Package ‘cito’

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Type Package

Title Building and Training Neural Networks

Version 1.1

Description The 'cito' package provides a user-friendly interface for training and interpreting deep neural networks (DNN). 'cito' simplifies the fitting of DNNs by supporting the familiar formula syntax, hyperparameter tuning under cross-validation, and helps to detect and handle convergence problems. DNNs can be trained on CPU, GPU and MacOS GPUs. In addition, 'cito' has many downstream functionalities such as various explainable AI (xAI) metrics (e.g. variable importance, partial dependence plots, accumulated local effect plots, and effect estimates) to interpret trained DNNs. 'cito' optionally provides confidence intervals (and p-values) for all xAI metrics and predictions. At the same time, 'cito' is computationally efficient because it is based on the deep learning framework 'torch'. The 'torch' package is native to R, so no Python installation or other API is required for this package.

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R topics documented:

ALE *Accumulated Local Effect Plot (ALE)*

Description

Performs an ALE for one or more features.

Usage

```
ALE(
  model,
  variable = NULL,
  data = NULL,
  K = 10,
  ALE_type = c("equidistant", "quantile"),
  plot = TRUE,
  parallel = FALSE,
  ...
)

## S3 method for class 'citodnn'
ALE(
  model,
  variable = NULL,
  data = NULL,
  K = 10,
  ALE_type = c("equidistant", "quantile"),
  plot = TRUE,
  parallel = FALSE,
  ...
)

## S3 method for class 'citodnnBootstrap'
ALE(
  model,
  variable = NULL,
  data = NULL,
  K = 10,
  ALE_type = c("equidistant", "quantile"),
  plot = TRUE,
  parallel = FALSE,
  ...
)
```

Arguments

`model`	a model created by `dnn`
`variable`	variable as string for which the PDP should be done
`data`	data on which ALE is performed on, if NULL training data will be used.
`K`	number of neighborhoods original feature space gets divided into
`ALE_type`	method on how the feature space is divided into neighborhoods.
`plot`	plot ALE or not
`parallel`	parallelize over bootstrap models or not
`...`	arguments passed to `predict`

Value

A list of plots made with 'ggplot2' consisting of an individual plot for each defined variable.

Explanation

Accumulated Local Effect plots (ALE) quantify how the predictions change when the features change. They are similar to partial dependency plots but are more robust to feature collinearity.

Mathematical details

If the defined variable is a numeric feature, the ALE is performed. Here, the non centered effect for feature j with k equally distant neighborhoods is defined as:

$\hat{\tilde{f}}_{j,ALE}(x) = \sum_{k=1}^{k_j(x)} \frac{1}{n_j(k)} \sum_{i:x_j^{(i)} \in N_j(k)} \left[\hat{f}(z_{k,j}, x_{\setminus j}^{(i)}) - \hat{f}(z_{k-1,j}, x_{\setminus j}^{(i)})\right]$

Where $N_j(k)$ is the k-th neighborhood and $n_j(k)$ is the number of observations in the k-th neighborhood.

The last part of the equation, $\left[\hat{f}(z_{k,j}, x_{\setminus j}^{(i)}) - \hat{f}(z_{k-1,j}, x_{\setminus j}^{(i)})\right]$ represents the difference in model prediction when the value of feature j is exchanged with the upper and lower border of the current neighborhood.

See Also

`PDP`

Examples

```
if(torch::torch_is_installed()){
library(cito)

# Build and train  Network
nn.fit<- dnn(Sepal.Length~., data = datasets::iris)

ALE(nn.fit, variable = "Petal.Length")
}
```

`analyze_training` *Visualize training of Neural Network*

Description

After training a model with cito, this function helps to analyze the training process and decide on best performing model. Creates a 'plotly' figure which allows to zoom in and out on training graph

Usage

```
analyze_training(object)
```

Arguments

`object`	a model created by dnn or cnn

Details

The baseline loss is the most important reference. If the model was not able to achieve a better (lower) loss than the baseline (which is the loss for a intercept only model), the model probably did not converge. Possible reasons include an improper learning rate, too few epochs, or too much regularization. See the ?dnn help or the `vignette("B-Training_neural_networks")`.

Value

a 'plotly' figure

Examples

```
if(torch::torch_is_installed()){
library(cito)
set.seed(222)
validation_set<- sample(c(1:nrow(datasets::iris)),25)

# Build and train  Network
nn.fit<- dnn(Sepal.Length~., data = datasets::iris[-validation_set,],validation = 0.1)

# show zoomable plot of training and validation losses
analyze_training(nn.fit)

# Use model on validation set
predictions <- predict(nn.fit, iris[validation_set,])

# Scatterplot
plot(iris[validation_set,]$Sepal.Length,predictions)
}
```

avgPool *Average pooling layer*

Description

creates a 'avgPool' 'citolayer' object that is used by create_architecture.

Usage

```
avgPool(kernel_size = NULL, stride = NULL, padding = NULL)
```

Arguments

kernel_size	(int or tuple) size of the kernel in this layer. Use a tuple if the kernel size isn't equal in all dimensions
stride	(int or tuple) stride of the kernel in this layer. NULL sets the stride equal to the kernel size. Use a tuple if the stride isn't equal in all dimensions
padding	(int or tuple) zero-padding added to both sides of the input. Use a tuple if the padding isn't equal in all dimensions

Details

This function creates a 'avgPool' 'citolayer' object that is passed to the create_architecture function. The parameters that aren't assigned here (and are therefore still NULL) are filled with the default values passed to create_architecture.

Value

S3 object of class "avgPool" "citolayer"

Author(s)

Armin Schenk

See Also

create_architecture

cito *'cito': Building and training neural networks*

Description

The 'cito' package provides a user-friendly interface for training and interpreting deep neural networks (DNN). 'cito' simplifies the fitting of DNNs by supporting the familiar formula syntax, hyperparameter tuning under cross-validation, and helps to detect and handle convergence problems. DNNs can be trained on CPU, GPU and MacOS GPUs. In addition, 'cito' has many downstream functionalities such as various explainable AI (xAI) metrics (e.g. variable importance, partial dependence plots, accumulated local effect plots, and effect estimates) to interpret trained DNNs. 'cito' optionally provides confidence intervals (and p-values) for all xAI metrics and predictions. At the same time, 'cito' is computationally efficient because it is based on the deep learning framework 'torch'. The 'torch' package is native to R, so no Python installation or other API is required for this package.

Details

Cito is built around its main function `dnn`, which creates and trains a deep neural network. Various tools for analyzing the trained neural network are available.

Installation

in order to install cito please follow these steps:

```
install.packages("cito")
```

```
library(torch)
```

```
install_torch(reinstall = TRUE)
```

```
library(cito)
```

cito functions and typical workflow

- `dnn`: train deep neural network
- `analyze_training`: check for convergence by comparing training loss with baseline loss
- `continue_training`: continues training of an existing cito dnn model for additional epochs
- `summary.citodnn`: extract xAI metrics/effects to understand how predictions are made
- `PDP`: plot the partial dependency plot for a specific feature
- `ALE`: plot the accumulated local effect plot for a specific feature

Check out the vignettes for more details on training NN and how a typical workflow with 'cito' could look like.

Examples

```
if(torch::torch_is_installed()){
library(cito)

# Example workflow in cito

## Build and train  Network
### softmax is used for multi-class responses (e.g., Species)
nn.fit<- dnn(Species~., data = datasets::iris, loss = "softmax")

## The training loss is below the baseline loss but at the end of the
## training the loss was still decreasing, so continue training for another 50
## epochs
nn.fit <- continue_training(nn.fit, epochs = 50L)

# Sturcture of Neural Network
print(nn.fit)

# Plot Neural Network
plot(nn.fit)
## 4 Input nodes (first layer) because of 4 features
## 3 Output nodes (last layer) because of 3 response species (one node for each
## level in the response variable).
## The layers between the input and output layer are called hidden layers (two
## of them)

## We now want to understand how the predictions are made, what are the
## important features? The summary function automatically calculates feature
## importance (the interpretation is similar to an anova) and calculates
## average conditional effects that are similar to linear effects:
summary(nn.fit)

## To visualize the effect (response-feature effect), we can use the ALE and
## PDP functions

# Partial dependencies
PDP(nn.fit, variable = "Petal.Length")

# Accumulated local effect plots
ALE(nn.fit, variable = "Petal.Length")



# Per se, it is difficult to get confidence intervals for our xAI metrics (or
# for the predictions). But we can use bootstrapping to obtain uncertainties
# for all cito outputs:
## Re-fit the neural network with bootstrapping
nn.fit<- dnn(Species~.,
             data = datasets::iris,
             loss = "softmax",
             epochs = 150L,
```

```
             verbose = FALSE,
             bootstrap = 20L)
## convergence can be tested via the analyze_training function
analyze_training(nn.fit)

## Summary for xAI metrics (can take some time):
summary(nn.fit)
## Now with standard errors and p-values
## Note: Take the p-values with a grain of salt! We do not know yet if they are
## correct (e.g. if you use regularization, they are likely conservative == too
## large)

## Predictions with bootstrapping:
dim(predict(nn.fit))
## predictions are by default averaged (over the bootstrap samples)



# Hyperparameter tuning (experimental feature)
hidden_values = matrix(c(5, 2,
                         4, 2,
                         10,2,
                         15,2), 4, 2, byrow = TRUE)
## Potential architectures we want to test, first column == number of nodes
print(hidden_values)

nn.fit = dnn(Species~.,
             data = iris,
             epochs = 30L,
             loss = "softmax",
             hidden = tune(values = hidden_values),
             lr = tune(0.00001, 0.1) # tune lr between range 0.00001 and 0.1
             )
## Tuning results:
print(nn.fit$tuning)

# test = Inf means that tuning was cancelled after only one fit (within the CV)


# Advanced: Custom loss functions and additional parameters
## Normal Likelihood with sd parameter:
custom_loss = function(pred, true) {
  logLik = torch::distr_normal(pred,
                               scale = torch::nnf_relu(scale)+
                                 0.001)$log_prob(true)
  return(-logLik$mean())
}

nn.fit<- dnn(Sepal.Length~.,
             data = datasets::iris,
             loss = custom_loss,
             verbose = FALSE,
             custom_parameters = list(scale = 1.0)
```

```
)
nn.fit$parameter$scale

## Multivariate normal likelihood with parametrized covariance matrix
## Sigma = L*L^t + D
## Helper function to build covariance matrix
create_cov = function(LU, Diag) {
  return(torch::torch_matmul(LU, LU$t()) + torch::torch_diag(Diag$exp()+0.01))
}

custom_loss_MVN = function(true, pred) {
  Sigma = create_cov(SigmaPar, SigmaDiag)
  logLik = torch::distr_multivariate_normal(pred,
                                            covariance_matrix = Sigma)$
    log_prob(true)
  return(-logLik$mean())
}


nn.fit<- dnn(cbind(Sepal.Length, Sepal.Width, Petal.Length)~.,
             data = datasets::iris,
             lr = 0.01,
             verbose = FALSE,
             loss = custom_loss_MVN,
             custom_parameters =
               list(SigmaDiag =  rep(0, 3),
                    SigmaPar = matrix(rnorm(6, sd = 0.001), 3, 2))
)
as.matrix(create_cov(nn.fit$loss$parameter$SigmaPar,
                     nn.fit$loss$parameter$SigmaDiag))

}
```

