Package 'tabnet'

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Title Fit 'TabNet' Models for Classification and Regression

Version 0.5.0

Description Implements the 'TabNet' model by Sercan O. Arik et al. (2019) <arXiv:1908.07442>
with 'Coherent Hierarchical Multi-label Classification Networks' by Giunchiglia et al.
<arXiv:2010.10151> and provides a consistent interface for fitting and creating
predictions. It's also fully compatible with the 'tidymodels' ecosystem.

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Encoding UTF-8

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URL https://mlverse.github.io/tabnet/,
https://github.com/mlverse/tabnet

BugReports https://github.com/mlverse/tabnet/issues

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NeedsCompilation no

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R **topics documented:**

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autoplot.tabnet_explain

Plot tabnet_explain mask importance heatmap

Description

Plot tabnet_explain mask importance heatmap

Usage

```
autoplot.tabnet_explain(
  object,
  type = c("mask_agg", "steps"),
  quantile = 1,
  ...
)
```

Arguments

object	A tabnet_explain object as a result of [tabnet_explain()](#).
type	a character value. Either "mask_agg" the default, for a single heatmap of aggregated mask importance per predictor along the dataset, or "steps" for one heatmap at each mask step.
quantile	numerical value between 0 and 1. Provides quantile clipping of the mask values
...	not used.

Details

Plot the tabnet_explain object mask importance per variable along the predicted dataset. type="mask_agg" output a single heatmap of mask aggregated values, type="steps" provides a plot faceted along the n_steps mask present in the model. quantile=.995 may be used for strong outlier clipping, in order to better highlight low values. quantile=1, the default, do not clip any values.

Value

A ggplot object.

Examples

```
library(ggplot2)
data("attrition", package = "modeldata")

## Single-outcome binary classification of `Attrition` in `attrition` dataset
attrition_fit <- tabnet_fit(Attrition ~. , data=attrition, epoch=11)
attrition_explain <- tabnet_explain(attrition_fit, attrition)
# Plot the model aggregated mask interpretation heatmap
autoplot(attrition_explain)

## Multi-outcome regression on `Sale_Price` and `Pool_Area` in `ames` dataset,
data("ames", package = "modeldata")
ids <- sample(nrow(ames), 256)
x <- ames[ids,-which(names(ames) %in% c("Sale_Price", "Pool_Area"))]
y <- ames[ids, c("Sale_Price", "Pool_Area")]
ames_fit <- tabnet_fit(x, y, epochs = 5, verbose=TRUE)
ames_explain <- tabnet_explain(ames_fit, x)
autoplot(ames_explain, quantile = 0.99)
```

---

autoplot.tabnet_fit   *Plot tabnet_fit model loss along epochs*

Description

Plot tabnet_fit model loss along epochs

Usage

```
autoplot.tabnet_fit(object, ...)

autoplot.tabnet_pretrain(object, ...)
```

Arguments

object	A tabnet_fit or tabnet_pretrain object as a result of tabnet_fit() or tabnet_pretrain().
...	not used.

Details

Plot the training loss along epochs, and validation loss along epochs if any. A dot is added on epochs where model snapshot is available, helping the choice of `from_epoch` value for later model training resume.

Value

A `ggplot` object.

Examples

```
library(ggplot2)
data("attrition", package = "modeldata")
attrition_fit <- tabnet_fit(Attrition ~. , data=attrition, valid_split=0.2, epoch=11)

# Plot the model loss over epochs
autoplot(attrition_fit)
```

---

check_compliant_node   *Check that Node object names are compliant*

Description

Check that Node object names are compliant

Usage

```
check_compliant_node(node)
```

Arguments

node   the Node object, or a dataframe ready to be parsed by `data.tree::as.Node()`

Value

node if it is compliant, else an Error with the column names to fix

Examples

```
library(dplyr)
library(data.tree)
data(starwars)
starwars_tree <- starwars %>%
  mutate(pathString = paste("tree", species, homeworld, `name`, sep = "/"))

# pre as.Node() check
```

```
try(check_compliant_node(starwars_tree))

# post as.Node() check
check_compliant_node(as.Node(starwars_tree))
```

