# Package 'sjSDM'

March 11, 2022

Type Package

Title Scalable Joint Species Distribution Modeling

```
Version 1.0.1
Date 2022-03-11
Description A scalable method to estimate joint Species Distribution Models (jSDMs) for big com-
      munity datasets based on a Monte Carlo approximation of the joint likelihood. The numeri-
      cal approximation is based on 'PyTorch' and 'reticu-
      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.
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      ggtern
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```

<pre>URL https://theoreticalecology.github.i</pre>	o/s-jSDM/
--	-----------

 $\pmb{BugReports} \ \, \texttt{https://github.com/TheoreticalEcology/s-jSDM/issues} \\$ 

**Roxygen** list(old\_usage = FALSE)

**VignetteBuilder** knitr **RdMacros** mathjaxr

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AccSGD

# **Description**

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

kappa long step

xi advantage parameter

small\_const small constant

weight\_decay 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.

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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**

Calculate type I anova in the following order:

Null, biotic, abiotic (environment), and spatial (if present).

Deviance for interactions (e.g. between space and environment) are also calculated and can be visualized via plot.sjSDManova.

# Usage

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

# Arguments

object model of object sjSDM

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

plemented

#### **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.
sites individual site R2s.

individual site by species negative-log-likelihood values.

Implemented S3 methods are print.sjSDManova and plot.sjSDManova

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#### See Also

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

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**

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

#### See Also

sjSDM

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#### **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
```

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```
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$env_weights, lambda = 0.01, alpha = 0.5),
              # we can do the same for the species-species associations
              biotic = bioticStruct(lambda = 0.01, alpha = 0.5),
              iter = 2L) # increase iter for your own data
summary(model)
coef(model)
getCov(model)
com = simulate_SDM(env = 3L, species = 15L, sites = 200L, correlation = TRUE)
XY = matrix(rnorm(400), 200, 2)
SPV = generateSpatialEV(XY)
model = sjSDM(Y = com$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)
```

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```
# Deep neural network
\mbox{\#\#} 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

check\_module

check module

# **Description**

check if module is loaded

# Usage

```
check_module()
```

DiffGrad

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)
```

# Arguments

betas betas eps eps

weight\_decay weight\_decay

## Value

Anonymous function that returns optimizer when called.

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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 = "relu",
   bias = TRUE,
   lambda = 0,
   alpha = 0.5,
   dropout = 0
)
```

# **Arguments**

matrix of environmental predictors data formula formula object for predictors hidden hidden units in layers, length of hidden corresponds to number of layers activation functions, can be of length one, or a vector of activation functions for activation 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:  $\lambda * (lasso + ridge)$ alpha weighting between lasso and ridge:  $(1 - \alpha) * |weights| + \alpha ||weights||^2$ 

#### Value

dropout

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

probability of dropout rate

formula	Model matrix formula
Χ	Model matrix of covariates
data	Raw data
l1_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.
activation	Character vector of activation functions.
bias	Logical vector whether to use bias or not in each hidden layer.

Implemented S3 methods include print.DNN

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$response,
              env = linear(data = com$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
```

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```
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)
```

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```
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),
              \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
getCov(model)
getWeights(model)
## End(Not run)
```

generateSpatialEV

Generate spatial eigenvectors

#### **Description**

function to generate spatial eigenvectors to account for spatial autocorrelation

#### 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.

getCov 15

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

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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

importance 17

#### **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
```

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#### **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

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#### 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

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#### **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.

install\_sjSDM 21

#### 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.

22 linear

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 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
```

linear 23

```
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)
```

24 linear

```
## 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)
```

logLik.sjSDM 25

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
```

26 plot.sjSDM

#### 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.

plot.sjSDM.DNN 27

#### Value

No return value, called for side effects.

# 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.

28 plot.sjSDManova

#### **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("Deviance", "Nagelkerke", "McFadden"),
    internal = FALSE,
    cols = c("#7FC97F", "#BEAED4", "#FDC086"),
    alpha = 0.15,
    env_deviance = NULL,
    ...
)
```

# **Arguments**

```
Χ
                  anova object from anova.sjSDM
                  unused argument
У
                  deviance, Nagelkerke or McFadden R-squared
type
internal
                  logical, plot internal or total structure
cols
                  colors for the groups
alpha
                  alpha for colors
                  environmental deviance
env_deviance
                  Additional arguments to pass to plot()
. . .
```

The internal = TRUE plot was heavily inspired by Leibold et al., 2022

plot.sjSDMimportance

# 29

#### 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,
    contour = FALSE,
    col.points = "#24526e",
    cex.points = 1.2,
    pch = 19,
    col.contour = "#ffbf02",
    ...
)
```

#### **Arguments**

```
x a model fitted by importance
y unused argument
contour plot contour or not
col.points point color
cex.points point size
pch point symbol
col.contour contour color
... Additional arguments to pass to plot()
```

#### Value

The visualized matrix is silently returned.

30 plot.sjSDM\_cv

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.

plotsjSDMcoef 31

# 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]== "Mamma1".
col	Define colors for groups, default is NULL.
slist	Select the species you want to plot, default is all, parameter is not supported yet.

# 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)
```

32 print.bioticStruct

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

object a model fitted by sjSDM newdata newdata for predictions

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

```
x object created by bioticStruct
```

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

print.DNN 33

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

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 = 0.01,
  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 Nagelkerke or McFadden

# Usage

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

# Arguments

model model

method Nagelkerke or McFadden

setWeights 37

### **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**

object of class sjSDM with DNN object

weights list of layer weights: list(env=list(matrix(...)), spatial=list(matrix(...)), sigma=matrix

see getWeights

### Value

No return value, weights are changed in place.

38 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 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 numer 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 39

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

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

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

```
sjSDM(
  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"
sjSDM.tune(object)
```

### **Arguments**

Y matrix of species occurences/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 family functions 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 number of cpu cores for the data loader, only necessary for large datasets parallel

control parameters for optimizer, see sjSDMControl control

which device to be used, "cpu" or "gpu" device

dtype which data type, most GPUs support only 32 bit floats.

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 speciesspecies 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:

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

s jSDM approximates this integral by M Monte-Carlo samples from the multivariate normal speciesspecies 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"

• 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  $\sim 0+$ .) 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 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)

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#### 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

```
update.sjSDM,sjSDM_cv,DNN,plot.sjSDM,print.sjSDM,predict.sjSDM,coef.sjSDM,summary.sjSDM,getCov,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), \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$env_weights, lambda = 0.01, alpha = 0.5),
              # we can do the same for the species-species associations
              biotic = bioticStruct(lambda = 0.01, alpha = 0.5),
              iter = 2L) # increase iter for your own data
summary(model)
coef(model)
getCov(model)
# Anova
com = simulate_SDM(env = 3L, species = 15L, sites = 200L, correlation = TRUE)
XY = matrix(rnorm(400), 200, 2)
SPV = generateSpatialEV(XY)
model = sjSDM(Y = com$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)
```

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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.

scheduler\_patience

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

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```
1r_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
                   defines spatial structure, object of type linear, or DNN
spatial
                   tuning strategy, random or grid search
tune
C۷
                   n-fold cross validation
tune_steps
                   number of tuning steps
alpha_cov
                   weighting of 11 and 12 on covariances: (1 - \alpha) * |cov| + \alpha ||cov||^2
```

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```
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
                   overall regularization strength on covariances
lambda_cov
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
                   blocks of parallel tuning steps
                   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
                        iter = 2L # we can pass arguments to sjSDM via...
```

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```
# 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, ...)
```

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## **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.

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