cnn *CNN*

Description

fits a custom convolutional neural network.

Usage

```
cnn(
  X,
  Y = NULL,
  architecture,
  loss = c("mse", "mae", "softmax", "cross-entropy", "gaussian", "binomial", "poisson"),
  optimizer = c("sgd", "adam", "adadelta", "adagrad", "rmsprop", "rprop"),
  lr = 0.01,
```

```
  alpha = 0.5,
  lambda = 0,
  validation = 0,
  batchsize = 32L,
  burnin = 10,
  shuffle = TRUE,
  epochs = 100,
  early_stopping = NULL,
  lr_scheduler = NULL,
  custom_parameters = NULL,
  device = c("cpu", "cuda", "mps"),
  plot = TRUE,
  verbose = TRUE
)
```

Arguments

X	predictor: array with dimension 3, 4 or 5 for 1D-, 2D- or 3D-convolutions, respectively. The first dimension are the samples, the second dimension the channels and the third - fifth dimension are the input dimensions
Y	response: vector, factor, numerical matrix or logical matrix
architecture	'citoarchitecture' object created by create_architecture
loss	loss after which network should be optimized. Can also be distribution from the stats package or own function, see details
optimizer	which optimizer used for training the network, for more adjustments to optimizer see config_optimizer
lr	learning rate given to optimizer
alpha	add L1/L2 regularization to training $(1-\alpha)*\|weights\|+\alpha\|\|weights\|\|^2$ will get added for each layer. Must be between 0 and 1
lambda	strength of regularization: lambda penalty, $\lambda*(L1+L2)$ (see alpha)
validation	percentage of data set that should be taken as validation set (chosen randomly)
batchsize	number of samples that are used to calculate one learning rate step
burnin	training is aborted if the trainings loss is not below the baseline loss after burnin epochs
shuffle	if TRUE, data in each batch gets reshuffled every epoch
epochs	epochs the training goes on for
early_stopping	if set to integer, training will stop if loss has gotten higher for defined number of epochs in a row, will use validation loss if available.
lr_scheduler	learning rate scheduler created with config_lr_scheduler
custom_parameters	List of parameters/variables to be optimized. Can be used in a custom loss function. See Vignette for example.
device	device on which network should be trained on.
plot	plot training loss
verbose	print training and validation loss of epochs

Value

an S3 object of class "citocnn" is returned. It is a list containing everything there is to know about the model and its training process. The list consists of the following attributes:

- `net` An object of class "nn_sequential" "nn_module", originates from the torch package and represents the core object of this workflow.
- `call` The original function call
- `loss` A list which contains relevant information for the target variable and the used loss function
- `data` Contains data used for training the model
- `weights` List of weights for each training epoch
- `use_model_epoch` Integer, which defines which model from which training epoch should be used for prediction.
- `loaded_model_epoch` Integer, shows which model from which epoch is loaded currently into model$net.
- `model_properties` A list of properties of the neural network, contains number of input nodes, number of output nodes, size of hidden layers, activation functions, whether bias is included and if dropout layers are included.
- `training_properties` A list of all training parameters that were used the last time the model was trained. It consists of learning rate, information about an learning rate scheduler, information about the optimizer, number of epochs, whether early stopping was used, if plot was active, lambda and alpha for L1/L2 regularization, batchsize, shuffle, was the data set split into validation and training, which formula was used for training and at which epoch did the training stop.
- `losses` A data.frame containing training and validation losses of each epoch

Convolutional neural networks:

Convolutional Neural Networks (CNNs) are a specialized type of neural network designed for processing structured grid data, such as images. The characterizing parts of the architecture are convolutional layers, pooling layers and fully-connected (linear) layers:

- Convolutional layers are the core building blocks of CNNs. They consist of filters (also called kernels), which are small, learnable matrices. These filters slide over the input data to perform element-wise multiplication, producing feature maps that capture local patterns and features. Multiple filters are used to detect different features in parallel. They help the network learn hierarchical representations of the input data by capturing low-level features (edges, textures) and gradually combining them (in subsequent convolutional layers) to form higher-level features.
- Pooling layers are used to downsample the spatial dimensions of the feature maps while retaining important information. Max pooling is a common pooling operation, where the maximum value in a local region of the input is retained, reducing the size of the feature maps.
- Fully-connected (linear) layers connect every neuron in one layer to every neuron in the next layer. These layers are found at the end of the network and are responsible for combining high-level features to make final predictions.

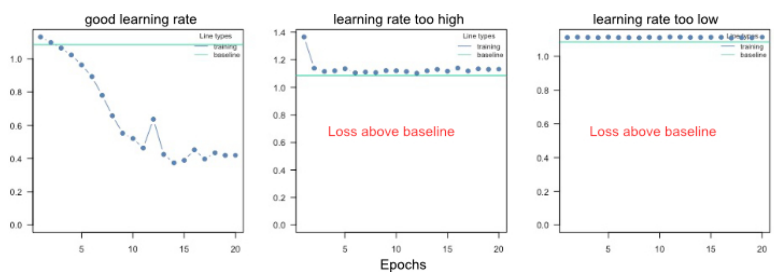
Loss functions / Likelihoods

We support loss functions and likelihoods for different tasks:

Name	Explanation	Example / Task
mse	mean squared error	Regression, predicting continuous values
mae	mean absolute error	Regression, predicting continuous values
softmax	categorical cross entropy	Multi-class, species classification
cross-entropy	categorical cross entropy	Multi-class, species classification
gaussian	Normal likelihood	Regression, residual error is also estimated (similar to `stats::lm()`)
binomial	Binomial likelihood	Classification/Logistic regression, mortality
Poisson	Poisson likelihood	Regression, count data, e.g. species abundances

Training and convergence of neural networks

Ensuring convergence can be tricky when training neural networks. Their training is sensitive to a combination of the learning rate (how much the weights are updated in each optimization step), the batch size (a random subset of the data is used in each optimization step), and the number of epochs (number of optimization steps). Typically, the learning rate should be decreased with the size of the neural networks (amount of learnable parameters). We provide a baseline loss (intercept only model) that can give hints about an appropriate learning rate:



If the training loss of the model doesn't fall below the baseline loss, the learning rate is either too high or too low. If this happens, try higher and lower learning rates.

A common strategy is to try (manually) a few different learning rates to see if the learning rate is on the right scale.

See the troubleshooting vignette (`vignette("B-Training_neural_networks")`) for more help on training and debugging neural networks.

