p3))
mu1 <- RH(X3, RH(X2, RH(X1, Beta1)))
mu2 <- RH(X3, RH(X2, RH(X1, Beta2)))
Y1 <- array(rnorm(n1 * n2 * n3, mu1), dim = c(n1, n2, n3))
Y2 <- array(rnorm(n1 * n2 * n3, mu2), dim = c(n1, n2, n3))

Y <- array(NA, c(dim(Y1), 2))
Y[,,, 1] <- Y1; Y[,,, 2] <- Y2;

fit <- softmaximin(X, Y, penalty = "lasso", alg = "npg")

##new data in matrix form
x <- matrix(rnorm(p1 * p2 * p3), nrow = 1)
predict(fit, x = x)[[15]]

##new data in tensor component form
X1 <- matrix(rnorm(p1), nrow = 1)
X2 <- matrix(rnorm(p2), nrow = 1)
X3 <- matrix(rnorm(p3), nrow = 1)
predict(fit, X = list(X1, X2, X3))[[15]]

```

**print.SMMA***Print Function for objects of Class SMMA*

## Description

This function will print some information about the SMMA object.

## Usage

```
## S3 method for class 'SMMA'
print(x, ...)
```

## Arguments

|     |               |
|-----|---------------|
| x   | a SMMA object |
| ... | ignored       |

## Author(s)

Adam Lund

## Examples

```

##size of example
n1 <- 65; n2 <- 26; n3 <- 13; p1 <- 13; p2 <- 5; p3 <- 4

##marginal design matrices (Kronecker components)
X1 <- matrix(rnorm(n1 * p1, 0, 0.5), n1, p1)
X2 <- matrix(rnorm(n2 * p2, 0, 0.5), n2, p2)
X3 <- matrix(rnorm(n3 * p3, 0, 0.5), n3, p3)
X <- list(X1, X2, X3)

component <- rbinom(p1 * p2 * p3, 1, 0.1)
Beta1 <- array(rnorm(p1 * p2 * p3, 0, .1) + component, c(p1, p2, p3))
Beta2 <- array(rnorm(p1 * p2 * p3, 0, .1) + component, c(p1, p2, p3))
mu1 <- RH(X3, RH(X2, RH(X1, Beta1)))
mu2 <- RH(X3, RH(X2, RH(X1, Beta2)))
Y1 <- array(rnorm(n1 * n2 * n3, mu1), dim = c(n1, n2, n3))
Y2 <- array(rnorm(n1 * n2 * n3, mu2), dim = c(n1, n2, n3))

Y <- array(NA, c(dim(Y1), 2))
Y[,,, 1] <- Y1; Y[,,, 2] <- Y2;

fit <- softmaximin(X, Y, penalty = "lasso", alg = "npg")
fit

```

## Description

This function is an implementation of the  $\rho$ -operator found in *Currie et al 2006*. It forms the basis of the GLAM arithmetic.

## Usage

```
RH(M, A)
```

## Arguments

- |   |  |
|---|--|
| M | a $n \times p_1$ matrix.                         |
| A | a 3d array of size $p_1 \times p_2 \times p_3$ . |

## Details

For details see *Currie et al 2006*. Note that this particular implementation is not used in the optimization routines underlying the gllasso procedure.

**Value**

A 3d array of size  $p_2 \times p_3 \times n$ .

**Author(s)**

Adam Lund

**References**

Currie, I. D., M. Durban, and P. H. C. Eilers (2006). Generalized linear array models with applications to multidimensional smoothing. *Journal of the Royal Statistical Society. Series B*. 68, 259-280.

**Examples**

```
n1 <- 65; n2 <- 26; n3 <- 13; p1 <- 13; p2 <- 5; p3 <- 4

##marginal design matrices (Kronecker components)
X1 <- matrix(rnorm(n1 * p1), n1, p1)
X2 <- matrix(rnorm(n2 * p2), n2, p2)
X3 <- matrix(rnorm(n3 * p3), n3, p3)

Beta <- array(rnorm(p1 * p2 * p3, 0, 1), c(p1 , p2, p3))
max(abs(c(RH(X3, RH(X2, RH(X1, Beta))))) - kronecker(X3, kronecker(X2, X1)) %*% c(Beta)))
```

**Description**

Efficient design matrix free procedure for solving a soft maximin problem for large scale array-tensor structured models, see *Lund et al., 2017*. Currently Lasso and SCAD penalized estimation is implemented.

**Usage**

```
softmaximin(X,
            Y,
            penalty = c("lasso", "scad"),
            nlambda = 30,
            lambda.min.ratio = 1e-04,
            lambda = NULL,
            penalty.factor = NULL,
            reltol = 1e-05,
            maxiter = 15000,
```