---

decision_width *Parameters for the tabnet model*

Description

Parameters for the tabnet model

Usage

```
decision_width(range = c(8L, 64L), trans = NULL)

attention_width(range = c(8L, 64L), trans = NULL)

num_steps(range = c(3L, 10L), trans = NULL)

feature_reusage(range = c(1, 2), trans = NULL)

num_independent(range = c(1L, 5L), trans = NULL)

num_shared(range = c(1L, 5L), trans = NULL)

momentum(range = c(0.01, 0.4), trans = NULL)

mask_type(values = c("sparsemax", "entmax"))
```

Arguments

range	the default range for the parameter value
trans	whether to apply a transformation to the parameter
values	possible values for factor parameters
	These functions are used with `tune` grid functions to generate candidates.

Value

A `dials` parameter to be used when tuning TabNet models.

---

nn_prune_head.tabnet_fit

Prune top layer(s) of a tabnet network

Description

Prune `head_size` last layers of a tabnet network in order to use the pruned module as a sequential embedding module.

Usage

```
nn_prune_head.tabnet_fit(x, head_size)

nn_prune_head.tabnet_pretrain(x, head_size)
```

Arguments

x	nn_network to prune
head_size	number of nn_layers to prune, should be less than 2

Value

a tabnet network with the top nn_layer removed

---

node_to_df   *Turn a Node object into predictor and outcome.*

Description

Turn a Node object into predictor and outcome.

Usage

```
node_to_df(x, drop_last_level = TRUE)
```

Arguments

x	Node object
drop_last_level	
	TRUE unused

Value

a named list of x and y, being respectively the predictor data-frame and the outcomes data-frame, as expected inputs for `hardhat::mold()` function.

Examples

```
library(dplyr)
library(data.tree)
data(starwars)
starwars_tree <- starwars %>%
  mutate(pathString = paste("tree", species, homeworld, `name`, sep = "/")) %>%
  as.Node()
node_to_df(starwars_tree)$x %>% head()
node_to_df(starwars_tree)$y %>% head()
```

---

tabnet   *Parsnip compatible tabnet model*

Description

Parsnip compatible tabnet model

Usage

```
tabnet(
  mode = "unknown",
  epochs = NULL,
  penalty = NULL,
  batch_size = NULL,
  learn_rate = NULL,
  decision_width = NULL,
  attention_width = NULL,
  num_steps = NULL,
  feature_reusage = NULL,
  virtual_batch_size = NULL,
  num_independent = NULL,
  num_shared = NULL,
  momentum = NULL
)
```

Arguments

mode	A single character string for the type of model. Possible values for this model are "unknown", "regression", or "classification".
epochs	(int) Number of training epochs.
penalty	This is the extra sparsity loss coefficient as proposed in the original paper. The bigger this coefficient is, the sparser your model will be in terms of feature selection. Depending on the difficulty of your problem, reducing this value could help (default 1e-3).

batch_size	(int) Number of examples per batch, large batch sizes are recommended. (default: 1024^2)
learn_rate	initial learning rate for the optimizer.
decision_width	(int) Width of the decision prediction layer. Bigger values gives more capacity to the model with the risk of overfitting. Values typically range from 8 to 64.
attention_width	
	(int) Width of the attention embedding for each mask. According to the paper n_d = n_a is usually a good choice. (default=8)
num_steps	(int) Number of steps in the architecture (usually between 3 and 10)
feature_reusage	
	(float) This is the coefficient for feature reusage in the masks. A value close to 1 will make mask selection least correlated between layers. Values range from 1.0 to 2.0.
virtual_batch_size	
	(int) Size of the mini batches used for "Ghost Batch Normalization" (default=256^2)
num_independent	
	Number of independent Gated Linear Units layers at each step of the encoder. Usual values range from 1 to 5.
num_shared	Number of shared Gated Linear Units at each step of the encoder. Usual values at each step of the decoder. range from 1 to 5
momentum	Momentum for batch normalization, typically ranges from 0.01 to 0.4 (default=0.02)

Value

A TabNet `parsnip` instance. It can be used to fit tabnet models using `parsnip` machinery.

Threading

TabNet uses `torch` as its backend for computation and `torch` uses all available threads by default.

