# Package 'sjSDM'

June 16, 2023

**Description** A scalable method to estimate joint Species Distribution Models (jSDMs) for big community datasets based on a Monte Carlo approximation of the joint likelihood. The numeri-

```
late', and can be run on CPUs and GPUs alike. The method is described in Pichler & Har-
      tig (2021) <doi:10.1111/2041-210X.13687>. The package contains various extensions, includ-
      ing support for different response families, ability to account for spatial autocorrela-
      tion, and deep neural networks instead of the linear predictor in jSDMs.
License GPL-3
Encoding UTF-8
LazyData true
Depends R (>= 3.0)
Imports reticulate,
      stats,
      mvtnorm,
      utils,
      rstudioapi,
      abind,
      graphics,
      grDevices,
      Metrics,
      parallel,
      mgcv,
      cli,
      crayon,
      ggplot2,
      checkmate,
      mathjaxr,
      ggtern
Suggests testthat,
      knitr,
      rmarkdown
RoxygenNote 7.2.3
URL https://theoreticalecology.github.io/s-jSDM/
```

Title Scalable Joint Species Distribution Modeling

cal approximation is based on 'PyTorch' and 'reticu-

Type Package

Version 1.0.5

$\pmb{BugReports} \   \texttt{https://github.com/TheoreticalEcology/s-jSDM/issues} \\$		
<b>Roxygen</b> list(old_usage = FALSE)		
VignetteBuilder knitr		
RdMacros mathjaxr		

# ${\sf R}$ topics documented:

AccSGD
AdaBound
Adamax
anova.sjSDM
bioticStruct
checkModel
check_module
coef.sjSDM
DiffGrad
DNN
generateSpatialEV
getCor
getCov
getImportance
getSe
getWeights
importance
installation_help
install_diagnostic
install_sjSDM
is_torch_available
linear
logLik.sjSDM
madgrad
new_image
plot.sjSDM
plot.sjSDM.DNN
plot.sjSDManova
plot.sjSDMimportance
plot.sjSDM_cv
plotInternalStructure
plotsjSDMcoef
predict.sjSDM
print.bioticStruct
print.DNN
print.linear
print.sjSDM
print.sjSDManova
print.sjSDMimportance
print.sjSDM_cv
RMSprop
Rsquared
setWeights
SGD

AccSGD 3

	simulate.sjSDM	40
	simulate_SDM	41
	sjSDM	42
	sjSDMControl	48
	sjSDM_cv	49
	summary.sjSDM	51
	summary.sjSDM_cv	51
	update.sjSDM	52
Index		53

# Description

AccSGD

accelerated stochastic gradient, see Kidambi et al., 2018 for details

AccSGD

# Usage

```
AccSGD(kappa = 1000, xi = 10, small_const = 0.7, weight_decay = 0)
```

# Arguments

long step
advantage parameter
small constant
12 penalty on weights

## Value

Anonymous function that returns optimizer when called.

## References

Kidambi, R., Netrapalli, P., Jain, P., & Kakade, S. (2018, February). On the insufficiency of existing momentum schemes for stochastic optimization. In 2018 Information Theory and Applications Workshop (ITA) (pp. 1-9). IEEE.

4 Adamax

AdaBound

AdaBound

## Description

adaptive gradient methods with dynamic bound of learning rate, see Luo et al., 2019 for details

## Usage

```
AdaBound(
    betas = c(0.9, 0.999),
    final_lr = 0.1,
    gamma = 0.001,
    eps = 1e-08,
    weight_decay = 0,
    amsbound = TRUE
)
```

## Arguments

```
betas betas

final_lr eps
gamma small_const
eps eps
weight_decay weight_decay
amsbound amsbound
```

#### Value

Anonymous function that returns optimizer when called.

### References

Luo, L., Xiong, Y., Liu, Y., & Sun, X. (2019). Adaptive gradient methods with dynamic bound of learning rate. arXiv preprint arXiv:1902.09843.

Adamax

Adamax

## Description

Adamax optimizer, see Kingma and Ba, 2014

## Usage

```
Adamax(betas = c(0.9, 0.999), eps = 1e-08, weight_decay = 0.002)
```

anova.sjSDM 5

#### **Arguments**

betas exponential decay rates

eps fuzz factor

weight\_decay 12 penalty on weights

#### Value

Anonymous function that returns optimizer when called.

#### References

Kingma, D. P., & Ba, J. (2014). Adam: A method for stochastic optimization. arXiv preprint arXiv:1412.6980.

anova.sjSDM Anova

## **Description**

Calculates type II anova.

Shared contributions (e.g. between space and environment) are also calculated (and divided proportionally) and can be optionally visualized via plot.sjSDManova with add\_shared=TRUE. The anova can get unstable for many species and few occurrences/observations. We recommend using large numbers for 'samples'.

## Usage

```
## S3 method for class 'sjSDM'
anova(object, samples = 5000L, ...)
```

## **Arguments**

object model of object sjSDM

samples Number of Monte Carlo samples

... optional arguments which are passed to the calculation of the logLikelihood

#### **Details**

Compute analysis of variance

#### Value

An S3 class of type 'sjSDManova' including the following components:

results Data frame of results.

to\_print Data frame, summarized results for type I anova.

N Number of observations (sites).spatial Logical, spatial model or not.species individual species R2s.

6 bioticStruct

```
sites individual site R2s.
```

individual site by species negative-log-likelihood values.

Implemented S3 methods are print.sjSDManova and plot.sjSDManova

#### See Also

```
plot.sjSDManova, print.sjSDManova, plotInternalStructure
```

bioticStruct biotic structure

## **Description**

define biotic (species-species) association (interaction) structure

## Usage

```
bioticStruct(
  df = NULL,
  lambda = 0,
  alpha = 0.5,
  on_diag = FALSE,
  reg_on_Cov = TRUE,
  inverse = FALSE,
  diag = FALSE
)
```

## **Arguments**

df degree of freedom for covariance parametrization, if NULL df is set to ncol(Y)/2

lambda penalty, strength of regularization:  $\lambda*(lasso+ridge)$ 

alpha weighting between lasso and ridge:  $(1-\alpha)*|covariances|+\alpha||covariances||^2$ 

on\_diag regularization on diagonals

reg\_on\_Cov regularization on covariance matrix

inverse regularization on the inverse covariance matrix diag use diagonal matrix with zeros (internal usage)

#### Value

An S3 class of type 'bioticStruct' including the following components:

11\_cov L1 regularization strength.12\_cov L2 regularization strength.

inverse Logical, use inverse covariance matrix or not.

diag Logical, use diagonal matrix or not.

reg\_on\_Cov Logical, regularize covariance matrix or not.

on\_diag Logical, regularize diagonals or not.

Implemented S3 methods include print.bioticStruct

bioticStruct 7

#### See Also

sjSDM

## **Examples**

```
## Not run:
# Basic workflow:
## simulate community:
com = simulate_SDM(env = 3L, species = 7L, sites = 100L)
## fit model:
model = sjSDM(Y = com$response,env = com$env_weights, iter = 50L)
# increase iter for your own data
coef(model)
summary(model)
getCov(model)
## plot results
species=c("sp1","sp2","sp3","sp4","sp5","sp6","sp7")
group=c("mammal","bird","fish","fish","mammal","amphibian","amphibian")
group = data.frame(species=species,group=group)
plot(model,group=group)
## calculate post-hoc p-values:
p = getSe(model)
summary(p)
## or turn on the option in the sjSDM function:
model = sjSDM(Y = com$response, env = com$env_weights, se = TRUE,
              family = binomial("probit"),
               iter = 2L)
summary(model)
## fit model with interactions:
model = sjSDM(Y = com$response,
              env = linear(data = com$env_weights, formula = ~X1:X2 + X3),
              se = TRUE,
              iter = 2L) # increase iter for your own data
summary(model)
## without intercept:
model = update(model, env_formula = ~0+X1:X2 + X3)
summary(model)
## predict with model:
preds = predict(model, newdata = com$env_weights)
## calculate R-squared:
R2 = Rsquared(model)
print(R2)
# With spatial terms:
## linear spatial model
```