```

steps = 1,
btmax = 100,
zeta = 2,
c = 0.001,
Delta0 = 1,
nu = 1,
alg = c("npg", "mfista"),
log = TRUE)

```

## Arguments

|                  |  |
|------------------|--|
| X                | A list containing the Kronecker components (1,2 or 3) of the Kronecker design matrix. These are matrices of sizes $n_i \times p_i$ .             |
| Y                | The response values, an array of size $n_1 \times \dots \times n_d \times G$ .   |
| penalty          | A string specifying the penalty. Possible values are "lasso", "scad".  |
| nlambda          | The number of lambda values.   |
| lambda.min.ratio | The smallest value for lambda, given as a fraction of $\lambda_{max}$ ; the (data dependent) smallest value for which all coefficients are zero. |
| lambda           | The sequence of penalty parameters for the regularization path.  |
| penalty.factor   | An array of size $p_1 \times \dots \times p_d$ . Is multiplied with each element in lambda to allow differential shrinkage on the coefficients.  |
| reltol           | The convergence tolerance for the inner loop.  |
| maxiter          | The maximum number of iterations allowed for each lambda value, when summing over all outer iterations for said lambda.                          |
| steps            | The number of steps used in the multi-step adaptive lasso algorithm for non-convex penalties. Automatically set to 1 when penalty = "lasso".     |
| btmax            | Maximum number of backtracking steps allowed in each iteration. Default is btmax = 100.  |
| zeta             | Constant controlling the softmax approximation accuracy. Must be strictly positive. Default is zeta = 2.   |
| c                | constant used in the NPG algorithm. Must be strictly positive. Default is c = 0.001.   |
| Delta0           | constant used to bound the stepsize. Must be strictly positive. Default is Delta0 = 1.   |
| nu               | constant used to control the stepsize. Must be positive. A small value gives a big stepsize. Default is nu = 1.                                  |
| alg              | string indicating which algortihm to use. Possible values are "npg", "mfista".   |
| log              | logical variable indicating wheter to use log-loss to or not. TRUE is default and yields the problem described below.                            |

## Details

In Lund *et al.*, 2017 the following mixed model setup for  $d$ -dimensional array data,  $d = 1, 2, 3$ , with known fixed group structure and tensor structured design matrix is considered: With  $G$  groups,

$g \in \{1, \dots, G\}$ ,  $n$  is the number of observations in each group,  $Y_g := (y_i, \dots, y_{i_n})^\top$  the group-specific  $n_1 \times \dots \times n_d$  response array and  $X$  a  $n \times p$  design matrix, with tensor structure

$$X = \bigotimes_{i=1}^d X_i,$$

where for  $d = 1, 2, 3$ ,  $X_1, \dots, X_d$  are the marginal  $n_i \times p_i$  design matrices (Kronecker components). Using the GLAM framework the model equation is

$$Y_g = \rho(X_d, \rho(X_{d-1}, \dots, \rho(X_1, B_g))) + E,$$

where  $\rho$  is the so called rotated  $H$ -transfrom (see Currie et al., 2006),  $B_g$  for each  $g$  is a random  $p_1 \times \dots \times p_d$  parameter array and  $E$  is  $n_1 \times \dots \times n_d$  error array uncorrelated with  $X$ . Note that for  $d = 1$  the model is a GLM.

In Lund et al., 2017 a penalized soft maximin problem, given as

$$\min_{\beta} \log \left( \sum_{g=1}^G \exp(-\zeta \hat{V}_g(\beta)) \right) + \lambda J(\beta),$$

is proposed where  $J$  is a proper and convex penalty,  $\zeta > 0$  and

$$\hat{V}_g(\beta) := \frac{1}{n} (2\beta^\top X^\top y_g - \beta^\top X^\top X \beta),$$

$y_g := \text{vec}(Y_g)$ , is the minimal empirical explained variance from Meinshausen and Bühlmann, 2015.

For  $d = 1, 2, 3$ , using only the marginal matrices  $X_1, X_2, \dots$  (for  $d = 1$  there is only one marginal), the function `softmaximin` solves the soft maximin problem for a sequence of penalty parameters  $\lambda_{\max} > \dots > \lambda_{\min} > 0$ . The underlying algorithm is based on a non-monotone proximal gradient method. We note that if  $J$  is not convex, as with the SCAD penalty, we use the multiple step adaptive lasso procedure to loop over the proximal algorithm, see Lund et al., 2017 for more details.

## Value

An object with S3 Class "SMMA".

|                      |   |
|----------------------|---|
| <code>spec</code>    | A string indicating the array dimension (1, 2 or 3) and the penalty.  |
| <code>coef</code>    | A $p_1 \times \dots \times p_d \times n_{\text{lambda}}$ matrix containing the estimates of the model coefficients ( <code>beta</code> ) for each <code>lambda</code> -value.   |
| <code>lambda</code>  | A vector containing the sequence of penalty values used in the estimation procedure.  |
| <code>Obj</code>     | A matrix containing the objective values for each iteration and each model.   |
| <code>df</code>      | The number of nonzero coefficients for each value of <code>lambda</code> .  |
| <code>dimcoef</code> | A vector giving the dimension of the model coefficient array $\beta$ .  |
| <code>dimobs</code>  | A vector giving the dimension of the observation (response) array $Y$ .   |
| <code>Iter</code>    | A list with 4 items: <code>bt_iter</code> is total number of backtracking steps performed, <code>bt_enter</code> is the number of times the backtracking is initiated, and <code>iter_mat</code> is a vector containing the number of iterations for each <code>lambda</code> value and <code>iter</code> is total number of iterations i.e. <code>sum(Iter)</code> . |

## Author(s)

Adam Lund

Maintainer: Adam Lund, <adam.lund@math.ku.dk>

## References

- Lund, A., S. W. Mogensen and N. R. Hansen (2017). Estimating Soft Maximin Effects in Heterogeneous Large-scale Array Data. *Preprint*.
- Meinshausen, N and P. Bühlmann (2015). Maximin effects in inhomogeneous large-scale data. *The Annals of Statistics*. 43, 4, 1801-1830.
- Currie, I. D., M. Durban, and P. H. C. Eilers (2006). Generalized linear array models with applications to multidimensional smoothing. *Journal of the Royal Statistical Society. Series B*. 68, 259-280.

## Examples