You can control the number of threads used by `torch` with:

```
torch::torch_set_num_threads(1)
torch::torch_set_num_interop_threads(1)
```

See Also

tabnet_fit

Examples

```
library(parsnip)
data("ames", package = "modeldata")
model <- tabnet() %>%
  set_mode("regression") %>%
  set_engine("torch")
model %>%
  fit(Sale_Price ~ ., data = ames)
```

---

tabnet_config *Configuration for TabNet models*

Description

Configuration for TabNet models

Usage

```
tabnet_config(
  batch_size = 1024^2,
  penalty = 0.001,
  clip_value = NULL,
  loss = "auto",
  epochs = 5,
  drop_last = FALSE,
  decision_width = NULL,
  attention_width = NULL,
  num_steps = 3,
  feature_reusage = 1.3,
  mask_type = "sparsemax",
  virtual_batch_size = 256^2,
  valid_split = 0,
  learn_rate = 0.02,
  optimizer = "adam",
  lr_scheduler = NULL,
  lr_decay = 0.1,
  step_size = 30,
  checkpoint_epochs = 10,
  cat_emb_dim = 1,
  num_independent = 2,
  num_shared = 2,
  num_independent_decoder = 1,
  num_shared_decoder = 1,
  momentum = 0.02,
  pretraining_ratio = 0.5,
  verbose = FALSE,
  device = "auto",
  importance_sample_size = NULL,
  early_stopping_monitor = "auto",
  early_stopping_tolerance = 0,
  early_stopping_patience = 0L,
  num_workers = 0L,
  skip_importance = FALSE
)
```

Arguments

`batch_size`	(int) Number of examples per batch, large batch sizes are recommended. (default: 1024^2)
`penalty`	This is the extra sparsity loss coefficient as proposed in the original paper. The bigger this coefficient is, the sparser your model will be in terms of feature selection. Depending on the difficulty of your problem, reducing this value could help (default 1e-3).
`clip_value`	If a float is given this will clip the gradient at clip_value. Pass NULL to not clip.
`loss`	(character or function) Loss function for training (default to mse for regression and cross entropy for classification)
`epochs`	(int) Number of training epochs.
`drop_last`	(logical) Whether to drop last batch if not complete during training
`decision_width`	(int) Width of the decision prediction layer. Bigger values gives more capacity to the model with the risk of overfitting. Values typically range from 8 to 64.
`attention_width`	
	(int) Width of the attention embedding for each mask. According to the paper n_d = n_a is usually a good choice. (default=8)
`num_steps`	(int) Number of steps in the architecture (usually between 3 and 10)
`feature_reusage`	
	(float) This is the coefficient for feature reusage in the masks. A value close to 1 will make mask selection least correlated between layers. Values range from 1.0 to 2.0.
`mask_type`	(character) Final layer of feature selector in the attentive_transformer block, either ″sparsemax″ or ″entmax″.Defaults to ″sparsemax″.
`virtual_batch_size`	
	(int) Size of the mini batches used for "Ghost Batch Normalization" (default=256^2)
`valid_split`	([0, 1)) The fraction of the dataset used for validation. (default = 0 means no split)
`learn_rate`	initial learning rate for the optimizer.
`optimizer`	the optimization method. currently only 'adam' is supported, you can also pass any torch optimizer function.
`lr_scheduler`	if NULL, no learning rate decay is used. If "step" decays the learning rate by `lr_decay` every `step_size` epochs. If "reduce_on_plateau" decays the learning rate by `lr_decay` when no improvement after `step_size` epochs. It can also be a torch::lr_scheduler function that only takes the optimizer as parameter. The step method is called once per epoch.
`lr_decay`	multiplies the initial learning rate by `lr_decay` every `step_size` epochs. Unused if `lr_scheduler` is a torch::lr_scheduler or NULL.
`step_size`	the learning rate scheduler step size. Unused if `lr_scheduler` is a torch::lr_scheduler or NULL.
`checkpoint_epochs`	
	checkpoint model weights and architecture every `checkpoint_epochs`. (default is 10). This may cause large memory usage. Use 0 to disable checkpoints.

