Package 'deepregression'

January 17, 2023

```
Title Fitting Deep Distributional Regression
```

Version 1.0.0

Description Allows for the specification of semi-

structured deep distributional regression models which are fitted in a neural network as proposed by Ruegamer et al. (2023) <doi:10.18637/jss.v105.i02>.

Predictors can be modeled using structured (penalized) linear effects, structured non-linear effects or using an unstructured deep network model.

```
Config/reticulate list( packages = list( list(package = ``six", pip = TRUE), list(package = ``tensorflow", version = ``2.10.0", pip = TRUE), list(package = ``tensorflow_probability", version = ``0.16", pip = TRUE), list(package = ``keras", version = ``2.10.0", pip = TRUE)) )
```

Depends R (>= 4.0.0), tensorflow (>= 2.2.0), tfprobability, keras (>= 2.2.0)

Suggests testthat, knitr, covr

Imports mgcv, dplyr, R6, reticulate (>= 1.14), Matrix, magrittr, tfruns, methods

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NeedsCompilation no

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 ${\sf check_and_install}$

Function to check python environment and install necessary packages

Description

If you encounter problems with installing the required python modules please make sure, that a correct python version is configured using py_discover_config and change the python version if required. Internally uses keras::install_keras.

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Usage

```
check_and_install(force = FALSE)
```

Arguments

force if TRUE, forces the installations

Value

Function that checks if a Python environment is available and contains TensorFlow. If not the recommended version is installed.

coef.drEnsemble

Method for extracting ensemble coefficient estimates

Description

Method for extracting ensemble coefficient estimates

Usage

```
## S3 method for class 'drEnsemble'
coef(object, which_param = 1, type = NULL, ...)
```

Arguments

object of class "drEnsemble"

which_param integer, indicating for which distribution parameter coefficients should be re-

turned (default is first parameter)

type either NULL (all types of coefficients are returned), "linear" for linear coeffi-

cients or "smooth" for coefficients of smooth terms

... further arguments supplied to coef.deepregression

Value

list of coefficient estimates of all ensemble members

combine_penalties 5

| compine | penalties |
|---------|-----------|

Function to combine two penalties

Description

Function to combine two penalties

Usage

```
combine_penalties(penalties, dims)
```

Arguments

penalties a list of penalties

dims dimensions of the parameters to penalize

Value

a TensorFlow penalty combining the two penalties

create_family

Function to create (custom) family

Description

Function to create (custom) family

Usage

```
create_family(tfd_dist, trafo_list, output_dim = 1L)
```

Arguments

tfd_dist a tensorflow probability distribution

trafo_list list of transformations h for each parameter (e.g, exp for a variance parameter)

output_dim integer defining the size of the response

Value

a function that can be used by tfpstar DistributionLambda to create a new distribuional layer

6 cv

create_penalty

Function to create mgcv-type penalty

Description

Function to create mgcv-type penalty

Usage

```
create_penalty(evaluated_gam_term, df, controls, Z = NULL)
```

Arguments

```
evaluated_gam_term
```

a list resulting from a smoothConstruct call

df integer; specified degrees-of-freedom for the gam term

controls list; further arguments defining the smooth

Z matrix; matrix for constraint(s)

Value

a list with penalty parameter and penalty matrix

С٧

Generic cv function

Description

Generic cv function

Usage

```
cv(x, ...)
```

Arguments

x model to do cv on

... further arguments passed to the class-specific function

deepregression 7

deepregression

Fitting Semi-Structured Deep Distributional Regression

Description

Fitting Semi-Structured Deep Distributional Regression

Usage

```
deepregression(
  у,
 list_of_formulas,
 list_of_deep_models = NULL,
  family = "normal",
  data,
  tf\_seed = as.integer(1991 - 5 - 4),
  return_prepoc = FALSE,
  subnetwork_builder = subnetwork_init,
 model_builder = keras_dr,
  fitting_function = utils::getFromNamespace("fit.keras.engine.training.Model",
    "keras"),
  additional_processors = list(),
  penalty_options = penalty_control(),
 orthog_options = orthog_control(),
 weight_options = weight_control(),
  formula_options = form_control(),
 output_dim = 1L,
  verbose = FALSE,
)
```

Arguments

y response variable

list_of_formulas

a named list of right hand side formulas, one for each parameter of the distribution specified in family; set to ~ 1 if the parameter should be treated as constant. Use the s()-notation from mgcv for specification of non-linear structured effects and d(...) for deep learning predictors (predictors in brackets are separated by commas), where d can be replaced by an name name of the names in list_of_deep_models, e.g., $\sim 1 + s(x) + my_deep_mod(a,b,c)$, where my_deep_mod is the name of the neural net specified in list_of_deep_models and a,b,c are features modeled via this network.

list_of_deep_models

a named list of functions specifying a keras model. See the examples for more details.