```
##size of example
n1 <- 65; n2 <- 26; n3 <- 13; p1 <- 13; p2 <- 5; p3 <- 4

##marginal design matrices (Kronecker components)
X1 <- matrix(rnorm(n1 * p1), n1, p1)
X2 <- matrix(rnorm(n2 * p2), n2, p2)
X3 <- matrix(rnorm(n3 * p3), n3, p3)
X <- list(X1, X2, X3)

component <- rbinom(p1 * p2 * p3, 1, 0.1)
Beta1 <- array(rnorm(p1 * p2 * p3, 0, 0.1) + component, c(p1 , p2, p3))
mu1 <- RH(X3, RH(X2, RH(X1, Beta1)))
Y1 <- array(rnorm(n1 * n2 * n3), dim = c(n1, n2, n3)) + mu1
Beta2 <- array(rnorm(p1 * p2 * p3, 0, 0.1) + component, c(p1 , p2, p3))
mu2 <- RH(X3, RH(X2, RH(X1, Beta2)))
Y2 <- array(rnorm(n1 * n2 * n3), dim = c(n1, n2, n3)) + mu2
Beta3 <- array(rnorm(p1 * p2 * p3, 0, 0.1) + component, c(p1 , p2, p3))
mu3 <- RH(X3, RH(X2, RH(X1, Beta3)))
Y3 <- array(rnorm(n1 * n2 * n3), dim = c(n1, n2, n3)) + mu3
Beta4 <- array(rnorm(p1 * p2 * p3, 0, 0.1) + component, c(p1 , p2, p3))
mu4 <- RH(X3, RH(X2, RH(X1, Beta4)))
Y4 <- array(rnorm(n1 * n2 * n3), dim = c(n1, n2, n3)) + mu4
Beta5 <- array(rnorm(p1 * p2 * p3, 0, 0.1) + component, c(p1 , p2, p3))
mu5 <- RH(X3, RH(X2, RH(X1, Beta5)))
Y5 <- array(rnorm(n1 * n2 * n3), dim = c(n1, n2, n3)) + mu5

Y <- array(NA, c(dim(Y1), 5))
Y[,,, 1] <- Y1; Y[,,, 2] <- Y2; Y[,,, 3] <- Y3; Y[,,, 4] <- Y4; Y[,,, 5] <- Y5;

fit <- softmaximin(X, Y, penalty = "lasso", alg = "npg")
Betafit <- fit$coef

modelno <- 15
```

```
m <- min(Betafit[, modelno], c(component))
M <- max(Betafit[, modelno], c(component))
plot(c(component), type="l", ylim = c(m, M))
lines(Betafit[, modelno], col = "red")
```

# Index

\*Topic **package**

SMMA, [5](#)

glamlasso\_RH (RH), [4](#)

H (RH), [4](#)

pga (SMMA), [5](#)

predict.SMMA, [2](#)

print.SMMA, [3](#)

RH, [4](#)

Rotate (RH), [4](#)

SMMA, [5](#)

softmaximin (SMMA), [5](#)