cat_emb_dim   Size of the embedding of categorical features. If int, all categorical features will
                   have same embedding size, if list of int, every corresponding feature will have
                   specific embedding size.

num_independent
                   Number of independent Gated Linear Units layers at each step of the encoder.
                   Usual values range from 1 to 5.

num_shared   Number of shared Gated Linear Units at each step of the encoder. Usual values
                   at each step of the decoder. range from 1 to 5

num_independent_decoder
                   For pretraining, number of independent Gated Linear Units layers Usual values
                   range from 1 to 5.

num_shared_decoder
                   For pretraining, number of shared Gated Linear Units at each step of the decoder.
                   Usual values range from 1 to 5.

momentum   Momentum for batch normalization, typically ranges from 0.01 to 0.4 (default=0.02)

pretraining_ratio
                   Ratio of features to mask for reconstruction during pretraining. Ranges from 0
                   to 1 (default=0.5)

verbose   (logical) Whether to print progress and loss values during training.

device   the device to use for training. "cpu" or "cuda". The default ("auto") uses to
                   "cuda" if it's available, otherwise uses "cpu".

importance_sample_size
                   sample of the dataset to compute importance metrics. If the dataset is larger than
                   1e5 obs we will use a sample of size 1e5 and display a warning.

early_stopping_monitor
                   Metric to monitor for early_stopping. One of "valid_loss", "train_loss" or "auto"
                   (defaults to "auto").

early_stopping_tolerance
                   Minimum relative improvement to reset the patience counter. 0.01 for 1% toler-
                   ance (default 0)

early_stopping_patience
                   Number of epochs without improving until stopping training. (default=5)

num_workers   (int, optional): how many subprocesses to use for data loading. 0 means that the
                   data will be loaded in the main process. (default: 0)

skip_importance
                   if feature importance calculation should be skipped (default: FALSE)

Value

A named list with all hyperparameters of the TabNet implementation.

tabnet_explain   *Interpretation metrics from a TabNet model*

Description

Interpretation metrics from a TabNet model

Usage

```
tabnet_explain(object, new_data)

## Default S3 method:
tabnet_explain(object, new_data)

## S3 method for class 'tabnet_fit'
tabnet_explain(object, new_data)

## S3 method for class 'tabnet_pretrain'
tabnet_explain(object, new_data)

## S3 method for class 'model_fit'
tabnet_explain(object, new_data)
```

Arguments

object	a TabNet fit object
new_data	a data.frame to obtain interpretation metrics.

Value

Returns a list with

- `M_explain`: the aggregated feature importance masks as detailed in TabNet's paper.
- `masks` a list containing the masks for each step.

Examples

```
set.seed(2021)

n <- 1000
x <- data.frame(
  x = rnorm(n),
  y = rnorm(n),
  z = rnorm(n)
)
```

```
y <- x$x

fit <- tabnet_fit(x, y, epochs = 20,
                  num_steps = 1,
                  batch_size = 512,
                  attention_width = 1,
                  num_shared = 1,
                  num_independent = 1)


 ex <- tabnet_explain(fit, x)
```

---

tabnet_fit	*Tabnet model*

Description

Fits the [TabNet: Attentive Interpretable Tabular Learning](#) model

Usage

```
tabnet_fit(x, ...)

## Default S3 method:
tabnet_fit(x, ...)

## S3 method for class 'data.frame'
tabnet_fit(
  x,
  y,
  tabnet_model = NULL,
  config = tabnet_config(),
  ...,
  from_epoch = NULL
)

## S3 method for class 'formula'
tabnet_fit(
  formula,
  data,
  tabnet_model = NULL,
  config = tabnet_config(),
  ...,
  from_epoch = NULL
)
```

```
## S3 method for class 'recipe'
tabnet_fit(
  x,
  data,
  tabnet_model = NULL,
  config = tabnet_config(),
  ...,
  from_epoch = NULL
)

## S3 method for class 'Node'
tabnet_fit(
  x,
  tabnet_model = NULL,
  config = tabnet_config(),
  ...,
  from_epoch = NULL
)
```