8 deepregression

| family | a character specifying the distribution. For information on possible distribution and parameters, see make_tfd_dist. Can also be a custom distribution. |
|-------------------------|---|
| data | data.frame or named list with input features |
| tf_seed | a seed for TensorFlow (only works with R version \geq 2.2.0) |
| return_prepoc | logical; if TRUE only the pre-processed data and layers are returned (default FALSE). |
| subnetwork_buil | der |
| | function to build each subnetwork (network for each distribution parameter; per default subnetwork_init). Can also be a list of the same size as list_of_formulas. |
| model_builder | function to build the model based on additive predictors (per default keras_dr). In order to work with the methods defined for the class deepregression, the model should behave like a keras model |
| fitting_function | on |
| | function to fit the instantiated model when calling fit. Per default the keras fit function. |
| additional_proc | |
| | a named list with additional processors to convert the formula(s). Can have an attribute "controls" to pass additional controls |
| penalty_options | |
| | options for smoothing and penalty terms defined by penalty_control |
| orthog_options | options for the orthgonalization defined by orthog_control |
| ${\tt weight_options}$ | options for layer weights defined by weight_control |
| formula_options | |
| | options for formula parsing (mainly used to make calculation more efficiently) |
| output_dim | dimension of the output, per default 1L |
| verbose | logical; whether to print progress of model initialization to console |
| | further arguments passed to the model_builder function |

References

Ruegamer, D. et al. (2023): deepregression: a Flexible Neural Network Framework for Semi-Structured Deep Distributional Regression. doi:10.18637/jss.v105.i02.

Examples

```
library(deepregression)

n <- 1000
data = data.frame(matrix(rnorm(4*n), c(n,4)))
colnames(data) <- c("x1","x2","x3","xa")
formula <- ~ 1 + deep_model(x1,x2,x3) + s(xa) + x1

deep_model <- function(x) x %>%
layer_dense(units = 32, activation = "relu", use_bias = FALSE) %>%
layer_dropout(rate = 0.2) %>%
layer_dense(units = 8, activation = "relu") %>%
```

distfun_to_dist

```
layer_dense(units = 1, activation = "linear")
y \leftarrow rnorm(n) + data$xa^2 + data$x1
mod <- deepregression(</pre>
  list_of_formulas = list(loc = formula, scale = ~ 1),
  data = data, y = y,
  list_of_deep_models = list(deep_model = deep_model)
)
if(!is.null(mod)){
# train for more than 10 epochs to get a better model
mod %>% fit(epochs = 10, early_stopping = TRUE)
mod %>% fitted() %>% head()
cvres <- mod %>% cv()
mod %>% get_partial_effect(name = "s(xa)")
mod %>% coef()
mod %>% plot()
}
mod <- deepregression(</pre>
  list_of_formulas = list(loc = ~1 + s(xa) + x1, scale = ~1,
                          dummy = ~-1 + deep_model(x1,x2,x3) %OZ% 1),
  data = data, y = y,
  list_of_deep_models = list(deep_model = deep_model),
  mapping = list(1,2,1:2)
)
```

distfun_to_dist

Function to define output distribution based on dist_fun

Description

Function to define output distribution based on dist_fun

Usage

```
distfun_to_dist(dist_fun, preds)
```

Arguments

dist_fun a distribution function as defined by make_tfd_dist preds tensors with predictions

Value

a symbolic tfp distribution

ensemble

Generic deep ensemble function

Description

Generic deep ensemble function

Usage

```
ensemble(x, ...)
```

Arguments

x model to ensemble

... further arguments passed to the class-specific function

ensemble.deepregression

Ensemblind deepregression models

Description

Ensemblind deepregression models

Usage

```
## S3 method for class 'deepregression'
ensemble(
 х,
 n_{ensemble} = 5,
 reinitialize = TRUE,
 mylapply = lapply,
 verbose = FALSE,
  patience = 20,
 plot = TRUE,
 print_members = TRUE,
  stop_if_nan = TRUE,
  save_weights = TRUE,
  callbacks = list(),
  save_fun = NULL,
 seed = seq_len(n_ensemble),
)
```