8 bioticStruct

```
XY = matrix(rnorm(200), 100, 2)
model = sjSDM(Y = com$response, env = linear(com$env_weights),
              spatial = linear(XY, ~0+X1:X2),
              iter = 50L) # increase iter for your own data
summary(model)
predict(model, newdata = com$env_weights, SP = XY)
R2 = Rsquared(model)
print(R2)
## Using spatial eigenvectors as predictors to account
## for spatial autocorrelation is a common approach:
SPV = generateSpatialEV(XY)
model = sjSDM(Y = com$response, env = linear(com$env_weights),
              spatial = linear(SPV, ~0+., lambda = 0.1),
              iter = 50L) # increase iter for your own data
summary(model)
predict(model, newdata = com$env_weights, SP = SPV)
## Visualize internal meta-community structure
an = anova(model)
plot(an, internal=TRUE)
## non-linear(deep neural network) model
model = sjSDM(Y = com$response, env = linear(com$env_weights),
              spatial = DNN(SPV, hidden = c(5L, 5L), ~0+.),
              iter = 2L) # increase iter for your own data
summary(model)
predict(model, newdata = com$env_weights, SP = SPV)
# Regularization
## lambda is the regularization strength
## alpha weights the lasso or ridge penalty:
## - alpha = 0 --> pure lasso
## - alpha = 1.0 --> pure ridge
model = sjSDM(Y = com$response,
              # mix of lasso and ridge
              env = linear(com$env_weights, lambda = 0.01, alpha = 0.5),
              # we can do the same for the species-species associations
              biotic = bioticStruct(lambda = 0.01, alpha = 0.5),
              iter = 2L) # increase iter for your own data
summary(model)
coef(model)
getCov(model)
# Anova
com = simulate_SDM(env = 3L, species = 15L, sites = 200L, correlation = TRUE)
XY = matrix(rnorm(400), 200, 2)
SPV = generateSpatialEV(XY)
model = sjSDM(Y = com$response, env = linear(com$env_weights),
              spatial = linear(SPV, ~0+.),
              iter = 50L) # increase iter for your own data
result = anova(model)
print(result)
```

checkModel 9

```
plot(result)
## visualize meta-community structure
plot(result, internal=TRUE)
# Deep neural network
## we can fit also a deep neural network instead of a linear model:
model = sjSDM(Y = com$response,
              env = DNN(com$env_weights, hidden = c(10L, 10L, 10L)),
              iter = 2L) # increase iter for your own data
summary(model)
getCov(model)
pred = predict(model, newdata = com$env_weights)
## extract weights
weights = getWeights(model)
## we can also assign weights:
setWeights(model, weights)
## with regularization:
model = sjSDM(Y = com$response,
              # mix of lasso and ridge
              env = DNN(com$env_weights, lambda = 0.01, alpha = 0.5),
              # we can do the same for the species-species associations
              biotic = bioticStruct(lambda = 0.01, alpha = 0.5),
              iter = 2L) # increase iter for your own data
getCov(model)
getWeights(model)
## End(Not run)
```

checkModel

check model check model and rebuild if necessary

## Description

check model check model and rebuild if necessary

#### Usage

```
checkModel(object)
```

## **Arguments**

object of class sjSDM

DiffGrad

check\_module

check module

## Description

check if module is loaded

## Usage

```
check_module()
```

coef.sjSDM

Return coefficients from a fitted sjSDM model

# Description

Return coefficients from a fitted sjSDM model

## Usage

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

## Arguments

object a model fitted by sjSDM

... optional arguments for compatibility with the generic function, no function im-

plemented

## Value

Matrix of environmental coefficients or list of environmental and spatial coefficients for spatial models.

DiffGrad

DiffGrad

## Description

DiffGrad

# Usage

```
DiffGrad(betas = c(0.9, 0.999), eps = 1e-08, weight_decay = 0)
```

DNN 11

#### **Arguments**

```
betas betas
eps eps
weight_decay weight_decay
```

#### Value

Anonymous function that returns optimizer when called.

DNN

Non-linear model (deep neural network) of environmental responses

## **Description**

specify the model to be fitted

## Usage

```
DNN(
  data = NULL,
  formula = NULL,
  hidden = c(10L, 10L, 10L),
  activation = "selu",
  bias = TRUE,
  lambda = 0,
  alpha = 0.5,
  dropout = 0
)
```

# Arguments

dropout

data matrix of environmental predictors formula formula object for predictors hidden units in layers, length of hidden corresponds to number of layers hidden activation activation functions, can be of length one, or a vector of activation functions for each layer. Currently supported: tanh, relu, leakyrelu, selu, or sigmoid bias whether use biases in the layers, can be of length one, or a vector (number of hidden layers including (last layer) but not first layer (intercept in first layer is specified by formula)) of logicals for each layer. lambda lambda penalty, strength of regularization:  $\lambda * (lasso + ridge)$ weighting between lasso and ridge:  $(1 - \alpha) * |weights| + \alpha ||weights||^2$ alpha

probability of dropout rate

DNN

#### Value

An S3 class of type 'DNN' including the following components:

formula Model matrix formula Χ Model matrix of covariates data Raw data 11\_coef L1 regularization strength, can be -99 if lambda = 0.0 12\_coef L2 regularization strength, can be -99 if lambda = 0.0 hidden Integer vector of hidden neurons in the deep neural network. Length of vector corresponds to the number of hidden layers. Character vector of activation functions. activation Logical vector whether to use bias or not in each hidden layer. bias

Implemented S3 methods include print.DNN

#### See Also

```
linear, sjSDM
```

## **Examples**

```
## Not run:
# Basic workflow:
## simulate community:
com = simulate_SDM(env = 3L, species = 7L, sites = 100L)
## fit model:
model = sjSDM(Y = com$response,env = com$env_weights, iter = 50L)
# increase iter for your own data
coef(model)
summary(model)
getCov(model)
## plot results
species=c("sp1","sp2","sp3","sp4","sp5","sp6","sp7")
group=c("mammal","bird","fish","fish","mammal","amphibian","amphibian")
group = data.frame(species=species,group=group)
plot(model,group=group)
## calculate post-hoc p-values:
p = getSe(model)
summary(p)
## or turn on the option in the sjSDM function:
model = sjSDM(Y = com$response, env = com$env_weights, se = TRUE,
              family = binomial("probit"),
              iter = 2L)
summary(model)
## fit model with interactions:
model = sjSDM(Y = com$response,
```

DNN 13

```
env = linear(data = com$env_weights, formula = ~X1:X2 + X3),
              se = TRUE,
              iter = 2L) # increase iter for your own data
summary(model)
## without intercept:
model = update(model, env_formula = ~0+X1:X2 + X3)
summary(model)
## predict with model:
preds = predict(model, newdata = com$env_weights)
## calculate R-squared:
R2 = Rsquared(model)
print(R2)
# With spatial terms:
## linear spatial model
XY = matrix(rnorm(200), 100, 2)
model = sjSDM(Y = com$response, env = linear(com$env_weights),
              spatial = linear(XY, ~0+X1:X2),
              iter = 50L) # increase iter for your own data
summary(model)
predict(model, newdata = com$env_weights, SP = XY)
R2 = Rsquared(model)
print(R2)
## Using spatial eigenvectors as predictors to account
## for spatial autocorrelation is a common approach:
SPV = generateSpatialEV(XY)
model = sjSDM(Y = com$response, env = linear(com$env_weights),
              spatial = linear(SPV, ~0+., lambda = 0.1),
              iter = 50L) # increase iter for your own data
summary(model)
predict(model, newdata = com$env_weights, SP = SPV)
## Visualize internal meta-community structure
an = anova(model)
plot(an, internal=TRUE)
## non-linear(deep neural network) model
model = sjSDM(Y = com$response, env = linear(com$env_weights),
              spatial = DNN(SPV, hidden = c(5L, 5L), \sim 0+.),
              iter = 2L) # increase iter for your own data
summary(model)
predict(model, newdata = com$env_weights, SP = SPV)
# Regularization
## lambda is the regularization strength
## alpha weights the lasso or ridge penalty:
## - alpha = 0 --> pure lasso
## - alpha = 1.0 --> pure ridge
model = sjSDM(Y = com$response,
              # mix of lasso and ridge
              env = linear(com$env_weights, lambda = 0.01, alpha = 0.5),
```

14 generateSpatialEV

```
# we can do the same for the species-species associations
              biotic = bioticStruct(lambda = 0.01, alpha = 0.5),
              iter = 2L) # increase iter for your own data
summary(model)
coef(model)
getCov(model)
# Anova
com = simulate_SDM(env = 3L, species = 15L, sites = 200L, correlation = TRUE)
XY = matrix(rnorm(400), 200, 2)
SPV = generateSpatialEV(XY)
model = sjSDM(Y = com$response, env = linear(com$env_weights),
              spatial = linear(SPV, ~0+.),
              iter = 50L) # increase iter for your own data
result = anova(model)
print(result)
plot(result)
## visualize meta-community structure
plot(result, internal=TRUE)
# Deep neural network
## we can fit also a deep neural network instead of a linear model:
model = sjSDM(Y = com$response,
              env = DNN(com$env_weights, hidden = c(10L, 10L, 10L)),
              iter = 2L) # increase iter for your own data
summary(model)
getCov(model)
pred = predict(model, newdata = com$env_weights)
## extract weights
weights = getWeights(model)
## we can also assign weights:
setWeights(model, weights)
## with regularization:
model = sjSDM(Y = com$response,
              # mix of lasso and ridge
              env = DNN(com$env_weights, lambda = 0.01, alpha = 0.5),
              # we can do the same for the species-species associations
              biotic = bioticStruct(lambda = 0.01, alpha = 0.5),
              iter = 2L) # increase iter for your own data
getCov(model)
getWeights(model)
## End(Not run)
```

getCor 15

## **Description**

Generates a Moran's eigenvector map of the distance matrix. See Dray, Legendre, and Peres-Neto, 2006 for more information.