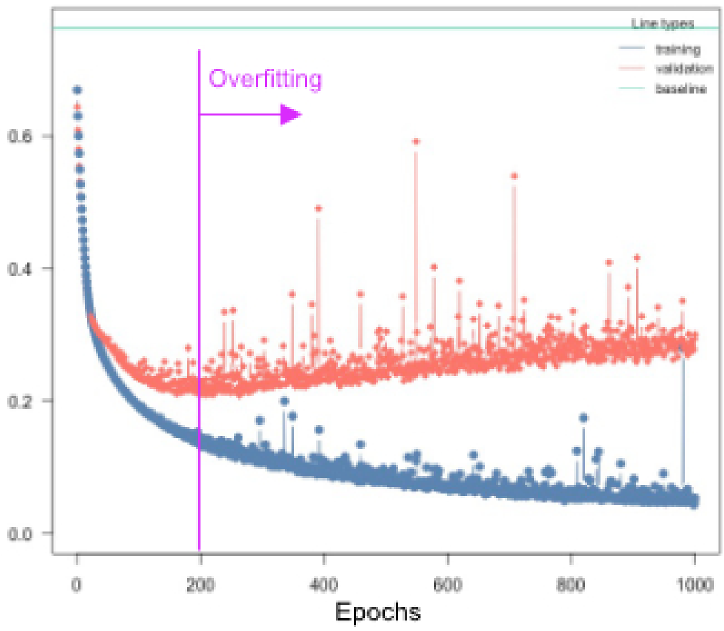
Finding the right architecture

As with the learning rate, there is no definitive guide to choosing the right architecture for the right task. However, there are some general rules/recommendations: In general, wider, and deeper neural networks can improve generalization - but this is a double-edged sword because it also increases the risk of overfitting. So, if you increase the width and depth of the network, you should also add regularization (e.g., by increasing the lambda parameter, which corresponds to the regularization strength). Furthermore, in Pichler & Hartig, 2023, we investigated the effects of the hyperparameters on the prediction performance as a function of the data size. For example, we found that the `selu` activation function outperforms `relu` for small data sizes (<100 observations).

We recommend starting with moderate sizes (like the defaults), and if the model doesn't generalize/converge, try larger networks along with a regularization that helps minimize the risk of overfitting (see `vignette("B-Training_neural_networks")`).

Overfitting

Overfitting means that the model fits the training data well, but generalizes poorly to new observations. We can use the validation argument to detect overfitting. If the validation loss starts to increase again at a certain point, it often means that the models are starting to overfit your training data:



Solutions:

- Re-train with epochs = point where model started to overfit
- Early stopping, stop training when model starts to overfit, can be specified using the `early_stopping=...` argument
- Use regularization (dropout or elastic-net, see next section)

Regularization

Elastic Net regularization combines the strengths of L1 (Lasso) and L2 (Ridge) regularization. It introduces a penalty term that encourages sparse weight values while maintaining overall weight shrinkage. By controlling the sparsity of the learned model, Elastic Net regularization helps avoid overfitting while allowing for meaningful feature selection. We advise using elastic net (e.g. lambda = 0.001 and alpha = 0.2).

Dropout regularization helps prevent overfitting by randomly disabling a portion of neurons during training. This technique encourages the network to learn more robust and generalized representations, as it prevents individual neurons from relying too heavily on specific input patterns. Dropout has been widely adopted as a simple yet effective regularization method in deep learning. In the case of 2D and 3D inputs whole feature maps are disabled. Since the torch package doesn't currently support feature map-wise dropout for 1D inputs, instead random neurons in the feature maps are disabled similar to dropout in linear layers.

By utilizing these regularization methods in your neural network training with the cito package, you can improve generalization performance and enhance the network's ability to handle unseen data. These techniques act as valuable tools in mitigating overfitting and promoting more robust and reliable model performance.

Custom Optimizer and Learning Rate Schedulers

When training a network, you have the flexibility to customize the optimizer settings and learning rate scheduler to optimize the learning process. In the cito package, you can initialize these configurations using the `config_lr_scheduler` and `config_optimizer` functions.

`config_lr_scheduler` allows you to define a specific learning rate scheduler that controls how the learning rate changes over time during training. This is beneficial in scenarios where you want to adaptively adjust the learning rate to improve convergence or avoid getting stuck in local optima.

Similarly, the `config_optimizer` function enables you to specify the optimizer for your network. Different optimizers, such as stochastic gradient descent (SGD), Adam, or RMSprop, offer various strategies for updating the network's weights and biases during training. Choosing the right optimizer can significantly impact the training process and the final performance of your neural network.

Training on graphic cards

If you have an NVIDIA CUDA-enabled device and have installed the CUDA toolkit version 11.3 and cuDNN 8.4, you can take advantage of GPU acceleration for training your neural networks. It is crucial to have these specific versions installed, as other versions may not be compatible. For detailed installation instructions and more information on utilizing GPUs for training, please refer to the mlverse: 'torch' documentation.

Note: GPU training is optional, and the package can still be used for training on CPU even without CUDA and cuDNN installations.

Author(s)

Armin Schenk, Maximilian Pichler

See Also

`predict.citocnn`, `plot.citocnn`, `coef.citocnn`, `print.citocnn`, `summary.citocnn`, `continue_training`, `analyze_training`

coef.citocnn *Returns list of parameters the neural network model currently has in use*

Description

Returns list of parameters the neural network model currently has in use

Usage

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

Arguments

object	a model created by cnn
...	nothing implemented yet

Value

list of weights of neural network

coef.citodnn *Returns list of parameters the neural network model currently has in use*

Description

Returns list of parameters the neural network model currently has in use

Usage

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

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

Arguments

object	a model created by dnn
...	nothing implemented yet

Value

list of weights of neural network

Examples

```
if(torch::torch_is_installed()){
library(cito)

set.seed(222)
validation_set<- sample(c(1:nrow(datasets::iris)),25)

# Build and train  Network
nn.fit<- dnn(Sepal.Length~., data = datasets::iris[-validation_set,])

# Sturcture of Neural Network
print(nn.fit)

#analyze weights of Neural Network
coef(nn.fit)
}
```

---

conditionalEffects *Calculate average conditional effects*

Description

Average conditional effects calculate the local derivatives for each observation for each feature. They are similar to marginal effects. And the average of these conditional effects is an approximation of linear effects (see Pichler and Hartig, 2023 for more details). You can use this function to either calculate main effects (on the diagonal, take a look at the example) or interaction effects (off-diagonals) between features.

To obtain uncertainties for these effects, enable the bootstrapping option in the `dnn(..)` function (see example).

Usage

```
conditionalEffects(
  object,
  interactions = FALSE,
  epsilon = 0.1,
  device = c("cpu", "cuda", "mps"),
  indices = NULL,
  data = NULL,
  type = "response",
  ...
)

## S3 method for class 'citodnn'
conditionalEffects(
  object,
```

```
  interactions = FALSE,
  epsilon = 0.1,
  device = c("cpu", "cuda", "mps"),
  indices = NULL,
  data = NULL,
  type = "response",
  ...
)

## S3 method for class 'citodnnBootstrap'
conditionalEffects(
  object,
  interactions = FALSE,
  epsilon = 0.1,
  device = c("cpu", "cuda", "mps"),
  indices = NULL,
  data = NULL,
  type = "response",
  ...
)
```

Arguments

`object`	object of class `citodnn`
`interactions`	calculate interactions or not (computationally expensive)
`epsilon`	difference used to calculate derivatives
`device`	which device
`indices`	of variables for which the ACE are calculated
`data`	data which is used to calculate the ACE
`type`	ACE on which scale (response or link)
`...`	additional arguments that are passed to the predict function

Value

an S3 object of class `"conditionalEffects"` is returned. The list consists of the following attributes:

`result`	3-dimensional array with the raw results
`mean`	Matrix, average conditional effects
`abs`	Matrix, summed absolute conditional effects
`sd`	Matrix, standard deviation of the conditional effects

Author(s)

Maximilian Pichler

References

Scholbeck, C. A., Casalicchio, G., Molnar, C., Bischl, B., & Heumann, C. (2022). Marginal effects for non-linear prediction functions. arXiv preprint arXiv:2201.08837.

Pichler, M., & Hartig, F. (2023). Can predictive models be used for causal inference?. arXiv preprint arXiv:2306.10551.

Examples

```
if(torch::torch_is_installed()){
library(cito)

# Build and train  Network
nn.fit = dnn(Sepal.Length~., data = datasets::iris)

# Calculate average conditional effects
ACE = conditionalEffects(nn.fit)

## Main effects (categorical features are not supported)
ACE

## With interaction effects:
ACE = conditionalEffects(nn.fit, interactions = TRUE)
## The off diagonal elements are the interaction effects
ACE[[1]]$mean
## ACE is a list, elements correspond to the number of response classes
## Sepal.length == 1 Response so we have only one
## list element in the ACE object

# Re-train NN with bootstrapping to obtain standard errors
nn.fit = dnn(Sepal.Length~., data = datasets::iris, bootstrap = 30L)
## The summary method calculates also the conditional effects, and if
## bootstrapping was used, it will also report standard errors and p-values:
summary(nn.fit)


}
```

---

config_lr_scheduler — *Creation of customized learning rate scheduler objects*

Description

Helps create custom learning rate schedulers for dnn.

Usage

```
config_lr_scheduler(
  type = c("lambda", "multiplicative", "reduce_on_plateau", "one_cycle", "step"),
  verbose = FALSE,
  ...
)
```

Arguments

`type`	String defining which type of scheduler should be used. See Details.
`verbose`	If TRUE, additional information about scheduler will be printed to console.
`...`	additional arguments to be passed to scheduler. See Details.

Details

different learning rate scheduler need different variables, these functions will tell you which variables can be set:

- lambda: `lr_lambda`
- multiplicative: `lr_multiplicative`
- reduce_on_plateau: `lr_reduce_on_plateau`
- one_cycle: `lr_one_cycle`
- step: `lr_step`

Value

object of class cito_lr_scheduler to give to `dnn`

Examples

```
if(torch::torch_is_installed()){
library(cito)

# create learning rate scheduler object
scheduler <- config_lr_scheduler(type = "step",
                        step_size = 30,
                        gamma = 0.15,
                        verbose = TRUE)

# Build and train  Network
nn.fit<- dnn(Sepal.Length~., data = datasets::iris, lr_scheduler = scheduler)

}
```

config_optimizer — *Creation of customized optimizer objects*

Description

Helps you create custom optimizer for dnn. It is recommended to set learning rate in dnn.

