## Package 'joinet'

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Version 1.0.0

Title Penalised Multivariate Regression ('Multi-Target Learning')

**Description** Implements penalised multivariate regression (i.e., for multiple outcomes and many features) by stacked generalisation (<doi:10.1093/bioinformatics/btab576>). For positively correlated outcomes, a single multivariate regression is typically more predictive than multiple univariate regressions. Includes functions for model fitting, extracting coefficients, outcome prediction, and performance measurement. For optional comparisons, install 'remMap' from GitHub (<https://github.com/cran/remMap>).

```
Depends R (>= 3.0.0)
```

Imports glmnet, palasso, cornet

**Suggests** knitr, rmarkdown, testthat, MASS, mice, earth, spls, MRCE, remMap, MultivariateRandomForest, SiER, mcen, GPM, RMTL, MTPS

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**Encoding UTF-8** 

VignetteBuilder knitr

RoxygenNote 7.3.2

URL https://github.com/rauschenberger/joinet,

https://rauschenberger.github.io/joinet/

BugReports https://github.com/rauschenberger/joinet/issues

NeedsCompilation no

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joinet-package

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#### **Description**

The R package joinet implements multivariate ridge and lasso regression using stacked generalisation. This multivariate regression typically outperforms univariate regression at predicting correlated outcomes. It provides predictive and interpretable models in high-dimensional settings.

#### **Details**

Use function joinet for model fitting. Type library(joinet) and then ?joinet or help("joinet)" to open its help file.

See the vignette for further examples. Type vignette("joinet") or browseVignettes("joinet") to open the vignette.

## Author(s)

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#### References

Armin Rauschenberger and Enrico Glaab (2021) "Predicting correlated outcomes from molecular data". *Bioinformatics* 37(21):3889–3895. doi:10.1093/bioinformatics/btab576. (Click here to access PDF.)

## See Also

Useful links:

- https://github.com/rauschenberger/joinet
- https://rauschenberger.github.io/joinet/
- Report bugs at https://github.com/rauschenberger/joinet/issues

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## **Examples**

```
## Not run:
#--- data simulation ---
n <- 50; p <- 100; q <- 3
X <- matrix(rnorm(n*p),nrow=n,ncol=p)</pre>
Y <- replicate(n=q,expr=rnorm(n=n,mean=rowSums(X[,1:5])))
# n samples, p inputs, q outputs
#--- model fitting ---
object <- joinet(Y=Y,X=X)</pre>
# slot "base": univariate
# slot "meta": multivariate
#--- make predictions ---
y_hat <- predict(object,newx=X)</pre>
# n x q matrix "base": univariate
# n x q matrix "meta": multivariate
#--- extract coefficients ---
coef <- coef(object)</pre>
# effects of inputs on outputs
# q vector "alpha": intercepts
# p x q matrix "beta": slopes
#--- model comparison ---
loss <- cv.joinet(Y=Y,X=X)</pre>
# cross-validated loss
# row "base": univariate
# row "meta": multivariate
## End(Not run)
```

coef.joinet

Extract Coefficients

## **Description**

Extracts pooled coefficients. (The meta learners linearly combines the coefficients from the base learners.)

#### Usage

```
## S3 method for class 'joinet'
coef(object, ...)
```

## Arguments

```
object joinet object
```

... further arguments (not applicable)

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#### Value

This function returns the pooled coefficients. The slot alpha contains the intercepts in a vector of length q, and the slot beta contains the slopes in a matrix with p rows (inputs) and q columns.

## **Examples**

```
## Not run:
n <- 50; p <- 100; q <- 3
X <- matrix(rnorm(n*p),nrow=n,ncol=p)
Y <- replicate(n=q,expr=rnorm(n=n,mean=rowSums(X[,1:5])))
object <- joinet(Y=Y,X=X)
coef <- coef(object)
## End(Not run)</pre>
```

cv.joinet

Model comparison

## **Description**

Compares univariate and multivariate regression.

#### Usage

```
cv.joinet(
 Υ,
 Χ,
  family = "gaussian",
  nfolds.ext = 5,
  nfolds.int = 10,
  foldid.ext = NULL,
  foldid.int = NULL,
  type.measure = "deviance",
  alpha.base = 1,
  alpha.meta = 1,
  compare = FALSE,
 mice = FALSE,
  cvpred = FALSE,
  times = FALSE,
)
```

## **Arguments**

Y outputs: numeric matrix with n rows (samples) and q columns (outputs)

X inputs: numeric matrix with n rows (samples) and p columns (inputs)