## Usage

```
generateSpatialEV(coords = NULL, threshold = 0)
```

## **Arguments**

coords matrix or data.frame of coordinates
threshold ignore distances greater than threshold

#### Value

Matrix of spatial eigenvectors.

## References

Dray, S., Legendre, P., & Peres-Neto, P. R. (2006). Spatial modelling: a comprehensive framework for principal coordinate analysis of neighbour matrices (PCNM). Ecological modelling, 196(3-4), 483-493.

getCor getCor

## Description

get species-species association correlation matrix

## Usage

```
getCor(object)
## S3 method for class 'sjSDM'
getCor(object)
```

## **Arguments**

object a model fitted by sjSDM, or sjSDM with DNN object

## Value

Matrix of dimensions species by species corresponding to the covariance (occurrence) matrix.

## See Also

sjSDM,DNN

16 getImportance

getCov getCov

## **Description**

get species-species association (covariance) matrix

## Usage

```
getCov(object)
## S3 method for class 'sjSDM'
getCov(object)
```

## Arguments

object a model fitted by sjSDM, or sjSDM with DNN object

#### Value

Matrix of dimensions species by species corresponding to the covariance (occurrence) matrix.

## See Also

sjSDM,DNN

getImportance

getImportance

## Description

variation partitioning with coefficients

## Usage

```
getImportance(beta, sp = NULL, association, covX, covSP = NULL)
```

## **Arguments**

beta abiotic weights
sp spatial weights
association species associations

covX environmental covariance matrix

covSP spatial covariance matrix

## Author(s)

Maximilian Pichler

getSe 17

getSe

Post hoc calculation of standard errors

## Description

Post hoc calculation of standard errors

## Usage

```
getSe(object, step_size = NULL, parallel = 0L)
```

## Arguments

object a model fitted by sjSDM

step\_size batch size for stochastic gradient descent

parallel number of cpu cores for the data loader, only necessary for large datasets

## Value

The object passed to this function but the object\$se field contains the standard errors now

getWeights

Get weights

# Description

return weights of each layer

# Usage

```
getWeights(object)
## S3 method for class 'sjSDM'
getWeights(object)
```

# Arguments

object of class sjSDM with DNN

#### Value

- layers list of layer weights
- sigma weight to construct covariance matrix

18 importance

#### **Description**

Computes standardized variance components with respect to abiotic, biotic, and spatial effect groups.

## Usage

```
importance(x, save_memory = TRUE, ...)
```

#### **Arguments**

x object fitted by sjSDM or a list with beta, the association matrix, and the correlation matrix of the predictors, see details below
save\_memory use torch backend to calculate importance with single precision floats
additional arguments

#### **Details**

This variance partitioning approach is based on Ovaskainen et al., 2017. For an example how to interpret the outputs, see Leibold et al., 2021. This function will be deprecated in the future. Please use plot(anova(model), internal=TRUE) (currently only supported for spatial models).

## Value

An S3 class of type 'sjSDMimportance' including the following components:

names Character vector, species names.

res Data frame of results.

spatial Logical, spatial model or not.

Implemented S3 methods include print.sjSDMimportance and plot.sjSDMimportance

#### Author(s)

Maximilian Pichler

## References

Ovaskainen, O., Tikhonov, G., Norberg, A., Guillaume Blanchet, F., Duan, L., Dunson, D., ... & Abrego, N. (2017). How to make more out of community data? A conceptual framework and its implementation as models and software. Ecology letters, 20(5), 561-576.

Leibold, M. A., Rudolph, F. J., Blanchet, F. G., De Meester, L., Gravel, D., Hartig, F., ... & Chase, J. M. (2021). The internal structure of metacommunities. Oikos.

## See Also

```
print.sjSDMimportance, plot.sjSDMimportance
```

installation\_help 19

#### **Examples**

```
## Not run:
library(sjSDM)
com = simulate_SDM(sites = 300L, species = 12L,
                   link = "identical", response = "identical")
Raw = com$response
SP = matrix(rnorm(300*2), 300, 2)
SPweights = matrix(rnorm(12L), 1L)
SPweights[1,1:6] = 0
Y = Raw + (SP[,1,drop=FALSE]*SP[,2,drop=FALSE]) %*% SPweights
Y = ifelse(Y > 0, 1, 0)
model = sjSDM(Y = Y,env = linear(com$env_weights, lambda = 0.001),
              spatial = linear(SP, formula = ~0+X1:X2, lambda = 0.001),
              biotic = bioticStruct(lambda = 0.001),iter = 40L)
imp = importance(model)
plot(imp)
## End(Not run)
```

installation\_help

Installation help

#### **Description**

Trouble shooting guide for the installation of the sjSDM package

We provide a function <code>install\_sjSDM</code> to install automatically all necessary python dependencies but it can fail sometimes because of individual system settings or if other python/conda installations get into the way.

#### 'PyTorch' Installation - Before you start

A few notes before you start with the installation (skip this point if you do not know 'conda'):

- existing 'conda' installations: make sure you have the latest conda3/miniconda3 version and remove unnecessary 'conda' installations.
- existing 'conda'/'virtualenv' environments (skip this point if you do not know 'conda'): we currently enforce the usage of a specific environment called 'r-sjsdm', so if you want use a custom environment it should be named 'r-sjsdm'

#### Windows - automatic installation

Sometimes the automatic 'miniconda' installation (via install\_sjSDM) doesn't work because of white spaces in the user's name. But you can easily download and install 'conda' on your own:

Download and install the latest 'conda' version

Afterwards run:

install\_sjSDM(version = c("gpu")) # or "cpu" if you do not have a proper gpu device Reload the package and run the example, if this doesn't work:

- · Restart RStudio
- Install manually 'pytorch', see the following section

20 installation\_help

#### Windows - manual installation

Download and install the latest 'conda' version:

- Install the latest 'conda' version
- Open the command window (cmd.exe hit windows key + r and write cmd)

Run in cmd.exe:

```
$ conda create --name r-sjsdm python=3.7
$ conda activate r-sjsdm
$ conda install pytorch torchvision cpuonly -c pytorch # cpu
$ conda install pytorch torchvision cudatoolkit=11.3 -c pytorch #gpu
$ python -m pip install pyro-ppl torch_optimizer madgrad
```

Restart R, try to run the example, and if this doesn't work:

- · Restart RStudio
- See the 'Help and bugs' section

#### **Linux - automatic installation**

Run in R:

 $install\_sjSDM(version = c("gpu")) # or "cpu" if you do not have a proper 'gpu' device Restart R try to run the example, if this doesn't work:$ 

- · Restart RStudio
- Install manually 'PyTorch', see the following section

#### Linux - manual installation

We strongly advise to use a 'conda' environment but a virtual env should also work. The only requirement is that it is named 'r-sjsdm'

Download and install the latest 'conda' version:

- Install the latest 'conda' version
- · Open your terminal

Run in your terminal:

```
$ conda create --name r-sjsdm python=3.7
$ conda activate r-sjsdm
$ conda install pytorch torchvision cpuonly -c pytorch # cpu
$ conda install pytorch torchvision cudatoolkit=11.3 -c pytorch #gpu
$ python -m pip install pyro-ppl torch_optimizer madgrad
```

Restart R try to run the example, if this doesn't work:

- Restart RStudio
- See the 'Help and bugs' section

install\_diagnostic 21

#### **MacOS** - automatic installation

Run in R:

```
install_sjSDM(version = c("cpu"))
```

Restart R try to run the example, if this doesn't work:

- · Restart RStudio
- Install manually 'PyTorch', see the following section

#### **MacOS** - manual installation

Download and install the latest 'conda' version:

- Install the latest 'conda' version
- · Open your terminal

Run in your terminal:

```
$ conda create --name r-sjsdm python=3.7
$ conda activate r-sjsdm
$ python -m pip install torch torchvision torchaudio
$ python -m pip install pyro-ppl torch_optimizer madgrad
```

Restart R try to run the example from, if this doesn't work:

- · Restart RStudio
- See the 'Help and bugs' section

## Help and bugs

To report bugs or ask for help, post a reproducible example via the sjSDM issue tracker with a copy of the install\_diagnostic output as a quote.