Usage

```
config_optimizer(
  type = c("adam", "adadelta", "adagrad", "rmsprop", "rprop", "sgd"),
  verbose = FALSE,
  ...
)
```

Arguments

type	character string defining which optimizer should be used. See Details.
verbose	If TRUE, additional information about scheduler will be printed to console
...	additional arguments to be passed to optimizer. See Details.

Details

different optimizer need different variables, this function will tell you how the variables are set. For more information see the corresponding functions:

- adam: optim_adam
- adadelta: optim_adadelta
- adagrad: optim_adagrad
- rmsprop: optim_rmsprop
- rprop: optim_rprop
- sgd: optim_sgd

Value

object of class cito_optim to give to dnn

Examples

```
if(torch::torch_is_installed()){
library(cito)

# create optimizer object
opt <- config_optimizer(type = "adagrad",
                        lr_decay = 1e-04,
```

```
                        weight_decay = 0.1,
                        verbose = TRUE)

# Build and train  Network
nn.fit<- dnn(Sepal.Length~., data = datasets::iris, optimizer = opt)

}
```

---

config_tuning *Config hyperparameter tuning*

Description

Config hyperparameter tuning

Usage

```
config_tuning(
  CV = 5,
  steps = 10,
  parallel = FALSE,
  NGPU = 1,
  cancel = TRUE,
  bootstrap_final = NULL,
  bootstrap_parallel = FALSE,
  return_models = FALSE
)
```

Arguments

`CV`	numeric, specifies k-folded cross validation
`steps`	numeric, number of random tuning steps
`parallel`	numeric, number of parallel cores (tuning steps are parallelized)
`NGPU`	numeric, set if more than one GPU is available, tuning will be parallelized over CPU cores and GPUs, only works for NCPU > 1
`cancel`	CV/tuning for specific hyperparameter set if model cannot reduce loss below baseline after burnin or returns NA loss
`bootstrap_final`	bootstrap final model, if all models should be boostrapped it must be set globally via the bootstrap argument in the `dnn()` function
`bootstrap_parallel`	should the bootstrapping be parallelized or not
`return_models`	return individual models

Details

Note that hyperparameter tuning can be expensive. We have implemented an option to parallelize hyperparameter tuning, including parallelization over one or more GPUs (the hyperparameter evaluation is parallelized, not the CV). This can be especially useful for small models. For example, if you have 4 GPUs, 20 CPU cores, and 20 steps (random samples from the random search), you could run ‘dnn(..., device="cuda",lr = tune(), batchsize=tune(), tuning=config_tuning(parallel=20, NGPU=4)’, which will distribute 20 model fits across 4 GPUs, so that each GPU will process 5 models (in parallel).

`continue_training` *Continues training of a model generated with* `dnn` *or* `cnn` *for additional epochs.*

Description

If the training/validation loss is still decreasing at the end of the training, it is often a sign that the NN has not yet converged. You can use this function to continue training instead of re-training the entire model.

Usage

```
continue_training(model, ...)

## S3 method for class 'citodnn'
continue_training(
  model,
  epochs = 32,
  data = NULL,
  device = NULL,
  verbose = TRUE,
  changed_params = NULL,
  ...
)

## S3 method for class 'citodnnBootstrap'
continue_training(
  model,
  epochs = 32,
  data = NULL,
  device = NULL,
  verbose = TRUE,
  changed_params = NULL,
  parallel = FALSE,
  ...
)
```

```
## S3 method for class 'citocnn'
continue_training(
  model,
  epochs = 32,
  X = NULL,
  Y = NULL,
  device = c("cpu", "cuda", "mps"),
  verbose = TRUE,
  changed_params = NULL,
  ...
)
```

Arguments

`model`	a model created by dnn or cnn
`...`	class-specific arguments
`epochs`	additional epochs the training should continue for
`data`	matrix or data.frame. If not provided data from original training will be used
`device`	can be used to overwrite device used in previous training
`verbose`	print training and validation loss of epochs
`changed_params`	list of arguments to change compared to original training setup, see dnn which parameter can be changed
`parallel`	train bootstrapped model in parallel
`X`	array. If not provided X from original training will be used
`Y`	vector, factor, numerical matrix or logical matrix. If not provided Y from original training will be used

Value

a model of class citodnn, citodnnBootstrap or citocnn created by dnn or cnn

Examples

```
if(torch::torch_is_installed()){
library(cito)

set.seed(222)
validation_set<- sample(c(1:nrow(datasets::iris)),25)

# Build and train  Network
nn.fit<- dnn(Sepal.Length~., data = datasets::iris[-validation_set,], epochs = 32)

# continue training for another 32 epochs
nn.fit<- continue_training(nn.fit,epochs = 32)

# Use model on validation set
predictions <- predict(nn.fit, iris[validation_set,])
```

```
}
```

---

conv *Convolutional layer*

Description

creates a 'conv' 'citolayer' object that is used by create_architecture.

Usage

```
conv(
  n_kernels = NULL,
  kernel_size = NULL,
  stride = NULL,
  padding = NULL,
  dilation = NULL,
  bias = NULL,
  activation = NULL,
  normalization = NULL,
  dropout = NULL
)
```

Arguments

n_kernels	(int) amount of kernels in this layer
kernel_size	(int or tuple) size of the kernels in this layer. Use a tuple if the kernel size isn't equal in all dimensions
stride	(int or tuple) stride of the kernels in this layer. NULL sets the stride equal to the kernel size. Use a tuple if the stride isn't equal in all dimensions
padding	(int or tuple) zero-padding added to both sides of the input. Use a tuple if the padding isn't equal in all dimensions
dilation	(int or tuple) dilation of the kernels in this layer. Use a tuple if the dilation isn't equal in all dimensions
bias	(boolean) if TRUE, adds a learnable bias to the kernels of this layer
activation	(string) activation function that is used after this layer. The following activation functions are supported: "relu", "leaky_relu", "tanh", "elu", "rrelu", "prelu", "softplus", "celu", "selu", "gelu", "relu6", "sigmoid", "softsign", "hardtanh", "tanhshrink", "softshrink", "hardshrink", "log_sigmoid"
normalization	(boolean) if TRUE, batch normalization is used after this layer
dropout	(float) dropout rate of this layer. Set to 0 for no dropout

Details

This function creates a 'conv' 'citolayer' object that is passed to the `create_architecture` function. The parameters that aren't assigned here (and are therefore still NULL) are filled with the default values passed to `create_architecture`.

Value

S3 object of class `"conv" "citolayer"`

Author(s)

Armin Schenk

See Also

`create_architecture`

`create_architecture` *CNN architecture*

Description

creates a 'citoarchitecture' object that is used by `cnn`.

Usage

```
create_architecture(
  ...,
  default_n_neurons = 10,
  default_n_kernels = 10,
  default_kernel_size = list(conv = 3, maxPool = 2, avgPool = 2),
  default_stride = list(conv = 1, maxPool = NULL, avgPool = NULL),
  default_padding = list(conv = 0, maxPool = 0, avgPool = 0),
  default_dilation = list(conv = 1, maxPool = 1),
  default_bias = list(conv = TRUE, linear = TRUE),
  default_activation = list(conv = "relu", linear = "relu"),
  default_normalization = list(conv = FALSE, linear = FALSE),
  default_dropout = list(conv = 0, linear = 0)
)
```

Arguments

`...` objects of class 'citolayer' created by `linear`, `conv`, `maxPool`, `avgPool` or `transfer`

`default_n_neurons`
(int) default value: amount of neurons in a linear layer

`default_n_kernels`
(int) default value: amount of kernels in a convolutional layer

default_kernel_size
: (int or tuple) default value: size of the kernels in convolutional and pooling layers. Use a tuple if the kernel size isn't equal in all dimensions

default_stride
: (int or tuple) default value: stride of the kernels in convolutional and pooling layers. NULL sets the stride equal to the kernel size. Use a tuple if the stride isn't equal in all dimensions

default_padding
: (int or tuple) default value: zero-padding added to both sides of the input. Use a tuple if the padding isn't equal in all dimensions

default_dilation
: (int or tuple) default value: dilation of the kernels in convolutional and maxPooling layers. Use a tuple if the dilation isn't equal in all dimensions

default_bias
: (boolean) default value: if TRUE, adds a learnable bias to neurons of linear and kernels of convolutional layers

default_activation
: (string) default value: activation function that is used after linear and convolutional layers. The following activation functions are supported: "relu", "leaky_relu", "tanh", "elu", "rrelu", "prelu", "softplus", "celu", "selu", "gelu", "relu6", "sigmoid", "softsign", "hardtanh", "tanhshrink", "softshrink", "hardshrink", "log_sigmoid"

default_normalization
: (boolean) default value: if TRUE, batch normalization is used after linear and convolutional layers

default_dropout
: (float) default value: dropout rate of linear and convolutional layers. Set to 0 for no dropout

Details

This function creates a 'citoarchitecture' object that provides the `cnn` function with all information about the architecture of the CNN that will be created and trained. The final architecture consists of the layers in the sequence they were passed to this function. All parameters of the 'citolayer' objects, that are still NULL because they haven't been specified at the creation of the layer, are filled with the given default parameters for their specific layer type (linear, conv, maxPool, avgPool). The default values can be changed by either passing a list with the values for specific layer types (in which case the defaults of layer types which aren't in the list remain the same) or by passing a single value (in which case the defaults for all layer types is set to that value).