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Arguments

x object of class "deepregression" to ensemble
n_ensemble numeric; number of ensemble members to fit

reinitialize logical; if TRUE (default), model weights are initialized randomly prior to fitting

each member. Fixed weights are not affected

mylapply lapply function to be used; defaults to lapply

verbose whether to print training in each fold patience number of patience for early stopping

plot whether to plot the resulting losses in each fold

print_members logical; print results for each member

stop_if_nan logical; whether to stop CV if NaN values occur

save_weights whether to save final weights of each ensemble member; defaults to TRUE

callbacks a list of callbacks used for fitting

save_fun function applied to the model in each fold to be stored in the final result

seed seed for reproducibility

... further arguments passed to object\$fit_fun

Value

object of class "drEnsemble", containing the original "deepregression" model together with a list of ensembling results (training history and, if save_weights is TRUE, the trained weights of each ensemble member)

| extractval | Formula helpers | |
|------------|-----------------|--|
| | | |

Description

Formula helpers

Usage

```
extractval(term, name, default_for_missing = FALSE, default = NULL)
extractlen(term, data)
form2text(form)
```

12 extractvar

Arguments

term formula term

name character; the value to extract

default_for_missing

logical; if TRUE, returns default if argument is missing

default value returned when missing

data a data.frame or list

form formula that is converted to a character string

Value

the value used for name

Examples

```
extractval("s(a, la = 2)", "la")
```

extractvar

Extract variable from term

Description

Extract variable from term

Usage

```
extractvar(term, allow_ia = FALSE)
```

Arguments

term specified in formula

allow_ia logical; whether to allow interaction of terms using the : notation

Value

variable as string

extract_pure_gam_part 13

Description

Extract the smooth term from a deepregression term specification

Usage

```
extract_pure_gam_part(term, remove_other_options = TRUE)
```

Arguments

```
term term specified in a formula remove_other_options logical; whether to remove other options withing the smooth term
```

Value

pure gam part of term

extract_S

Convenience function to extract penalty matrix and value

Description

Convenience function to extract penalty matrix and value

Usage

```
extract_S(x)
```

Arguments

x evaluated smooth term object

family_to_trafo

family_to_tfd

Character-tfd mapping function

Description

Character-tfd mapping function

Usage

```
family_to_tfd(family)
```

Arguments

family

character defining the distribution

Value

a tfp distribution

family_to_trafo

Character-to-transformation mapping function

Description

Character-to-transformation mapping function

Usage

```
family_to_trafo(family, add_const = 1e-08)
```

Arguments

family character defining the distribution

add_const see make_tfd_dist

Value

a list of transformation for each distribution parameter

fitted.drEnsemble 15

| fitted.drEnsemble | Method for extracting the fitted values of an ensemble |
|-----------------------|--|
| TITTEU. UI EIISEIIDIE | Method for extracting the fitted values of an ensemble |

Description

Method for extracting the fitted values of an ensemble

Usage

```
## S3 method for class 'drEnsemble'
fitted(object, apply_fun = tfd_mean, ...)
```

Arguments

object a deepregression model

apply_fun function applied to fitted distribution, per default tfd_mean

... arguments passed to the predict function

Value

list of fitted values for each ensemble member

form_control

Options for formula parsing

Description

Options for formula parsing

Usage

```
form_control(precalculate_gamparts = TRUE, check_form = TRUE)
```

Arguments

```
precalculate_gamparts
```

logical; if TRUE (default), additive parts are pre-calculated and can later be used more efficiently. Set to FALSE only if no smooth effects are in the formula(s) and a formula is very large so that extracting all terms takes long or might fail

check_form logical; if TRUE (default), the formula is checked in process_terms

Value

Returns a list with options

16 from_preds_to_dist

from_dist_to_loss

Function to transform a distribution layer output into a loss function

Description

Function to transform a distribution layer output into a loss function

Usage

```
from_dist_to_loss(
  family,
  ind_fun = function(x) tfd_independent(x),
  weights = NULL
)
```

Arguments

family see ?deepregression

ind_fun function applied to the model output before calculating the log-likelihood. Per

default independence is assumed by applying tfd_independent.