# Description

Print information about available conda environments, python configs, and pytorch versions.

## Usage

```
install_diagnostic()
```

## **Details**

If the trouble shooting guide installation\_help did not help with the installation, please create an issue on issue tracker with the output of this function as a quote.

#### Value

No return value, called to extract dependency information.

is\_torch\_available

#### See Also

```
installation_help, install_sjSDM
```

 $install\_sjSDM$ 

Install sjSDM and its dependencies

## **Description**

Install sjSDM and its dependencies

#### Usage

```
install_sjSDM(
  conda = "auto",
  version = c("cpu", "gpu"),
  restart_session = TRUE,
  ...
)
```

## Arguments

```
conda path to conda

version version = "cpu" for CPU version, or "gpu" for GPU version. (note MacOS users have to install 'cuda' binaries by themselves)

restart_session

Restart R session after installing (note this will only occur within RStudio).

... not supported
```

## Value

No return value, called for side effects (installation of 'python' dependencies).

```
is_torch_available is_torch_available
```

## **Description**

```
is_torch_available
```

#### Usage

```
is_torch_available()
```

#### **Details**

check whether torch is available

#### Value

Logical, is torch module available or not.

linear 23

linear

Linear model of environmental response

## **Description**

specify the model to be fitted

## Usage

```
linear(data = NULL, formula = NULL, lambda = 0, alpha = 0.5)
```

#### **Arguments**

data matrix of environmental predictors formula formula object for predictors

lambda lambda penalty, strength of regularization:  $\lambda * (lasso + ridge)$ 

alpha weighting between lasso and ridge:  $(1-\alpha)*|coefficients|+\alpha||coefficients||^2$ 

#### Value

An S3 class of type 'linear' including the following components:

formula Model matrix formula

X Model matrix of covariates

data Raw data

11\_coef L1 regularization strength, can be -99 if lambda = 0.0 12\_coef L2 regularization strength, can be -99 if lambda = 0.0

Implemented S3 methods include print.linear

## See Also

```
DNN, sjSDM
```

## **Examples**

```
## Not run:

# Basic workflow:

## simulate community:
com = simulate_SDM(env = 3L, species = 7L, sites = 100L)

## fit model:
model = sjSDM(Y = com$response,env = com$env_weights, iter = 50L)
# increase iter for your own data

coef(model)
summary(model)
getCov(model)

## plot results
```

24 linear

```
species=c("sp1", "sp2", "sp3", "sp4", "sp5", "sp6", "sp7")
group=c("mammal","bird","fish","fish","mammal","amphibian","amphibian")
group = data.frame(species=species,group=group)
plot(model,group=group)
## calculate post-hoc p-values:
p = getSe(model)
summary(p)
## or turn on the option in the sjSDM function:
model = sjSDM(Y = com$response, env = com$env_weights, se = TRUE,
              family = binomial("probit"),
              iter = 2L)
summary(model)
## fit model with interactions:
model = sjSDM(Y = com$response,
              env = linear(data = com$env_weights, formula = ~X1:X2 + X3),
              se = TRUE,
              iter = 2L) # increase iter for your own data
summary(model)
## without intercept:
model = update(model, env_formula = ~0+X1:X2 + X3)
summary(model)
## predict with model:
preds = predict(model, newdata = com$env_weights)
## calculate R-squared:
R2 = Rsquared(model)
print(R2)
# With spatial terms:
## linear spatial model
XY = matrix(rnorm(200), 100, 2)
model = sjSDM(Y = com$response, env = linear(com$env_weights),
              spatial = linear(XY, ~0+X1:X2),
              iter = 50L) # increase iter for your own data
summary(model)
predict(model, newdata = com$env_weights, SP = XY)
R2 = Rsquared(model)
print(R2)
\#\# Using spatial eigenvectors as predictors to account
## for spatial autocorrelation is a common approach:
SPV = generateSpatialEV(XY)
model = sjSDM(Y = com$response, env = linear(com$env_weights),
              spatial = linear(SPV, ~0+., lambda = 0.1),
              iter = 50L) # increase iter for your own data
summary(model)
predict(model, newdata = com$env_weights, SP = SPV)
## Visualize internal meta-community structure
an = anova(model)
plot(an, internal=TRUE)
```

linear 25

```
## non-linear(deep neural network) model
model = sjSDM(Y = com$response, env = linear(com$env_weights),
              spatial = DNN(SPV, hidden = c(5L, 5L), \sim 0+.),
              iter = 2L) # increase iter for your own data
summary(model)
predict(model, newdata = com$env_weights, SP = SPV)
# Regularization
## lambda is the regularization strength
## alpha weights the lasso or ridge penalty:
## - alpha = 0 --> pure lasso
## - alpha = 1.0 --> pure ridge
model = sjSDM(Y = com$response,
              # mix of lasso and ridge
              env = linear(com$env_weights, lambda = 0.01, alpha = 0.5),
              \ensuremath{\text{\#}} we can do the same for the species-species associations
              biotic = bioticStruct(lambda = 0.01, alpha = 0.5),
              iter = 2L) # increase iter for your own data
summary(model)
coef(model)
getCov(model)
# Anova
com = simulate_SDM(env = 3L, species = 15L, sites = 200L, correlation = TRUE)
XY = matrix(rnorm(400), 200, 2)
SPV = generateSpatialEV(XY)
model = sjSDM(Y = com$response, env = linear(com$env_weights),
              spatial = linear(SPV, ~0+.),
              iter = 50L) # increase iter for your own data
result = anova(model)
print(result)
plot(result)
## visualize meta-community structure
plot(result, internal=TRUE)
# Deep neural network
## we can fit also a deep neural network instead of a linear model:
model = sjSDM(Y = com$response,
              env = DNN(com$env_weights, hidden = c(10L, 10L, 10L)),
              iter = 2L) # increase iter for your own data
summary(model)
getCov(model)
pred = predict(model, newdata = com$env_weights)
## extract weights
weights = getWeights(model)
## we can also assign weights:
setWeights(model, weights)
```

26 madgrad

logLik.sjSDM

Extract negative-log-Likelihood from a fitted sjSDM model

## **Description**

Extract negative-log-Likelihood from a fitted sjSDM model

## Usage

```
## S3 method for class 'sjSDM'
logLik(object, individual = FALSE, ...)
```

## **Arguments**

object a model fitted by sjSDM

individual returns internal ll structure, mostly for internal useage

... optional arguments passed to internal logLik function (only used if individual=TRUE)

#### Value

Numeric value or numeric matrix if individual is true.

madgrad madgrad

## **Description**

stochastic gradient descent optimizer

## Usage

```
madgrad(momentum = 0.9, weight_decay = 0, eps = 1e-06)
```

# **Arguments**

```
momentum strength of momentum weight_decay 12 penalty on weights eps epsilon
```

new\_image 27

#### Value

Anonymous function that returns optimizer when called.

#### References

Defazio, A., & Jelassi, S. (2021). Adaptivity without Compromise: A Momentumized, Adaptive, Dual Averaged Gradient Method for Stochastic Optimization. arXiv preprint arXiv:2101.11075.

new\_image

new\_image function

## **Description**

```
new_image function
```

### Usage

```
new_image(
  z,
  cols = (grDevices::colorRampPalette(c("white", "#24526E"), bias = 1.5))(10),
  range = c(0.5, 1)
)
```

## **Arguments**

```
z z matrix

cols cols for gradient

range rescale to range
```

plot.sjSDM

Coefficients plot

#### **Description**

Plotting coefficients returned by sjSDM model. This function only for model fitted by linear, fitted by DNN is not yet supported.