Value

S3 object of class `"citoarchitecture"`

Author(s)

Armin Schenk

See Also

`cnn`, `linear`, `conv`, `maxPool`, `avgPool`, `transfer`, `print.citoarchitecture`, `plot.citoarchitecture` dnn *DNN*

Description

fits a custom deep neural network using the Multilayer Perceptron architecture. dnn() supports the formula syntax and allows to customize the neural network to a maximal degree.

Usage

```
dnn(
  formula = NULL,
  data = NULL,
  hidden = c(50L, 50L),
  activation = "selu",
  bias = TRUE,
  dropout = 0,
 loss = c("mse", "mae", "softmax", "cross-entropy", "gaussian", "binomial", "poisson",
    "mvp", "nbinom"),
  validation = 0,
  lambda = 0,
  alpha = 0.5,
  optimizer = c("sgd", "adam", "adadelta", "adagrad", "rmsprop", "rprop"),
  lr = 0.01,
  batchsize = NULL,
  burnin = 30,
  baseloss = NULL,
  shuffle = TRUE,
  epochs = 100,
  bootstrap = NULL,
  bootstrap_parallel = FALSE,
  plot = TRUE,
  verbose = TRUE,
  lr_scheduler = NULL,
  custom_parameters = NULL,
  device = c("cpu", "cuda", "mps"),
  early_stopping = FALSE,
  tuning = config_tuning(),
  X = NULL,
  Y = NULL
)
```

Arguments

formula	an object of class "formula": a description of the model that should be fitted
data	matrix or data.frame with features/predictors and response variable
hidden	hidden units in layers, length of hidden corresponds to number of layers

activation
: activation functions, can be of length one, or a vector of different activation functions for each layer

bias
: whether use biases in the layers, can be of length one, or a vector (number of hidden layers + 1 (last layer)) of logicals for each layer.

dropout
: dropout rate, probability of a node getting left out during training (see nn_dropout)

loss
: loss after which network should be optimized. Can also be distribution from the stats package or own function, see details

validation
: percentage of data set that should be taken as validation set (chosen randomly)

lambda
: strength of regularization: lambda penalty, $\lambda * (L1 + L2)$ (see alpha)

alpha
: add L1/L2 regularization to training $(1 - \alpha) * |weights| + \alpha ||weights||^2$ will get added for each layer. Must be between 0 and 1

optimizer
: which optimizer used for training the network, for more adjustments to optimizer see config_optimizer

lr
: learning rate given to optimizer

batchsize
: number of samples that are used to calculate one learning rate step, default is 10% of the training data

burnin
: training is aborted if the trainings loss is not below the baseline loss after burnin epochs

baseloss
: baseloss, if null baseloss corresponds to intercept only models

shuffle
: if TRUE, data in each batch gets reshuffled every epoch

epochs
: epochs the training goes on for

bootstrap
: bootstrap neural network or not, numeric corresponds to number of bootstrap samples

bootstrap_parallel
: parallelize (CPU) bootstrapping

plot
: plot training loss

verbose
: print training and validation loss of epochs

lr_scheduler
: learning rate scheduler created with config_lr_scheduler

custom_parameters
: List of parameters/variables to be optimized. Can be used in a custom loss function. See Vignette for example.

device
: device on which network should be trained on. mps correspond to M1/M2 GPU devices.

early_stopping
: if set to integer, training will stop if loss has gotten higher for defined number of epochs in a row, will use validation loss is available.

tuning
: tuning options created with config_tuning

X
: Feature matrix or data.frame, alternative data interface

Y
: Response vector, factor, matrix or data.frame, alternative data interface

Value

an S3 object of class "cito.dnn" is returned. It is a list containing everything there is to know about the model and its training process. The list consists of the following attributes:

- `net` An object of class "nn_sequential" "nn_module", originates from the torch package and represents the core object of this workflow.
- `call` The original function call
- `loss` A list which contains relevant information for the target variable and the used loss function
- `data` Contains data used for training the model
- `weigths` List of weights for each training epoch
- `use_model_epoch` Integer, which defines which model from which training epoch should be used for prediction. 1 = best model, 2 = last model
- `loaded_model_epoch` Integer, shows which model from which epoch is loaded currently into model$net.
- `model_properties` A list of properties of the neural network, contains number of input nodes, number of output nodes, size of hidden layers, activation functions, whether bias is included and if dropout layers are included.
- `training_properties` A list of all training parameters that were used the last time the model was trained. It consists of learning rate, information about an learning rate scheduler, information about the optimizer, number of epochs, whether early stopping was used, if plot was active, lambda and alpha for L1/L2 regularization, batchsize, shuffle, was the data set split into validation and training, which formula was used for training and at which epoch did the training stop.
- `losses` A data.frame containing training and validation losses of each epoch

Activation functions

Supported activation functions: "relu", "leaky_relu", "tanh", "elu", "rrelu", "prelu", "softplus", "celu", "selu", "gelu", "relu6", "sigmoid", "softsign", "hardtanh", "tanhshrink", "softshrink", "hardshrink", "log_sigmoid"

Loss functions / Likelihoods

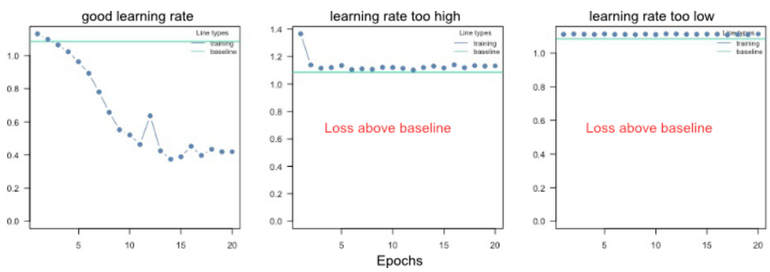
We support loss functions and likelihoods for different tasks:

Name	Explanation	Example / Task
mse	mean squared error	Regression, predicting continuous values
mae	mean absolute error	Regression, predicting continuous values
softmax	categorical cross entropy	Multi-class, species classification
cross-entropy	categorical cross entropy	Multi-class, species classification
gaussian	Normal likelihood	Regression, residual error is also estimated (similar to `stats::lm()`)
binomial	Binomial likelihood	Classification/Logistic regression, mortality

poisson	Poisson likelihood	Regression, count data, e.g. species abundances
nbinom	Negative binomial likelihood	Regression, count data with dispersion parameter
mvp	multivariate probit model	joint species distribution model, multi species (presence absence)

Training and convergence of neural networks

Ensuring convergence can be tricky when training neural networks. Their training is sensitive to a combination of the learning rate (how much the weights are updated in each optimization step), the batch size (a random subset of the data is used in each optimization step), and the number of epochs (number of optimization steps). Typically, the learning rate should be decreased with the size of the neural networks (depth of the network and width of the hidden layers). We provide a baseline loss (intercept only model) that can give hints about an appropriate learning rate:



If the training loss of the model doesn't fall below the baseline loss, the learning rate is either too high or too low. If this happens, try higher and lower learning rates.

A common strategy is to try (manually) a few different learning rates to see if the learning rate is on the right scale.

See the troubleshooting vignette (`vignette("B-Training_neural_networks")`) for more help on training and debugging neural networks.

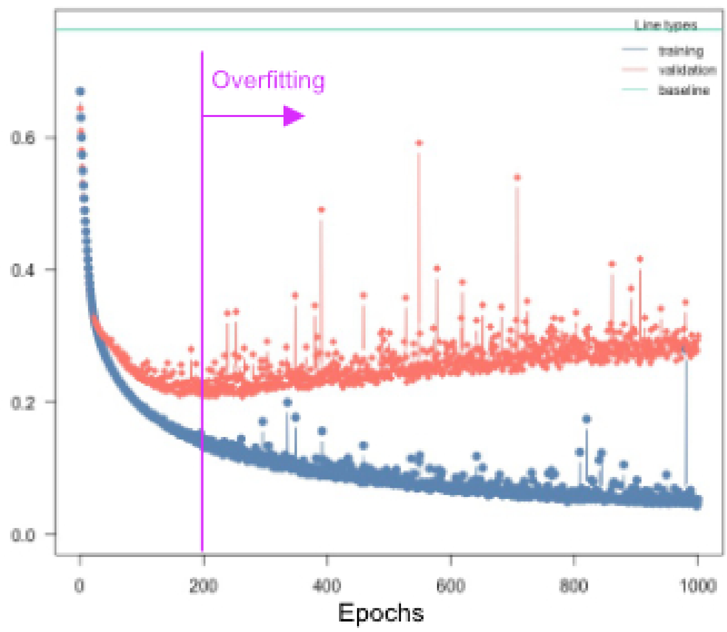
Finding the right architecture

As with the learning rate, there is no definitive guide to choosing the right architecture for the right task. However, there are some general rules/recommendations: In general, wider, and deeper neural networks can improve generalization - but this is a double-edged sword because it also increases the risk of overfitting. So, if you increase the width and depth of the network, you should also add regularization (e.g., by increasing the lambda parameter, which corresponds to the regularization strength). Furthermore, in Pichler & Hartig, 2023, we investigated the effects of the hyperparameters on the prediction performance as a function of the data size. For example, we found that the `selu` activation function outperforms `relu` for small data sizes (<100 observations).