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family	distribution: vector of length $1$ or $q$ with entries "gaussian", "binomial" or "poisson"
nfolds.ext	number of external folds
nfolds.int	number of internal folds
foldid.ext	external fold identifiers: vector of length $\boldsymbol{n}$ with entries between $1$ and nfolds.ext; or NULL
foldid.int	internal fold identifiers: vector of length $\boldsymbol{n}$ with entries between 1 and nfolds.int; or NULL
type.measure	loss function: vector of length 1 or $q$ with entries "deviance", "class", "mse" or "mae" (see cv.glmnet)
alpha.base	elastic net mixing parameter for base learners: numeric between $0 \ ({\rm ridge})$ and $1 \ ({\rm lasso})$
alpha.meta	elastic net mixing parameter for meta learners: numeric between $0$ (ridge) and $1$ (lasso)
compare	experimental arguments: character vector with entries "mnorm", "spls", "mrce", "sier", "mtps", "rmtl", "gpm" and others (requires packages spls, MRCE, SiER, MTPS, RMTL or GPM)
mice	missing data imputation: logical (mice=TRUE requires package mice)
cvpred	return cross-validated predictions: logical
times	measure computation time: logical
	further arguments passed to glmnet and cv.glmnet

#### Value

This function returns a matrix with q columns, including the cross-validated loss from the univariate models (base), the multivariate models (meta), and the intercept-only models (none).

## **Examples**

```
## Not run:
n <- 50; p <- 100; q <- 3
X <- matrix(rnorm(n*p),nrow=n,ncol=p)</pre>
Y <- replicate(n=q,expr=rnorm(n=n,mean=rowSums(X[,1:5])))
cv.joinet(Y=Y,X=X)
## End(Not run)
## Not run:
# correlated features
n <- 50; p <- 100; q <- 3
mu <- rep(0,times=p)</pre>
Sigma <- 0.90^abs(col(diag(p))-row(diag(p)))</pre>
X <- MASS::mvrnorm(n=n,mu=mu,Sigma=Sigma)</pre>
mu <- rowSums(X[,sample(seq_len(p),size=5)])</pre>
Y <- replicate(n=q,expr=rnorm(n=n,mean=mu))</pre>
#Y <- t(MASS::mvrnorm(n=q,mu=mu,Sigma=diag(n)))</pre>
cv.joinet(Y=Y,X=X)
## End(Not run)
```

joinet joinet

```
## Not run:
# other distributions
n <- 50; p <- 100; q <- 3
X <- matrix(rnorm(n*p),nrow=n,ncol=p)</pre>
eta <- rowSums(X[,1:5])
Y <- replicate(n=q,expr=rbinom(n=n,size=1,prob=1/(1+exp(-eta))))
cv.joinet(Y=Y,X=X,family="binomial")
Y <- replicate(n=q,expr=rpois(n=n,lambda=exp(scale(eta))))
cv.joinet(Y=Y,X=X,family="poisson")
## End(Not run)
## Not run:
# uncorrelated outcomes
n <- 50; p <- 100; q <- 3
X <- matrix(rnorm(n*p),nrow=n,ncol=p)</pre>
y <- rnorm(n=n,mean=rowSums(X[,1:5]))</pre>
Y <- cbind(y,matrix(rnorm(n*(q-1)),nrow=n,ncol=q-1))
cv.joinet(Y=Y,X=X)
## End(Not run)
## Not run:
# sparse and dense models
n <- 50; p <- 100; q <- 3
X <- matrix(rnorm(n*p),nrow=n,ncol=p)</pre>
Y <- replicate(n=q,expr=rnorm(n=n,mean=rowSums(X[,1:5])))
set.seed(1) # fix folds
cv.joinet(Y=Y,X=X,alpha.base=1) # lasso
set.seed(1)
cv.joinet(Y=Y,X=X,alpha.base=0) # ridge
## End(Not run)
```

joinet

Multivariate Elastic Net Regression

#### **Description**

Implements multivariate elastic net regression.

## Usage

```
joinet(
   Y,
   X,
   family = "gaussian",
   nfolds = 10,
   foldid = NULL,
   type.measure = "deviance",
   alpha.base = 1,
```

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. . .

```
alpha.meta = 1,
weight = NULL,
sign = NULL,
...
)
```