## Usage

```
## S3 method for class 'sjSDM' plot(x, ...)
```

## **Arguments**

```
x a model fitted by sjSDM
```

... Additional arguments to pass to plotsjSDMcoef.

28 plot.sjSDM.DNN

#### Value

ggplot2 object for linear sjSDM model and nothing for DNN sjSDM model.

## Author(s)

CAI Wang

## See Also

```
plotsjSDMcoef
```

## **Examples**

```
## Not run:
library(sjSDM)
# simulate community:
com = simulate_SDM(env = 6L, species = 7L, sites = 100L)

# fit model:
model = sjSDM(Y = com$response,env = com$env_weights, iter = 2L,se = TRUE)

#create a group dataframe for plot
species=c("sp1","sp2","sp3","sp4","sp5","sp6","sp7")
group=c("mammal","bird","fish","fish","mammal","amphibian","amphibian")
group = data.frame(species=species,group=group)

plot(model,group=group)

## End(Not run)
```

 ${\tt plot.sjSDM.DNN}$ 

Training history

## **Description**

Plot training loss history

## Usage

```
## S3 method for class 'sjSDM.DNN' plot(x, ...)
```

## **Arguments**

```
x a model fitted by sjSDM with DNN object... passed to plot
```

## Value

No return value, called for side effects.

plot.sjSDManova 29

#### **Examples**

```
## Not run:
library(sjSDM)
# simulate community:
com = simulate_SDM(env = 6L, species = 7L, sites = 100L)

# fit model:
model = sjSDM(Y = com$response,env = com$env_weights, iter = 2L,se = TRUE)

#create a group dataframe for plot
species=c("sp1","sp2","sp3","sp4","sp5","sp6","sp7")
group=c("mammal","bird","fish","fish","mammal","amphibian","amphibian")
group = data.frame(species=species,group=group)

plot(model,group=group)

## End(Not run)
```

plot.sjSDManova

Plot anova results

## Description

Plot anova results

# Usage

```
## S3 method for class 'sjSDManova'
plot(
    x,
    y,
    type = c("McFadden", "Deviance", "Nagelkerke"),
    internal = FALSE,
    add_shared = FALSE,
    cols = c("#7FC97F", "#BEAED4", "#FDC086"),
    alpha = 0.15,
    env_deviance = NULL,
    suppress_plotting = FALSE,
    ...
)
```

#### **Arguments**

```
x anova object from anova.sjSDM
y unused argument
type deviance, Nagelkerke or McFadden R-squared
internal logical, plot internal or total structure
add_shared Add shared contributions when plotting the internal structure
cols colors for the groups
alpha alpha for colors
```

```
env_deviance environmental deviance
suppress_plotting
return plots but don't plot them
... Additional arguments to pass to plot()
The internal = TRUE plot was heavily inspired by Leibold et al., 2022
```

#### Value

List with the following components:

If internal=TRUE:

plots ggplot objects for sites and species.

data List of data.frames with the shown results.

else:

VENN Matrix of shown results.

#### References

Leibold, M. A., Rudolph, F. J., Blanchet, F. G., De Meester, L., Gravel, D., Hartig, F., ... & Chase, J. M. (2022). The internal structure of metacommunities. Oikos, 2022(1).

```
plot.sjSDMimportance Plotimportance
```

# Description

Plot importance

#### Usage

```
## S3 method for class 'sjSDMimportance'
plot(x, y, col.points = "#24526e", cex.points = 1.2, ...)
```

## **Arguments**

```
x a model fitted by importance
y unused argument
col.points point color
cex.points point size
... Additional arguments to pass to plot()
```

## Value

The visualized matrix is silently returned.

plot.sjSDM\_cv 31

plot.sjSDM_cv	Plot elastic net tuning	

#### **Description**

Plot elastic net tuning

#### Usage

```
## S3 method for class 'sjSDM_cv'
plot(x, y, perf = c("logLik", "AUC", "AUC_macro"), resolution = 6, k = 3, ...)
```

## **Arguments**

x a model fitted by sjSDM\_cv

y unused argument

perf performance measurement to plot

resolution resolution of grid

k number of knots for the gm

... Additional arguments to pass to plot()

## Value

Named vector of optimized regularization parameters.

#### Without space:

lambda\_cov Regularization strength in the bioticStruct object.

alpha\_cov Weigthing between L1 and L2 in the bioticStruct object.

lambda\_coef Regularization strength in the linear or DNN object.

alpha\_coef Weigthing between L1 and L2 in the linear or DNN object.

# With space:

lambda\_cov Regularization strength in the bioticStruct object.

alpha\_cov Weigthing between L1 and L2 in the bioticStruct object.

lambda\_coef Regularization strength in the linear or DNN object.

alpha\_coef Weigthing between L1 and L2 in the linear or DNN object.

lambda\_spatial Regularization strength in the linear or DNN object for the spatial component.

alpha\_spatial Weighing between L1 and L2 in thelinear or DNN object for the spatial com-

ponent.

32 plotInternalStructure

```
plotInternalStructure Plot internal metacommunity structure
```

## **Description**

Plot internal metacommunity structure

## Usage

```
plotInternalStructure(
  object,
  Rsquared = c("McFadden", "Nagelkerke"),
  add_shared = FALSE,
  env_deviance = NULL,
  suppress_plotting = FALSE
)
```

## **Arguments**

object anova object from anova.sjSDM

Rsquared which R squared should be used, McFadden or Nagelkerke (McFadden is de-

fault)

add\_shared split shared components, default is TRUE

env\_deviance environmental deviance

 $suppress\_plotting$ 

should the plots be suppressed or not.

Plots and returns the internal metacommunity structure of species and sites (see

Leibold et al., 2022). Plots were heavily inspired by Leibold et al., 2022

#### Value

List with the following components:

plots ggplot objects for sites and species.

data List of data.frames with the internal metacommunity structure.

## References

Leibold, M. A., Rudolph, F. J., Blanchet, F. G., De Meester, L., Gravel, D., Hartig, F., ... & Chase, J. M. (2022). The internal structure of metacommunities. Oikos, 2022(1).

plotsjSDMcoef 33

## Description

Plotting coefficients returned by sjSDM model. This function only for model fitted by linear, fitted by DNN is not yet supported.

# Usage

```
plotsjSDMcoef(object, wrap_col = NULL, group = NULL, col = NULL, slist = NULL)
```

#### **Arguments**

object	a model fitted by sjSDM
wrap_col	Scales argument passed to wrap_col
group	Define the taxonomic characteristics of a species, you need to provide a dataframe with column1 named "species" and column2 named "group", default is NULL. For example, group[1,1]== "sp1", group[1,2]== "Mammal".
col	Define colors for groups, default is NULL.
slist	Select the species you want to plot, default is all, parameter is not supported yet.

#### Value

```
ggplot2 object
```

#### Author(s)

CAI Wang

# **Examples**

```
## Not run:
library(sjSDM)
# simulate community:
com = simulate_SDM(env = 6L, species = 7L, sites = 100L)

# fit model:
model = sjSDM(Y = com$response,env = com$env_weights, iter = 2L,se = TRUE)

#create a group dataframe for plot
species=c("sp1","sp2","sp3","sp4","sp5","sp6","sp7")
group=c("mammal","bird","fish","fish","mammal","amphibian","amphibian")
group = data.frame(species=species,group=group)

## End(Not run)
```

print.bioticStruct 34

predict.sjSDM

Predict from a fitted sjSDM model

## **Description**

Predict from a fitted sjSDM model

## Usage

```
## S3 method for class 'sjSDM'
predict(
  object,
  newdata = NULL,
  SP = NULL,
  type = c("link", "raw"),
  dropout = FALSE,
```

#### **Arguments**

a model fitted by sjSDM object newdata for predictions newdata

SP spatial predictors (e.g. X and Y coordinates)

type raw or link

dropout use dropout for predictions or not, only supported for DNNs

optional arguments for compatibility with the generic function, no function im-. . .

plemented

## Value

Matrix of predictions (sites by species)

print.bioticStruct

Print a bioticStruct object

#### **Description**

Print a bioticStruct object

# Usage

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

# **Arguments**

object created by bioticStruct Χ

optional arguments for compatibility with the generic function, no function im-

plemented

print.DNN 35

print.DNN

Print a DNN object

# Description

Print a DNN object

## Usage

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

# **Arguments**

x object created by DNN

... optional arguments for compatibility with the generic function, no function implemented

print.linear

Print a linear object

# Description

Print a linear object

# Usage

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

# Arguments

x object created by linear

... optional arguments for compatibility with the generic function, no function implemented

## Value

Invisible formula object

36 print.sjSDManova

print.sjSDM

Print a fitted sjSDM model

## Description

Print a fitted sjSDM model

## Usage

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

# **Arguments**

x a model fitted by sjSDM

... optional arguments for compatibility with the generic function, no function implemented

## Value

No return value

print.sjSDManova

Print sjSDM anova

## Description

Print sjSDM anova

## Usage

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

# Arguments

x an object of anova.sjSDM

... optional arguments for compatibility with the generic function, no function implemented

#### Value

The above matrix is silently returned

```
print.sjSDMimportance Print importance
```

### Description

Print importance

# Usage

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

# Arguments

x an object of importance

... optional arguments for compatibility with the generic function, no function implemented

### Value

The matrix above is silently returned

print.sjSDM\_cv

Print a fitted sjSDM\_cv model

### Description

Print a fitted sjSDM\_cv model

### Usage

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

### **Arguments**

x a model fitted by sjSDM\_cv

... optional arguments for compatibility with the generic function, no function implemented

#### Value

Above data frame is silently returned.