We recommend starting with moderate sizes (like the defaults), and if the model doesn't generalize/converge, try larger networks along with a regularization that helps minimize the risk of overfitting (see `vignette("B-Training_neural_networks")`).

Overfitting

Overfitting means that the model fits the training data well, but generalizes poorly to new observations. We can use the validation argument to detect overfitting. If the validation loss starts to increase again at a certain point, it often means that the models are starting to overfit your training data:



Solutions:

- Re-train with epochs = point where model started to overfit
- Early stopping, stop training when model starts to overfit, can be specified using the `early_stopping=...` argument
- Use regularization (dropout or elastic-net, see next section)

Regularization

Elastic Net regularization combines the strengths of L1 (Lasso) and L2 (Ridge) regularization. It introduces a penalty term that encourages sparse weight values while maintaining overall weight shrinkage. By controlling the sparsity of the learned model, Elastic Net regularization helps avoid overfitting while allowing for meaningful feature selection. We advise using elastic net (e.g. lambda = 0.001 and alpha = 0.2).

Dropout regularization helps prevent overfitting by randomly disabling a portion of neurons during training. This technique encourages the network to learn more robust and generalized representations, as it prevents individual neurons from relying too heavily on specific input patterns. Dropout has been widely adopted as a simple yet effective regularization method in deep learning.

By utilizing these regularization methods in your neural network training with the cito package, you can improve generalization performance and enhance the network's ability to handle unseen data. These techniques act as valuable tools in mitigating overfitting and promoting more robust and reliable model performance.

Uncertainty

We can use bootstrapping to generate uncertainties for all outputs. Bootstrapping can be enabled by setting `bootstrap = ...` to the number of bootstrap samples to be used. Note, however, that the computational cost can be excessive.

In some cases it may be worthwhile to parallelize bootstrapping, for example if you have a GPU and the neural network is small. Parallelization for bootstrapping can be enabled by setting the `bootstrap_parallel = ...` argument to the desired number of calls to run in parallel.

Custom Optimizer and Learning Rate Schedulers

When training a network, you have the flexibility to customize the optimizer settings and learning rate scheduler to optimize the learning process. In the cito package, you can initialize these configurations using the `config_lr_scheduler` and `config_optimizer` functions.

`config_lr_scheduler` allows you to define a specific learning rate scheduler that controls how the learning rate changes over time during training. This is beneficial in scenarios where you want to adaptively adjust the learning rate to improve convergence or avoid getting stuck in local optima.

Similarly, the `config_optimizer` function enables you to specify the optimizer for your network. Different optimizers, such as stochastic gradient descent (SGD), Adam, or RMSprop, offer various strategies for updating the network's weights and biases during training. Choosing the right optimizer can significantly impact the training process and the final performance of your neural network.

Hyperparameter tuning

We have implemented experimental support for hyperparameter tuning. We can mark hyperparameters that should be tuned by cito by setting their values to `tune()`, for example `dnn (..., lr = tune()`. `tune()` is a function that creates a range of random values for the given hyperparameter. You can change the maximum and minimum range of the potential hyperparameters or pass custom values to the `tune(values = c(....))` function. The following table lists the hyperparameters that can currently be tuned:

Hyperparameter	Example	Details
hidden	`dnn(...,hidden=tune(10, 20, fixed='depth'))`	Depth and width can be both tuned or only one o
bias	`dnn(..., bias=tune())`	Should the bias be turned on or off for all hidden
lambda	`dnn(..., lambda = tune(0.0001, 0.1))`	lambda will be tuned within the range (0.0001, 0.
alpha	`dnn(..., lambda = tune(0.2, 0.4))`	alpha will be tuned within the range (0.2, 0.4)
activation	`dnn(..., activation = tune())`	activation functions of the hidden layers will be t
dropout	`dnn(..., dropout = tune())`	Dropout rate will be tuned (globally for all layers
lr	`dnn(..., lr = tune())`	Learning rate will be tuned
batchsize	`dnn(..., batchsize = tune())`	batch size will be tuned
epochs	`dnn(..., batchsize = tune())`	batchsize will be tuned

The hyperparameters are tuned by random search (i.e., random values for the hyperparameters within a specified range) and by cross-validation. The exact tuning regime can be specified with config_tuning.

Note that hyperparameter tuning can be expensive. We have implemented an option to parallelize hyperparameter tuning, including parallelization over one or more GPUs (the hyperparameter evaluation is parallelized, not the CV). This can be especially useful for small models. For example, if you have 4 GPUs, 20 CPU cores, and 20 steps (random samples from the random search), you could run `dnn(..., device="cuda",lr = tune(), batchsize=tune(), tuning=config_tuning(parallel=20, NGPU=4)`, which will distribute 20 model fits across 4 GPUs, so that each GPU will process 5 models (in parallel).

As this is an experimental feature, we welcome feature requests and bug reports on our github site.

For the custom values, all hyperparameters except for the hidden layers require a vector of values. Hidden layers expect a two-column matrix where the first column is the number of hidden nodes and the second column corresponds to the number of hidden layers.

How neural networks work

In Multilayer Perceptron (MLP) networks, each neuron is connected to every neuron in the previous layer and every neuron in the subsequent layer. The value of each neuron is computed using a weighted sum of the outputs from the previous layer, followed by the application of an activation function. Specifically, the value of a neuron is calculated as the weighted sum of the outputs of the neurons in the previous layer, combined with a bias term. This sum is then passed through an activation function, which introduces non-linearity into the network. The calculated value of each neuron becomes the input for the neurons in the next layer, and the process continues until the output layer is reached. The choice of activation function and the specific weight values determine the network's ability to learn and approximate complex relationships between inputs and outputs.

Therefore the value of each neuron can be calculated using: $a(\sum_j w_j * a_j)$. Where w_j is the weight and a_j is the value from neuron j to the current one. a() is the activation function, e.g. $relu(x) = max(0, x)$

Training on graphic cards

If you have an NVIDIA CUDA-enabled device and have installed the CUDA toolkit version 11.3 and cuDNN 8.4, you can take advantage of GPU acceleration for training your neural networks. It is crucial to have these specific versions installed, as other versions may not be compatible. For detailed installation instructions and more information on utilizing GPUs for training, please refer to the mlverse: 'torch' documentation.

Note: GPU training is optional, and the package can still be used for training on CPU even without CUDA and cuDNN installations.

Author(s)

Christian Amesoeder, Maximilian Pichler

See Also

`predict.citodnn`, `plot.citodnn`, `coef.citodnn`,`print.citodnn`, `summary.citodnn`, `continue_training`, `analyze_training`, `PDP`, `ALE`,

Examples

```
if(torch::torch_is_installed()){
library(cito)

# Example workflow in cito

## Build and train  Network
### softmax is used for multi-class responses (e.g., Species)
nn.fit<- dnn(Species~., data = datasets::iris, loss = "softmax")

## The training loss is below the baseline loss but at the end of the
## training the loss was still decreasing, so continue training for another 50
## epochs
nn.fit <- continue_training(nn.fit, epochs = 50L)

# Sturcture of Neural Network
print(nn.fit)

# Plot Neural Network
plot(nn.fit)
## 4 Input nodes (first layer) because of 4 features
## 3 Output nodes (last layer) because of 3 response species (one node for each
## level in the response variable).
## The layers between the input and output layer are called hidden layers (two
## of them)

## We now want to understand how the predictions are made, what are the
## important features? The summary function automatically calculates feature
## importance (the interpretation is similar to an anova) and calculates
## average conditional effects that are similar to linear effects:
summary(nn.fit)

## To visualize the effect (response-feature effect), we can use the ALE and
## PDP functions

# Partial dependencies
PDP(nn.fit, variable = "Petal.Length")

# Accumulated local effect plots
ALE(nn.fit, variable = "Petal.Length")



# Per se, it is difficult to get confidence intervals for our xAI metrics (or
# for the predictions). But we can use bootstrapping to obtain uncertainties
# for all cito outputs:
## Re-fit the neural network with bootstrapping
nn.fit<- dnn(Species~.,
             data = datasets::iris,
             loss = "softmax",
             epochs = 150L,
```

```
             verbose = FALSE,
             bootstrap = 20L)
## convergence can be tested via the analyze_training function
analyze_training(nn.fit)

## Summary for xAI metrics (can take some time):
summary(nn.fit)
## Now with standard errors and p-values
## Note: Take the p-values with a grain of salt! We do not know yet if they are
## correct (e.g. if you use regularization, they are likely conservative == too
## large)

## Predictions with bootstrapping:
dim(predict(nn.fit))
## predictions are by default averaged (over the bootstrap samples)



# Hyperparameter tuning (experimental feature)
hidden_values = matrix(c(5, 2,
                         4, 2,
                         10,2,
                         15,2), 4, 2, byrow = TRUE)
## Potential architectures we want to test, first column == number of nodes
print(hidden_values)

nn.fit = dnn(Species~.,
             data = iris,
             epochs = 30L,
             loss = "softmax",
             hidden = tune(values = hidden_values),
             lr = tune(0.00001, 0.1) # tune lr between range 0.00001 and 0.1
             )
## Tuning results:
print(nn.fit$tuning)

# test = Inf means that tuning was cancelled after only one fit (within the CV)


# Advanced: Custom loss functions and additional parameters
## Normal Likelihood with sd parameter:
custom_loss = function(pred, true) {
  logLik = torch::distr_normal(pred,
                               scale = torch::nnf_relu(scale)+
                                 0.001)$log_prob(true)
  return(-logLik$mean())
}

nn.fit<- dnn(Sepal.Length~.,
             data = datasets::iris,
             loss = custom_loss,
             verbose = FALSE,
             custom_parameters = list(scale = 1.0)
```

```
)
nn.fit$parameter$scale

## Multivariate normal likelihood with parametrized covariance matrix
## Sigma = L*L^t + D
## Helper function to build covariance matrix
create_cov = function(LU, Diag) {
  return(torch::torch_matmul(LU, LU$t()) + torch::torch_diag(Diag$exp()+0.01))
}

custom_loss_MVN = function(true, pred) {
  Sigma = create_cov(SigmaPar, SigmaDiag)
  logLik = torch::distr_multivariate_normal(pred,
                                            covariance_matrix = Sigma)$
    log_prob(true)
  return(-logLik$mean())
}


nn.fit<- dnn(cbind(Sepal.Length, Sepal.Width, Petal.Length)~.,
             data = datasets::iris,
             lr = 0.01,
             verbose = FALSE,
             loss = custom_loss_MVN,
             custom_parameters =
               list(SigmaDiag =  rep(0, 3),
                    SigmaPar = matrix(rnorm(6, sd = 0.001), 3, 2))
)
as.matrix(create_cov(nn.fit$loss$parameter$SigmaPar,
                     nn.fit$loss$parameter$SigmaDiag))

}
```