Arguments

x	Depending on the context:
	- A **data frame** of predictors. - A **matrix** of predictors. - A **recipe** specifying a set of preprocessing steps created from recipes::recipe().
	The predictor data should be standardized (e.g. centered or scaled). The model treats categorical predictors internally thus, you don't need to make any treatment.
...	Model hyperparameters. Any hyperparameters set here will update those set by the config argument. See tabnet_config() for a list of all possible hyperparameters.
y	When x is a **data frame** or **matrix**, y is the outcome specified as:
	- A **data frame** with 1 or many numeric column (regression) or 1 or many categorical columns (classification) . - A **matrix** with 1 column. - A **vector**, either numeric or categorical.
tabnet_model	A previously fitted TabNet model object to continue the fitting on. if NULL (the default) a brand new model is initialized.
config	A set of hyperparameters created using the tabnet_config function. If no argument is supplied, this will use the default values in tabnet_config().
from_epoch	When a tabnet_model is provided, restore the network weights from a specific epoch. Default is last available checkpoint for restored model, or last epoch for in-memory model.
formula	A formula specifying the outcome terms on the left-hand side, and the predictor terms on the right-hand side.

data   When a **recipe** or **formula** is used, data is specified as:

- A **data frame** containing both the predictors and the outcome.

Value

A TabNet model object. It can be used for serialization, predictions, or further fitting.

Fitting a pre-trained model

When providing a parent tabnet_model parameter, the model fitting resumes from that model weights at the following epoch:

- last fitted epoch for a model already in torch context
- Last model checkpoint epoch for a model loaded from file
- the epoch related to a checkpoint matching or preceding the from_epoch value if provided The model fitting metrics append on top of the parent metrics in the returned TabNet model.

Multi-outcome

TabNet allows multi-outcome prediction, which is usually named multi-label classification or multi-output classification when outcomes are categorical. Multi-outcome currently expect outcomes to be either all numeric or all categorical.

Threading

TabNet uses torch as its backend for computation and torch uses all available threads by default.

You can control the number of threads used by torch with:

```
torch::torch_set_num_threads(1)
torch::torch_set_num_interop_threads(1)
```

Examples

```
data("ames", package = "modeldata")
data("attrition", package = "modeldata")
ids <- sample(nrow(attrition), 256)

## Single-outcome regression using formula specification
fit <- tabnet_fit(Sale_Price ~ ., data = ames, epochs = 1)

## Single-outcome classification using data-frame specification
attrition_x <- attrition[,-which(names(attrition) == "Attrition")]
fit <- tabnet_fit(attrition_x, attrition$Attrition, epochs = 1, verbose = TRUE)

## Multi-outcome regression on `Sale_Price` and `Pool_Area` in `ames` dataset using formula,
ames_fit <- tabnet_fit(Sale_Price + Pool_Area ~ ., data = ames[ids,], epochs = 2, valid_split = 0.2)

## Multi-label classification on `Attrition` and `JobSatisfaction` in
```

```
## `attrition` dataset using recipe
library(recipes)
rec <- recipe(Attrition + JobSatisfaction ~ ., data = attrition[ids,]) %>%
  step_normalize(all_numeric(), -all_outcomes())

attrition_fit <- tabnet_fit(rec, data = attrition[ids,], epochs = 2, valid_split = 0.2)

## Hierarchical classification on  `acme`
data(acme, package = "data.tree")

acme_fit <- tabnet_fit(acme, epochs = 2, verbose = TRUE)

# Note: Dataset number of rows and model number of epochs should be increased
# for publication-level results.
```

---

tabnet_nn   *TabNet Model Architecture*

Description

This is a nn_module representing the TabNet architecture from Attentive Interpretable Tabular Deep Learning.