Rsquared Rsquared

**RMSprop** 

RMSprop

### **Description**

RMSprop optimizer

### Usage

```
RMSprop(
  alpha = 0.99,
  eps = 1e-08,
  weight_decay = 1e-04,
  momentum = 0.1,
  centered = FALSE
)
```

# Arguments

alpha decay factor eps fuzz factor

weight\_decay 12 penalty on weights

momentum momentum centered centered or not

### Value

Anonymous function that returns optimizer when called.

Rsquared

R-squared

# Description

calculate R-squared following McFadden or Nagelkerke

### Usage

```
Rsquared(model, method = c("McFadden", "Nagelkerke"))
```

# Arguments

model model

method McFadden or Nagelkerke

setWeights 39

#### **Details**

Calculate R-squared following Nagelkerke or McFadden:

```
• Nagelkerke: R^2 = 1 - \exp(2/N \cdot (\log \mathcal{L}_0 - \log \mathcal{L}_1))
```

• McFadden: 
$$R^2 = 1 - log \mathcal{L}_1 / log \mathcal{L}_0$$

#### Value

R-squared as numeric value

### Author(s)

Maximilian Pichler

setWeights

Set weights

### Description

set layer weights and sigma in sjSDM with DNN object

### Usage

```
setWeights(object, weights)
## S3 method for class 'sjSDM'
setWeights(object, weights = NULL)
```

### **Arguments**

#### Value

No return value, weights are changed in place.

40 simulate.sjSDM

SGD SGD

### **Description**

stochastic gradient descent optimizer

### Usage

```
SGD(momentum = 0.5, dampening = 0, weight_decay = 0, nesterov = TRUE)
```

#### **Arguments**

momentum strength of momentum

dampening decay

weight\_decay 12 penalty on weights

nesterov Mesterov momentum or not

#### Value

Anonymous function that returns optimizer when called.

simulate.sjSDM Generates

Generates simulations from sjSDM model

### **Description**

Simulate nsim responses from the fitted model following a multivariate probit model. So currently only supported for family = stats::binomial("probit")

### Usage

```
## S3 method for class 'sjSDM'
simulate(object, nsim = 1, seed = NULL, ...)
```

### **Arguments**

object a model fitted by sjSDM nsim number of simulations

seed seed for random number generator

... optional arguments for compatibility with the generic function, no functionality

implemented

### Value

Array of simulated species occurrences of dimension order [nsim, sites, species]

simulate\_SDM 41

simulate\_SDM

Simulate joint Species Distribution Models

### **Description**

Simulate species distributions

### Usage

```
simulate_SDM(
  env = 5L,
  sites = 100L,
  species = 5L,
  correlation = TRUE,
  weight_range = c(-1, 1),
  link = "probit",
  response = "pa",
  sparse = NULL,
  tolerance = 0.05,
  iter = 20L,
  seed = NULL
)
```

### **Arguments**

env number of environment variables

sites number of sites species number of species

correlation correlated species TRUE or FALSE, can be also a function or a matrix

weight\_range sample true weights from uniform range, default -1,1

link probit, logit or identical

response pa (presence-absence) or count

sparse sparse rate

tolerance tolerance for sparsity check iter tries until sparse rate is achieved seed random seed. Default = 42

#### **Details**

Probit is not possible for abundance response (response = 'count')

### Value

List of simulation results:

env Number of environmental covariates

species Number of species sites Number of sites

link Which link

response\_type Which response type

response Species occurrence matrix correlation Species covariance matrix

species\_weights

Species-environment coefficients

env\_weights Environmental covariates

corr\_acc Method to calculate sign accurracy

#### Author(s)

Maximilian Pichler

sjSDM

Fitting scalable joint Species Distribution Models (sjSDM)

### **Description**

sjSDM is used to fit joint Species Distribution models (jSDMs) using the central processing unit (CPU) or the graphical processing unit (GPU). The default is a multivariate probit model based on a Monte-Carlo approximation of the joint likelihood. sjSDM can be used to fit linear but also deep neural networks and supports the well known formula syntax.

### Usage

```
siSDM(
 Y = NULL,
 env = NULL,
 biotic = bioticStruct(),
  spatial = NULL,
  family = stats::binomial("probit"),
  iter = 100L,
  step_size = NULL,
 learning_rate = 0.01,
  se = FALSE,
  sampling = 100L,
 parallel = 0L,
 control = sjSDMControl(),
 device = "cpu",
 dtype = "float32";
  seed = 758341678
)
sjSDM.tune(object)
```

#### **Arguments**

Υ	matrix of species occurrences/responses in range
env	matrix of environmental predictors, object of type linear or DNN
biotic	defines biotic (species-species associations) structure, object of type bioticStruct
spatial	defines spatial structure, object of type linear or DNN
family	error distribution with link function, see details for supported distributions
iter	number of fitting iterations
step_size	batch size for stochastic gradient descent, if NULL then step_size is set to: step_size = 0.1*nrow(X)
learning_	_rate learning rate for Adamax optimizer
se	calculate standard errors for environmental coefficients
sampling	number of sampling steps for Monte Carlo integration
parallel	number of cpu cores for the data loader, only necessary for large datasets
control	control parameters for optimizer, see sjSDMControl
device	which device to be used, "cpu" or "gpu"
dtype	which data type, most GPUs support only 32 bit floats.
seed	and for renders exerctions
	seed for random operations
object	object of type sjSDM_cv

#### **Details**

The function fits per default a multivariate probit model via Monte-Carlo integration (see Chen et al., 2018) of the joint likelihood for all species.

### Model description:

The most common jSDM structure describes the site (i=1,...,I) by species (j=1,...,J) matrix  $Y_{ij}$  as a function of environmental covariates  $X_{in}(n=1,...,N)$  covariates), and the species-species covariance matrix  $\Sigma$  accounts for correlations in  $e_{ij}$ :

$$g(Z_{ij}) = \beta_{j0} + \sum_{n=1}^{N} X_{in} \beta_{nj} + e_{ij}$$

with g(.) as link function. For the multivariate probit model, the link function is:

$$Y_{ij} = 1(Z_{ij} > 0)$$

The probability to observe the occurrence vector  $\mathbf{Y}_{i}$  is:

$$Pr(\mathbf{Y_i}|\mathbf{X_i}\boldsymbol{\beta}, \boldsymbol{\Sigma}) = \int_{\mathbf{A_{iJ}}} ... \int_{\mathbf{A_{i1}}} \phi_{\mathbf{J}}(\mathbf{Y_i^*}; \mathbf{X_i}\boldsymbol{\beta}, \boldsymbol{\Sigma}) \mathbf{dY_{i1}^*}...\mathbf{dY_{iJ}^*}$$

in the interval  $A_{ij}$  with  $(-\inf, 0]$  if  $Y_{ij} = 0$  and  $[0, +\inf)$  if  $Y_{ij} = 1$ .

and  $\phi$  being the density function of the multivariate normal distribution.