e *Embeddings*

Description

Can be used for categorical variables, a more efficient alternative to one-hot encoding

Usage

```
e(dim = 1L, weights = NULL, train = TRUE, lambda = 0, alpha = 1)
```

Arguments

`dim`	integer, embedding dimension
`weights`	matrix, to use custom embedding matrices

`train`	logical, should the embeddings be trained or not
`lambda`	regularization strength on the embeddings
`alpha`	mix between L1 and L2 regularization

`findReTrmClasses` *list of specials – taken from enum.R*

Description

list of specials – taken from enum.R

Usage

```
findReTrmClasses()
```

`linear` *Linear layer*

Description

creates a 'linear' 'citolayer' object that is used by `create_architecture`.

Usage

```
linear(
  n_neurons = NULL,
  bias = NULL,
  activation = NULL,
  normalization = NULL,
  dropout = NULL
)
```

Arguments

`n_neurons`	(int) amount of hidden neurons in this layer
`bias`	(boolean) if TRUE, adds a learnable bias to the neurons of this layer
`activation`	(string) activation function that is used after this layer. The following activation functions are supported: "relu", "leaky_relu", "tanh", "elu", "rrelu", "prelu", "softplus", "celu", "selu", "gelu", "relu6", "sigmoid", "softsign", "hardtanh", "tanhshrink", "softshrink", "hardshrink", "log_sigmoid"
`normalization`	(boolean) if TRUE, batch normalization is used after this layer
`dropout`	(float) dropout rate of this layer. Set to 0 for no dropout

Details

This function creates a 'linear' 'citolayer' object that is passed to the create_architecture function. The parameters that aren't assigned here (and are therefore still NULL) are filled with the default values passed to create_architecture.

Value

S3 object of class "linear" "citolayer"

Author(s)

Armin Schenk

See Also

create_architecture

---

maxPool *Maximum pooling layer*

Description

creates a 'maxPool' 'citolayer' object that is used by create_architecture.

Usage

```
maxPool(kernel_size = NULL, stride = NULL, padding = NULL, dilation = NULL)
```

Arguments

kernel_size	(int or tuple) size of the kernel in this layer. Use a tuple if the kernel size isn't equal in all dimensions
stride	(int or tuple) stride of the kernel in this layer. NULL sets the stride equal to the kernel size. Use a tuple if the stride isn't equal in all dimensions
padding	(int or tuple) zero-padding added to both sides of the input. Use a tuple if the padding isn't equal in all dimensions
dilation	(int or tuple) dilation of the kernel in this layer. Use a tuple if the dilation isn't equal in all dimensions

Details

This function creates a 'maxPool' 'citolayer' object that is passed to the create_architecture function. The parameters that aren't assigned here (and are therefore still NULL) are filled with the default values passed to create_architecture.

Value

S3 object of class "maxPool" "citolayer"

Author(s)

Armin Schenk

See Also

create_architecture

PDP *Partial Dependence Plot (PDP)*

Description

Calculates the Partial Dependency Plot for one feature, either numeric or categorical. Returns it as a plot.

Usage

```
PDP(
  model,
  variable = NULL,
  data = NULL,
  ice = FALSE,
  resolution.ice = 20,
  plot = TRUE,
  parallel = FALSE,
  ...
)

## S3 method for class 'citodnn'
PDP(
  model,
  variable = NULL,
  data = NULL,
  ice = FALSE,
  resolution.ice = 20,
  plot = TRUE,
  parallel = FALSE,
  ...
)

## S3 method for class 'citodnnBootstrap'
PDP(
  model,
```

```
    variable = NULL,
    data = NULL,
    ice = FALSE,
    resolution.ice = 20,
    plot = TRUE,
    parallel = FALSE,
    ...
)
```

Arguments

`model`	a model created by `dnn`
`variable`	variable as string for which the PDP should be done. If none is supplied it is done for all variables.
`data`	specify new data PDP should be performed . If NULL, PDP is performed on the training data.
`ice`	Individual Conditional Dependence will be shown if TRUE
`resolution.ice`	resolution in which ice will be computed
`plot`	plot PDP or not
`parallel`	parallelize over bootstrap models or not
`...`	arguments passed to `predict`

Value

A list of plots made with 'ggplot2' consisting of an individual plot for each defined variable.

Description

Performs a Partial Dependency Plot (PDP) estimation to analyze the relationship between a selected feature and the target variable.

The PDP function estimates the partial function $\hat{f}_S$:

$\hat{f}_S(x_S) = \frac{1}{n}\sum_{i=1}^n \hat{f}(x_S, x_C^{(i)})$

with a Monte Carlo Estimation:

$\hat{f}_S(x_S) = \frac{1}{n}\sum_{i=1}^n \hat{f}(x_S, x_C^{(i)})$ using a Monte Carlo estimation method. It calculates the average prediction of the target variable for different values of the selected feature while keeping other features constant.

For categorical features, all data instances are used, and each instance is set to one level of the categorical feature. The average prediction per category is then calculated and visualized in a bar plot.

If the `ice` parameter is set to `TRUE`, the Individual Conditional Expectation (ICE) curves are also shown. These curves illustrate how each individual data sample reacts to changes in the feature value. Please note that this option is not available for categorical features. Unlike PDP, the ICE curves are computed using a value grid instead of utilizing every value of every data entry.

Note: The PDP analysis provides valuable insights into the relationship between a specific feature and the target variable, helping to understand the feature's impact on the model's predictions. If a categorical feature is analyzed, all data instances are used and set to each level. Then an average is calculated per category and put out in a bar plot.

If ice is set to true additional the individual conditional dependence will be shown and the original PDP will be colored yellow. These lines show, how each individual data sample reacts to changes in the feature. This option is not available for categorical features. Unlike PDP the ICE curves are computed with a value grid instead of utilizing every value of every data entry.

See Also

ALE

Examples

```
if(torch::torch_is_installed()){
library(cito)

# Build and train  Network
nn.fit<- dnn(Sepal.Length~., data = datasets::iris)

PDP(nn.fit, variable = "Petal.Length")
}
```

---

plot.citoarchitecture *Plot the CNN architecture*

Description

Plot the CNN architecture

Usage

```
## S3 method for class 'citoarchitecture'
plot(x, input_shape, output_shape, ...)
```

Arguments

x	an object of class citoarchitecture created by create_architecture
input_shape	a vector with the dimensions of a single sample (e.g. c(3,28,28))
output_shape	the number of nodes in the output layer
...	additional arguments

Value

nothing

plot.citocnn — *Plot the CNN architecture*

Description

Plot the CNN architecture

Usage

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

Arguments

`x`	a model created by cnn
`...`	additional arguments

Value

original object x

plot.citodnn — *Creates graph plot which gives an overview of the network architecture.*

Description

Creates graph plot which gives an overview of the network architecture.