Usage

```
tabnet_nn(
  input_dim,
  output_dim,
  n_d = 8,
  n_a = 8,
  n_steps = 3,
  gamma = 1.3,
  cat_idxs = c(),
  cat_dims = c(),
  cat_emb_dim = 1,
  n_independent = 2,
  n_shared = 2,
  epsilon = 1e-15,
  virtual_batch_size = 128,
  momentum = 0.02,
  mask_type = "sparsemax"
)
```

Arguments

input_dim   Initial number of features.

output_dim   Dimension of network output examples : one for regression, 2 for binary classi-
                fication etc.. Vector of those dimensions in case of multi-output.

n_d	Dimension of the prediction layer (usually between 4 and 64).
n_a	Dimension of the attention layer (usually between 4 and 64).
n_steps	Number of successive steps in the network (usually between 3 and 10).
gamma	Float above 1, scaling factor for attention updates (usually between 1 and 2).
cat_idxs	Index of each categorical column in the dataset.
cat_dims	Number of categories in each categorical column.
cat_emb_dim	Size of the embedding of categorical features if int, all categorical features will have same embedding size if list of int, every corresponding feature will have specific size.
n_independent	Number of independent GLU layer in each GLU block of the encoder.
n_shared	Number of independent GLU layer in each GLU block of the encoder.
epsilon	Avoid log(0), this should be kept very low.
virtual_batch_size	
	Batch size for Ghost Batch Normalization.
momentum	Float value between 0 and 1 which will be used for momentum in all batch norm.
mask_type	Either "sparsemax" or "entmax" : this is the masking function to use.

---

tabnet_pretrain	*Tabnet model*

Description

Pretrain the TabNet: Attentive Interpretable Tabular Learning model on the predictor data exclusively (unsupervised training).

Usage

```
tabnet_pretrain(x, ...)

## Default S3 method:
tabnet_pretrain(x, ...)

## S3 method for class 'data.frame'
tabnet_pretrain(
  x,
  y,
  tabnet_model = NULL,
  config = tabnet_config(),
  ...,
  from_epoch = NULL
)

## S3 method for class 'formula'
```

```
tabnet_pretrain(
  formula,
  data,
  tabnet_model = NULL,
  config = tabnet_config(),
  ...,
  from_epoch = NULL
)

## S3 method for class 'recipe'
tabnet_pretrain(
  x,
  data,
  tabnet_model = NULL,
  config = tabnet_config(),
  ...,
  from_epoch = NULL
)

## S3 method for class 'Node'
tabnet_pretrain(
  x,
  tabnet_model = NULL,
  config = tabnet_config(),
  ...,
  from_epoch = NULL
)
```

Arguments

x
: Depending on the context:

    - A **data frame** of predictors.
    - A **matrix** of predictors.
    - A **recipe** specifying a set of preprocessing steps created from recipes::recipe().

    The predictor data should be standardized (e.g. centered or scaled). The model treats categorical predictors internally thus, you don't need to make any treatment.

...
: Model hyperparameters. Any hyperparameters set here will update those set by the config argument. See tabnet_config() for a list of all possible hyperparameters.

y
: (optional) When x is a **data frame** or **matrix**, y is the outcome

tabnet_model
: A pretrained TabNet model object to continue the fitting on. if NULL (the default) a brand new model is initialized.

config
: A set of hyperparameters created using the tabnet_config function. If no argument is supplied, this will use the default values in tabnet_config().

from_epoch	When a `tabnet_model` is provided, restore the network weights from a specific epoch. Default is last available checkpoint for restored model, or last epoch for in-memory model.
formula	A formula specifying the outcome terms on the left-hand side, and the predictor terms on the right-hand side.
data	When a **recipe** or **formula** is used, `data` is specified as: • A **data frame** containing both the predictors and the outcome.

Value

A TabNet model object. It can be used for serialization, predictions, or further fitting.

outcome

Outcome value are accepted here only for consistent syntax with `tabnet_fit`, but by design the outcome, if present, is ignored during pre-training.

pre-training from a previous model

When providing a parent `tabnet_model` parameter, the model pretraining resumes from that model weights at the following epoch:

- last pretrained epoch for a model already in torch context
- Last model checkpoint epoch for a model loaded from file
- the epoch related to a checkpoint matching or preceding the `from_epoch` value if provided The model pretraining metrics append on top of the parent metrics in the returned TabNet model.

Threading

TabNet uses `torch` as its backend for computation and `torch` uses all available threads by default.

You can control the number of threads used by `torch` with:

```
torch::torch_set_num_threads(1)
torch::torch_set_num_interop_threads(1)
```

Examples

```
data("ames", package = "modeldata")
pretrained <- tabnet_pretrain(Sale_Price ~ ., data = ames, epochs = 1)
```

Index