#### **Arguments**

Υ	outputs: numeric matrix with $n$ rows (samples) and $q$ columns (outputs)
Χ	inputs: numeric matrix with $n$ rows (samples) and $p$ columns (inputs)
family	distribution: vector of length $1$ or $q$ with entries "gaussian", "binomial" or "poisson" $ \\$
nfolds	number of folds
foldid	fold identifiers: vector of length $\boldsymbol{n}$ with entries between $1$ and nfolds; or NULL (balance)
type.measure	loss function: vector of length $1$ or $q$ with entries "deviance", "class", "mse" or "mae" (see ${\tt cv.glmnet})$
alpha.base	elastic net mixing parameter for base learners: numeric between $0\ (\mathrm{ridge})$ and $1\ (\mathrm{lasso})$
alpha.meta	elastic net mixing parameter for meta learners: numeric between $\boldsymbol{0}$ (ridge) and $\boldsymbol{1}$ (lasso)
weight	input-output relations: matrix with $p$ rows (inputs) and $q$ columns (outputs) with entries $0$ (exclude) and $1$ (include), or NULL (see details)
sign	output-output relations: matrix with $q$ rows ("meta-inputs") and $q$ columns (outputs), with entries $-1$ (negative), $0$ (none), $1$ (positive) and $NA$ (any), or NULL (see details)
	further arguments passed to glmnet

#### **Details**

**input-output relations:** In this matrix with p rows and q columns, the entry in the jth row and the kth column indicates whether the jth input may be used for modelling the kth output (where 0 means "exclude" and 1 means "include"). By default (sign=NULL), all entries are set to 1.

**output-output relations:** In this matrix with q rows and q columns, the entry in the lth row and the kth column indicates how the lth output may be used for modelling the kth output (where -1 means negative effect, 0 means no effect, 1 means positive effect, and NA means any effect).

There are three short-cuts for filling up this matrix: (1) sign=1 sets all entries to 1 (non-negativity constraints). This is useful if all pairs of outcomes are assumed to be *positively* correlated (potentially after changing the sign of some outcomes). (2) code=NA sets all diagonal entries to 1 and all off-diagonal entries to NA (no constraints). (3) sign=NULL uses Spearman correlation to determine the entries, with -1 for significant negative, 0 for insignificant, 1 for significant positive correlations.

elastic net: alpha.base controls input-output effects, alpha.meta controls output-output effects; lasso renders sparse models (alpha=1), ridge renders dense models (alpha=0)

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#### Value

This function returns an object of class joinet. Available methods include predict, coef, and weights. The slots base and meta each contain q cv.glmnet-like objects.

#### References

Armin Rauschenberger and Enrico Glaab (2021) "Predicting correlated outcomes from molecular data". *Bioinformatics* 37(21):3889–3895. doi:10.1093/bioinformatics/btab576. (Click here to access PDF.)

#### See Also

```
cv. joinet, vignette
```

## Examples

```
## Not run:
n <- 50; p <- 100; q <- 3
X <- matrix(rnorm(n*p),nrow=n,ncol=p)
Y <- replicate(n=q,expr=rnorm(n=n,mean=rowSums(X[,1:5])))
object <- joinet(Y=Y,X=X)
## End(Not run)
## Not run:
browseVignettes("joinet") # further examples
## End(Not run)</pre>
```

predict.joinet

Make Predictions

## **Description**

Predicts outcome from features with stacked model.

## Usage

```
## S3 method for class 'joinet'
predict(object, newx, type = "response", ...)
```

#### **Arguments**

```
object joinet object

newx covariates: numeric matrix with n rows (samples) and p columns (variables)

type character "link" or "response"

... further arguments (not applicable)
```

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## Value

This function returns predictions from base and meta learners. The slots base and meta each contain a matrix with n rows (samples) and q columns (variables).

#### **Examples**

```
## Not run:
n <- 50; p <- 100; q <- 3
X <- matrix(rnorm(n*p),nrow=n,ncol=p)
Y <- replicate(n=q,expr=rnorm(n=n,mean=rowSums(X[,1:5])))
Y[,1] <- 1*(Y[,1]>median(Y[,1]))
object <- joinet(Y=Y,X=X,family=c("binomial","gaussian","gaussian"))
predict(object,newx=X)
## End(Not run)</pre>
```

weights.joinet

Extract Weights

## **Description**

Extracts coefficients from the meta learner, i.e. the weights for the base learners.

## Usage

```
## S3 method for class 'joinet'
weights(object, ...)
```

## **Arguments**

```
object joinet object
... further arguments (not applicable)
```

## Value

This function returns a matrix with 1+q rows and q columns. The first row contains the intercepts, and the other rows contain the slopes, which are the effects of the outcomes in the row on the outcomes in the column.

#### **Examples**

```
## Not run:
n <- 50; p <- 100; q <- 3
X <- matrix(rnorm(n*p),nrow=n,ncol=p)
Y <- replicate(n=q,expr=rnorm(n=n,mean=rowSums(X[,1:5])))
object <- joinet(Y=Y,X=X)
weights(object)
## End(Not run)</pre>
```

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