The probability of  $Y_i$  requires to integrate over  $Y_i^*$  which has no closed analytical expression for more than two species which makes the evaluation of the likelihood computationally costly and needs a numerical approximation. The previous equation can be expressed more generally as:

$$\mathcal{L}(\beta, \Sigma; \mathbf{Y_i}, \mathbf{X_i}) = \int_{\Omega} \prod_{i=1}^{J} \mathbf{Pr}(\mathbf{Y_{ij}} | \mathbf{X_i} \beta + \zeta) \mathbf{Pr}(\zeta | \mathbf{\Sigma}) d\zeta$$

sjSDM approximates this integral by M Monte-Carlo samples from the multivariate normal species-species covariance. After integrating out the covariance term, the remaining part of the likelihood can be calculated as in an univariate case and the average of the M samples are used to get an approximation of the integral:

$$\mathcal{L}(\beta, \Sigma; \mathbf{Y_i}, \mathbf{X_i}) \approx \frac{1}{M} \mathbf{\Sigma_{m=1}^M} \prod_{i=1}^{J} \mathbf{Pr}(\mathbf{Y_{ij}}|\mathbf{X_i}\beta + \zeta_m)$$

with  $\zeta_m \sim MVN(0, \Sigma)$ .

sjSDM uses 'PyTorch' to run optionally the model on the graphical processing unit (GPU). Python dependencies needs to be installed before being able to use the sjSDM function. We provide a function which installs automatically python and the python dependencies. See install\_sjSDM, vignette("Dependencies", package = "sjSDM")

See Pichler and Hartig, 2020 for benchmark results.

#### Supported distributions:

Currently supported distributions and link functions:

```
• binomial: "probit" or "logit"
```

• poisson: "log"

• "nbinom": "log"

• gaussian: "identity"

### Space:

We can extend the model to account for spatial auto-correlation between the sites by:

$$g(Z_{ij}) = \beta_{j0} + \sum_{n=1}^{N} X_{in} \beta_{nj} + \sum_{m=1}^{M} S_{im} \alpha_{mj} + e_{ij}$$

There are two ways to generate spatial predictors S:

- trend surface model using spatial coordinates in a polynomial: linear(data=Coords, ~0+poly(X, Y, degree = 2))
- eigenvector spatial filtering using spatial eigenvectors. Spatial eigenvectors can be generated by the generateSpatialEV function:

```
SPV = generateSpatialEV(Coords)
```

Then we use, for example, the first 20 spatial eigenvectors:

linear(data=SPV[,1:20], ~0+.)

It is important to set the intercept to 0 in the spatial term (e.g. via ~0+.) because the intercept is already set in the environmental object.

### **Installation:**

install\_sjSDM should be theoretically able to install conda and 'PyTorch' automatically. If sjSDM still does not work after reloading RStudio, you can try to solve this on your following our trouble shooting guide installation\_help. If the problem remains, please create an issue on issue tracker with a copy of the install\_diagnostic output as a quote.

#### Value

An S3 class of type 'sjSDM' including the following components:

cl Model call

formula Formula object for environmental covariates.

names Names of environmental covariates.

species Names of species (can be NULL if columns of Y are not named).

get\_model Method which builds and returns the underlying 'python' model.

logLik negative log-Likelihood of the model and the regularization loss.

model The actual model.

settings List of model settings, see arguments of sjSDM.

family Response family.

time Runtime.

data List of Y, X (and spatial) model matrices.

sessionInfo Output of sessionInfo.

weights List of model coefficients (environmental (and spatial)).

sigma Lower triangular weight matrix for the covariance matrix.

history History of iteration losses.

se Matrix of standard errors, if se = FALSE the field 'se' is NULL.

Implemented S3 methods include summary.sjSDM, plot.sjSDM, print.sjSDM, predict.sjSDM, and coef.sjSDM. For other methods, see section 'See Also'.

sjSDM. tune returns an S3 object of class 'sjSDM', see above for information about values.

### Author(s)

Maximilian Pichler

### References

Chen, D., Xue, Y., & Gomes, C. P. (2018). End-to-end learning for the deep multivariate probit model. arXiv preprint arXiv:1803.08591.

Pichler, M., & Hartig, F. (2021). A new joint species distribution model for faster and more accurate inference of species associations from big community data. Methods in Ecology and Evolution, 12(11), 2159-2173.

#### See Also

```
getCor, getCov, update.sjSDM, sjSDM_cv, DNN, plot.sjSDM, print.sjSDM, predict.sjSDM,
coef.sjSDM, summary.sjSDM, simulate.sjSDM, getSe, anova.sjSDM, importance
```

# **Examples**

```
## Not run:

# Basic workflow:
## simulate community:
com = simulate_SDM(env = 3L, species = 7L, sites = 100L)

## fit model:
model = sjSDM(Y = com$response,env = com$env_weights, iter = 50L)
# increase iter for your own data

coef(model)
summary(model)
```

```
getCov(model)
## plot results
species=c("sp1","sp2","sp3","sp4","sp5","sp6","sp7")
group=c("mammal","bird","fish","fish","mammal","amphibian","amphibian")
group = data.frame(species=species,group=group)
plot(model,group=group)
## calculate post-hoc p-values:
p = getSe(model)
summary(p)
## or turn on the option in the sjSDM function:
model = sjSDM(Y = com$response, env = com$env_weights, se = TRUE,
              family = binomial("probit"),
              iter = 2L)
summary(model)
## fit model with interactions:
model = sjSDM(Y = com$response,
              env = linear(data = com$env_weights, formula = ~X1:X2 + X3),
              se = TRUE,
              iter = 2L) # increase iter for your own data
summary(model)
## without intercept:
model = update(model, env_formula = ~0+X1:X2 + X3)
summary(model)
## predict with model:
preds = predict(model, newdata = com$env_weights)
## calculate R-squared:
R2 = Rsquared(model)
print(R2)
# With spatial terms:
## linear spatial model
XY = matrix(rnorm(200), 100, 2)
model = sjSDM(Y = com$response, env = linear(com$env_weights),
              spatial = linear(XY, ~0+X1:X2),
              iter = 50L) # increase iter for your own data
summary(model)
predict(model, newdata = com$env_weights, SP = XY)
R2 = Rsquared(model)
print(R2)
## Using spatial eigenvectors as predictors to account
## for spatial autocorrelation is a common approach:
SPV = generateSpatialEV(XY)
model = sjSDM(Y = com$response, env = linear(com$env_weights),
              spatial = linear(SPV, ~0+., lambda = 0.1),
              iter = 50L) # increase iter for your own data
summary(model)
predict(model, newdata = com$env_weights, SP = SPV)
```

```
## Visualize internal meta-community structure
an = anova(model)
plot(an, internal=TRUE)
## non-linear(deep neural network) model
model = sjSDM(Y = com$response, env = linear(com$env_weights),
              spatial = DNN(SPV, hidden = c(5L, 5L), ~0+.),
              iter = 2L) # increase iter for your own data
summarv(model)
predict(model, newdata = com$env_weights, SP = SPV)
# Regularization
## lambda is the regularization strength
## alpha weights the lasso or ridge penalty:
## - alpha = 0 --> pure lasso
## - alpha = 1.0 --> pure ridge
model = sjSDM(Y = com$response,
              # mix of lasso and ridge
              env = linear(com$env_weights, lambda = 0.01, alpha = 0.5),
              # we can do the same for the species-species associations
              biotic = bioticStruct(lambda = 0.01, alpha = 0.5),
              iter = 2L) # increase iter for your own data
summary(model)
coef(model)
getCov(model)
com = simulate_SDM(env = 3L, species = 15L, sites = 200L, correlation = TRUE)
XY = matrix(rnorm(400), 200, 2)
SPV = generateSpatialEV(XY)
model = sjSDM(Y = com$response, env = linear(com$env_weights),
              spatial = linear(SPV, ~0+.),
              iter = 50L) # increase iter for your own data
result = anova(model)
print(result)
plot(result)
## visualize meta-community structure
plot(result, internal=TRUE)
# Deep neural network
## we can fit also a deep neural network instead of a linear model:
model = sjSDM(Y = com$response,
              env = DNN(com$env_weights, hidden = c(10L, 10L, 10L)),
              iter = 2L) # increase iter for your own data
summary(model)
getCov(model)
pred = predict(model, newdata = com$env_weights)
## extract weights
weights = getWeights(model)
```

48 sjSDMControl

sjSDMControl

sjSDM control object

### **Description**

sjSDM control object

# Usage

```
sjSDMControl(
  optimizer = RMSprop(),
  scheduler = 0,
  lr_reduce_factor = 0.99,
  early_stopping_training = 0,
  mixed = FALSE
)
```