Usage

```
## S3 method for class 'citodnn'
plot(x, node_size = 1, scale_edges = FALSE, ...)

## S3 method for class 'citodnnBootstrap'
plot(x, node_size = 1, scale_edges = FALSE, which_model = 1, ...)
```

Arguments

`x`	a model created by dnn
`node_size`	size of node in plot
`scale_edges`	edge weight gets scaled according to other weights (layer specific)
`...`	no further functionality implemented yet
`which_model`	which model from the ensemble should be plotted

Value

A plot made with 'ggraph' + 'igraph' that represents the neural network

Examples

```
if(torch::torch_is_installed()){
library(cito)

set.seed(222)
validation_set<- sample(c(1:nrow(datasets::iris)),25)

# Build and train  Network
nn.fit<- dnn(Sepal.Length~., data = datasets::iris[-validation_set,])

plot(nn.fit)
}
```

---

predict.citocnn *Predict from a fitted cnn model*

Description

Predict from a fitted cnn model

Usage

```
## S3 method for class 'citocnn'
predict(
  object,
  newdata = NULL,
  type = c("link", "response", "class"),
  device = c("cpu", "cuda", "mps"),
  ...
)
```

Arguments

object	a model created by cnn
newdata	new data for predictions
type	which value should be calculated, either raw response, output of link function or predicted class (in case of classification)
device	device on which network should be trained on.
...	additional arguments

Value

prediction matrix

`predict.citodnn` *Predict from a fitted dnn model*

Description

Predict from a fitted dnn model

Usage

```
## S3 method for class 'citodnn'
predict(
  object,
  newdata = NULL,
  type = c("link", "response", "class"),
  device = c("cpu", "cuda", "mps"),
  reduce = c("mean", "median", "none"),
  ...
)

## S3 method for class 'citodnnBootstrap'
predict(
  object,
  newdata = NULL,
  type = c("link", "response", "class"),
  device = c("cpu", "cuda", "mps"),
  reduce = c("mean", "median", "none"),
  ...
)
```

Arguments

`object`	a model created by dnn
`newdata`	new data for predictions
`type`	type of predictions. The default is on the scale of the linear predictor, "response" is on the scale of the response, and "class" means that class predictions are returned (if it is a classification task)
`device`	device on which network should be trained on.
`reduce`	predictions from bootstrapped model are by default reduced (mean, optional median or none)
`...`	additional arguments

Value

prediction matrix

Examples

```
if(torch::torch_is_installed()){
library(cito)

set.seed(222)
validation_set<- sample(c(1:nrow(datasets::iris)),25)

# Build and train  Network
nn.fit<- dnn(Sepal.Length~., data = datasets::iris[-validation_set,])

# Use model on validation set
predictions <- predict(nn.fit, iris[validation_set,])
# Scatterplot
plot(iris[validation_set,]$Sepal.Length,predictions)
# MAE
mean(abs(predictions-iris[validation_set,]$Sepal.Length))
}
```

`print.avgPool` *Print pooling layer*

Description

Print pooling layer

Usage

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

Arguments

`x`	an object of class avgPool
`input_shape`	input shape
`...`	further arguments, not supported yet

print.citoarchitecture *Print class citoarchitecture*

Description

Print class citoarchitecture

Usage

```
## S3 method for class 'citoarchitecture'
print(x, input_shape, output_shape, ...)
```

Arguments

`x`	an object created by `create_architecture`
`input_shape`	a vector with the dimensions of a single sample (e.g. c(3,28,28))
`output_shape`	the number of nodes in the output layer
`...`	additional arguments

Value

original object

print.citocnn *Print class citocnn*

Description

Print class citocnn

Usage

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

Arguments

`x`	a model created by `cnn`
`...`	additional arguments

Value

original object x

print.citodnn *Print class citodnn*

Description

Print class citodnn

Usage

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

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

Arguments

x	a model created by dnn
...	additional arguments

Value

original object x gets returned

Examples

```
if(torch::torch_is_installed()){
library(cito)

set.seed(222)
validation_set<- sample(c(1:nrow(datasets::iris)),25)

# Build and train  Network
nn.fit<- dnn(Sepal.Length~., data = datasets::iris[-validation_set,])

# Structure of Neural Network
print(nn.fit)
}
```

print.conditionalEffects *Print average conditional effects*

Description

Print average conditional effects

Usage

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

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

Arguments

x	print ACE calculated by conditionalEffects
...	optional arguments for compatibility with the generic function, no function implemented

Value

Matrix with average conditional effects

print.conv *Print conv layer*

Description

Print conv layer

Usage

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

Arguments

x	an object of class conv
input_shape	input shape
...	further arguments, not supported yet

print.linear *Print linear layer*

Description

Print linear layer

Usage

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

Arguments

x	an object of class linear
input_shape	input shape
...	further arguments, not supported yet

print.maxPool *Print pooling layer*

Description

Print pooling layer

Usage

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

Arguments

x	an object of class maxPool
input_shape	input shape
...	further arguments, not supported yet

print.summary.citodnn *Print method for class summary.citodnn*

Description

Print method for class summary.citodnn

Usage

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

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

Arguments

`x`	a summary object created by `summary.citodnn`
`...`	additional arguments

Value

List with Matrices for importance, average CE, absolute sum of CE, and standard deviation of the CE

print.transfer *Print transfer model*

Description

Print transfer model

Usage

```
## S3 method for class 'transfer'
print(x, input_shape, output_shape, ...)
```

Arguments

`x`	an object of class transfer
`input_shape`	input shape
`output_shape`	output shape
`...`	further arguments, not supported yet

residuals.citodnn *Extract Model Residuals*

Description

Returns residuals of training set.

Usage

```
## S3 method for class 'citodnn'
residuals(object, ...)
```

Arguments

`object`	a model created by dnn
`...`	no additional arguments implemented

Value

residuals of training set

simulate_shapes *Data Simulation for CNN*

Description

generates images of rectangles and ellipsoids

Usage

```
simulate_shapes(n, size, channels = 1)
```

Arguments

`n`	number of images
`size`	size of the (quadratic) images
`channels`	number of channels the generated data has (in each channel a new rectangle/ellipsoid is created)

Details

This function generates simple data to demonstrate the usage of cnn(). The generated images are of centered rectangles and ellipsoids with random widths and heights.

Value

array of dimension (n, 1, size, size)

Author(s)

Armin Schenk

`summary.citocnn` *Summary citocnn*

Description

currently the same as the print.citocnn method.

Usage

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

Arguments

`object`	a model created by `cnn`
`...`	additional arguments

Value

original object x

`summary.citodnn` *Summarize Neural Network of class citodnn*

Description

Performs a Feature Importance calculation based on Permutations

Usage

```
## S3 method for class 'citodnn'
summary(object, n_permute = NULL, device = NULL, ...)

## S3 method for class 'citodnnBootstrap'
summary(object, n_permute = NULL, device = NULL, adjust_se = FALSE, ...)
```

Arguments

`object`	a model of class citodnn created by `dnn`
`n_permute`	number of permutations performed. Default is $3 * \sqrt{n}$, where n euqals then number of samples in the training set
`device`	for calculating variable importance and conditional effects
`...`	additional arguments
`adjust_se`	adjust standard errors for importance (standard errors are multiplied with 1/sqrt(3))

Details

Performs the feature importance calculation as suggested by Fisher, Rudin, and Dominici (2018), and the mean and standard deviation of the average conditional Effects as suggested by Pichler & Hartig (2023).

Feature importances are in their interpretation similar to a ANOVA. Main and interaction effects are absorbed into the features. Also, feature importances are prone to collinearity between features, i.e. if two features are collinear, the importances might be overestimated.

Average conditional effects (ACE) are similar to marginal effects and approximate linear effects, i.e. their interpretation is similar to effects in a linear regression model.

The standard deviation of the ACE informs about the non-linearity of the feature effects. Higher values correlate with stronger non-linearities.

For each feature n permutation get done and original and permuted predictive mean squared error (e_{perm} & e_{orig}) get evaluated with $FI_j = e_{perm}/e_{orig}$. Based on Mean Squared Error.

Value

summary.citodnn returns an object of class "summary.citodnn", a list with components

---

`sumTerms` *combine a list of formula terms as a sum*

Description

combine a list of formula terms as a sum

Usage

```
sumTerms(termList)
```

Arguments

`termList`	a list of formula terms

transfer — *Transfer learning*

Description

creates a 'transfer' 'citolayer' object that is used by create_architecture.

Usage

```
transfer(
  name = c("alexnet", "inception_v3", "mobilenet_v2", "resnet101", "resnet152",
   "resnet18", "resnet34", "resnet50", "resnext101_32x8d", "resnext50_32x4d", "vgg11",
    "vgg11_bn", "vgg13", "vgg13_bn", "vgg16", "vgg16_bn", "vgg19", "vgg19_bn",
    "wide_resnet101_2", "wide_resnet50_2"),
  pretrained = TRUE,
  freeze = TRUE
)
```

Arguments

`name`	The name of the pretrained model
`pretrained`	if FALSE, random weights are used instead of the pretrained weights
`freeze`	if TRUE, the weights of the pretrained model (except the "classifier" part at the end) aren't changed in the training anymore. Only works if pretrained=TRUE

Details

This function creates a 'transfer' 'citolayer' object that is passed to the create_architecture function. With this object the pretrained models that are available in the 'torchvision' package can be used in cito. When 'freeze' is set to TRUE, only the weights of the last part of the network (consisting of one or more linear layers) are adjusted in the training. There mustn't be any other citolayers before the transfer citolayer object when calling create_architecture. If there are any citolayers after the transfer citolayer, the linear classifier part of the pretrained model is replaced with the specified citolayers.

Value

S3 object of class `"transfer" "citolayer"`

Author(s)

Armin Schenk

See Also

create_architecture

tune *Tune hyperparameter*

Description

Control hyperparameter tuning

Usage

```
tune(
  lower = NULL,
  upper = NULL,
  fixed = NULL,
  additional = NULL,
  values = NULL
)
```

Arguments

lower	numeric, numeric vector, character, lower boundaries of tuning space
upper	numeric, numeric vector, character, upper boundaries of tuning space
fixed	character, used for multi-dimensional hyperparameters such as hidden, which dimensions should be fixed
additional	numeric, additional control parameter which sets the value of the fixed argument
values	custom values from which hyperparameters are sampled, must be a matrix for hidden layers (first column == nodes, second column == number of layers)

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