### **Arguments**

optimizer object of type RMSprop, Adamax, SGD, AccSGD, madgrad, or AdaBound

scheduler reduce Ir on plateau scheduler or not (0 means no scheduler, > 0 number of

epochs before reducing learning rate)

lr\_reduce\_factor

factor to reduce learning rate in scheduler

early\_stopping\_training

number of epochs without decrease in training loss before invoking early stop-

ping (0 means no early stopping).

mixed mixed (half-precision) training or not. Only recommended for GPUs > 2000

series

### Value

List with the following fields:

optimizer Function which returns an optimizer. scheduler\_boolean

Logical, use scheduler or not.

sjSDM\_cv 49

```
scheduler_patience
```

Integer, number of epochs to wait before applying plateau scheduler.

lr\_reduce\_factor

Numerical, learning rate reduce factor.

mixed Logical, use mixed training or not.

early\_stopping\_training

Numerical, early stopping after n epochs.

sjSDM\_cv

Cross validation of elastic net tuning

#### **Description**

Cross validation of elastic net tuning

### Usage

```
sjSDM_cv(
  Υ,
  env = NULL,
  biotic = bioticStruct(),
  spatial = NULL,
  tune = c("random", "grid"),
  CV = 5L,
  tune\_steps = 20L,
  alpha_cov = seq(0, 1, 0.1),
  alpha_coef = seq(0, 1, 0.1),
  alpha_spatial = seq(0, 1, 0.1),
  lambda\_cov = 2^seq(-10, -1, length.out = 20),
  lambda_coef = 2^seq(-10, -0.5, length.out = 20),
  lambda_spatial = 2^seq(-10, -0.5, length.out = 20),
  device = "cpu",
  n_cores = NULL,
  n_gpu = NULL,
  sampling = 5000L,
  blocks = 1L,
)
```

# Arguments

Υ	species occurrence matrix
env	matrix of environmental predictors or object of type linear, or DNN
biotic	defines biotic (species-species associations) structure, object of type bioticStruct. Alpha and lambda have no influence
spatial	defines spatial structure, object of type linear, or DNN
tune	tuning strategy, random or grid search
CV	n-fold cross validation or list of test indices
tune_steps	number of tuning steps

50 sjSDM\_cv

```
weighting of 11 and 12 on covariances: (1 - \alpha) * |cov| + \alpha ||cov||^2
alpha_cov
                   weighting of 11 and 12 on coefficients: (1 - \alpha) * |coef| + \alpha ||coef||^2
alpha_coef
                   weighting of 11 and 12 on spatial coefficients: (1 - \alpha) * |coef_s p| + \alpha ||coef_s p||^2
alpha_spatial
lambda_cov
                   overall regularization strength on covariances
lambda_coef
                   overall regularization strength on coefficients
lambda_spatial
                   overall regularization strength on spatial coefficients
device
                   device, default cpu
n_cores
                   number of cores for parallelization
                   number of GPUs
n_gpu
sampling
                   number of sampling steps for Monte Carlo integration
                   blocks of parallel tuning steps
blocks
                   arguments passed to sjSDM, see sjSDM
```

#### Value

An S3 class of type 'sjSDM\_cv' including the following components:

tune\_results Data frame with tuning results.

short\_summary Data frame with averaged tuning results.

summary Data frame with summarized averaged results.

settings List of tuning settings, see the arguments in DNN.

data List of Y, env (and spatial) objects.

config List of sjSDM settings, see arguments of sjSDM.

spatial Logical, spatial model or not.

Implemented S3 methods include sjSDM.tune, plot.sjSDM\_cv, print.sjSDM\_cv, and summary.sjSDM\_cv

#### See Also

```
plot.sjSDM_cv, print.sjSDM_cv, summary.sjSDM_cv, sjSDM.tune
```

#### **Examples**

```
## Not run:
# simulate sparse community:
com = simulate_SDM(env = 5L, species = 25L, sites = 50L, sparse = 0.5)
# tune regularization:
tune_results = sjSDM_cv(Y = com$response,
                        env = com$env_weights,
                        tune = "random", # random steps in tune-paramter space
                        CV = 2L, # 3-fold cross validation
                        tune\_steps = 2L,
                        alpha_cov = seq(0, 1, 0.1),
                        alpha_coef = seq(0, 1, 0.1),
                        lambda_cov = seq(0, 0.1, 0.001),
                        lambda_coef = seq(0, 0.1, 0.001),
                        n_{cores} = 2L,
                        sampling = 100L,
                        # small models can be also run in parallel on the GPU
```

summary.sjSDM 51

```
iter = 2L # we can pass arguments to sjSDM via...
)

# print overall results:
tune_results

# summary (mean values over CV for each tuning step)
summary(tune_results)

# visualize tuning and best points:
# best = plot(tune_results, perf = "logLik")

# fit model with best regularization paramter:
model = sjSDM.tune(tune_results)

summary(model)

## End(Not run)
```

summary.sjSDM

Return summary of a fitted sjSDM model

### **Description**

Return summary of a fitted sjSDM model

### Usage

```
## S3 method for class 'sjSDM'
summary(object, ...)
```

#### **Arguments**

object a model fitted by sjSDM

... optional arguments for compatibility with the generic function, no functionality

implemented

### Value

The above matrix is silently returned.

summary.sjSDM\_cv

Return summary of a fitted sjSDM\_cv model

### Description

Return summary of a fitted sjSDM\_cv model

### Usage

```
## S3 method for class 'sjSDM_cv'
summary(object, ...)
```

52 update.sjSDM

### **Arguments**

object a model fitted by sjSDM\_cv

... optional arguments for compatibility with the generic function, no functionality

implemented

#### Value

Above data frame is silently returned.

update.sjSDM

Update and re-fit a model call

### **Description**

Update and re-fit a model call

### Usage

```
## S3 method for class 'sjSDM'
update(object, env_formula = NULL, spatial_formula = NULL, biotic = NULL, ...)
```

### **Arguments**

object of class 'sjSDM'

env\_formula new environmental formula

spatial\_formula

new spatial formula

biotic new biotic config
... additional arguments

### Value

An S3 class of type 'sjSDM'. See  ${\tt sjSDM}$  for more information.

# **Index**

poisson, 44

```
AccSGD, 3, 48
                                                   predict.sjSDM, 34, 45
AdaBound, 4, 48
                                                   print.bioticStruct, 6, 34
Adamax, 4, 48
                                                   print.DNN, 12, 35
anova.sjSDM, 5, 29, 32, 36, 45
                                                   print.linear, 23, 35
                                                   print.sjSDM, 36, 45
binomial, 44
                                                   print.sjSDM_cv, 37, 50
bioticStruct, 6, 31, 34, 43, 49
                                                   print.sjSDManova, 6, 36
                                                   print.sjSDMimportance, 18, 37
check_module, 10
checkModel. 9
                                                   RMSprop, 38, 48
coef.sjSDM, 10, 45
                                                   Rsquared, 38
DiffGrad, 10
                                                   sessionInfo, 45
DNN, 11, 15–17, 23, 28, 31, 35, 39, 43, 45, 49,
                                                   setWeights, 39
                                                   SGD, 40, 48
                                                   simulate.sjSDM, 40, 45
gaussian, 44
                                                   simulate_SDM, 41
generateSpatialEV, 14, 44
                                                   sjSDM, 5, 7, 10, 12, 15–18, 23, 26–28, 33, 34,
getCor, 15, 45
                                                             36, 39, 40, 42, 44, 45, 50–52
getCov, 16, 45
                                                   sjSDM. tune, 45, 50
getImportance, 16
                                                   sjSDM_cv, 31, 37, 43, 45, 49, 52
getSe, 17, 45
                                                   sjSDMControl, 43, 48
getWeights, 17, 39
                                                   summary.sjSDM, 45, 51
                                                   summary.sjSDM_cv, 50, 51
importance, 18, 30, 37, 45
install_diagnostic, 21, 21, 44
                                                   update.sjSDM, 45, 52
install_sjSDM, 19, 22, 22, 44
installation_help, 19, 21, 22, 44
is_torch_available, 22
linear, 12, 23, 31, 35, 43, 49
logLik.sjSDM, 26
madgrad, 26, 48
new_image, 27
plot.sjSDM, 27, 45
plot.sjSDM.DNN, 28
plot.sjSDM_cv, 31, 50
plot.sjSDManova, 5, 6, 29
plot.sjSDMimportance, 18, 30
plotInternalStructure, 6, 32
plotsjSDMcoef, 27, 28, 33
```