weights sample weights

Value

loss function

from_preds_to_dist

Define Predictor of a Deep Distributional Regression Model

Description

Define Predictor of a Deep Distributional Regression Model

Usage

```
from_preds_to_dist(
    list_pred_param,
    family = NULL,
    output_dim = 1L,
    mapping = NULL,
    from_family_to_distfun = make_tfd_dist,
    from_distfun_to_dist = distfun_to_dist,
    add_layer_shared_pred = function(x, units) layer_dense(x, units = units, use_bias = FALSE),
    trafo_list = NULL
)
```

gam_plot_data 17

Arguments

list_pred_param

list of input-output(-lists) generated from subnetwork_init

family see ?deepregression; if NULL, concatenated list_pred_param entries are

returned (after applying mapping if provided)

output_dim dimension of the output

mapping a list of integers. The i-th list item defines which element elements of list_pred_param

are used for the i-th parameter. For example, mapping = list(1,2,1:2) means

that list_pred_param[[1]] is used for the first distribution parameter, list_pred_param[[2]]

for the second distribution parameter and list_pred_param[[3]] for both distribution parameters (and then added once to list_pred_param[[1]] and once

to list_pred_param[[2]])

from_family_to_distfun

function to create a dist_fun (see ?distfun_to_dist) from the given charac-

ter family

from_distfun_to_dist

function creating a tfp distribution based on the prediction tensors and dist_fun.

See ?distfun_to_dist

add_layer_shared_pred

layer to extend shared layers defined in mapping

trafo_list a list of transformation function to convert the scale of the additive predictors to

the respective distribution parameter

Value

a list with input tensors and output tensors that can be passed to, e.g., keras_model

gam_plot_data used by gam_processor

Description

used by gam_processor

Usage

```
gam_plot_data(pp, weights, grid_length = 40, pe_fun = pe_gen)
```

Arguments

pp processed term weights layer weights

grid_length length for grid for evaluating basis
pe_fun function used to generate partial effects

get_distribution

Function to return the fitted distribution

Description

Function to return the fitted distribution

Usage

```
get_distribution(x, data = NULL, force_float = FALSE)
```

Arguments

x the fitted deepregression object

data an optional data set

force_float forces conversion into float tensors

get_ensemble_distribution

Obtain the conditional ensemble distribution

Description

Obtain the conditional ensemble distribution

Usage

```
get_ensemble_distribution(object, data = NULL, topK = NULL, ...)
```

Arguments

object of class "drEnsemble"

data data for which to return the fitted distribution

topK not implemented yet

... further arguments currently ignored

Value

tfd_distribution of the ensemble, i.e., a mixture of the ensemble member's predicted distributions conditional on data

get_gamdata 19

get_gamdata

Extract property of gamdata

Description

Extract property of gamdata

Usage

```
get_gamdata(
   term,
   param_nr,
   gamdata,
   what = c("data_trafo", "predict_trafo", "input_dim", "partial_effect", "sp_and_S",
        "df")
)
```

Arguments

term term in formula

param_nr integer; number of the distribution parameter

gamdata list as returned by precalc_gam what string specifying what to return

Value

property of the gamdata object as defined by what

```
get_gamdata_reduced_nr
```

Extract number in matching table of reduced gam term

Description

Extract number in matching table of reduced gam term

Usage

```
get_gamdata_reduced_nr(term, param_nr, gamdata)
```

Arguments

term in formula

param_nr integer; number of the distribution parameter

gamdata list as returned by precalc_gam

Value

integer with number of gam term in matching table

get_gam_part

Extract gam part from wrapped term

Description

Extract gam part from wrapped term

Usage

```
get_gam_part(term, wrapper = "vc")
```

Arguments

term cha

character; gam model term

wrapper

character; function name that is wrapped around the gam part

get_layernr_by_opname Function to return layer number given model and name

Description

Function to return layer number given model and name

Usage

```
get_layernr_by_opname(mod, name, partial_match = FALSE)
```

Arguments

mod

deepregression model

name

character

partial_match

logical; whether to also check for a partial match

get_layernr_trainable 21

get_layernr_trainable Function to return layer numbers with trainable weights

Description

Function to return layer numbers with trainable weights

Usage

```
get_layernr_trainable(mod, logic = FALSE)
```

Arguments

mod deepregression model

logical logical; TRUE: return logical vector; FALSE (default) index

get_layer_by_opname Function to return layer given model and name

Description

Function to return layer given model and name

Usage

```
get_layer_by_opname(mod, name, partial_match = FALSE)
```

Arguments

mod deepregression model

name character

partial_match logical; whether to also check for a partial match

22 get_partial_effect

get_names_pfc

Extract term names from the parsed formula content

Description

Extract term names from the parsed formula content

Usage

```
get_names_pfc(pfc)
```

Arguments

pfc

parsed formula content

Value

vector of term names

get_partial_effect

Return partial effect of one smooth term

Description

Return partial effect of one smooth term

Usage

```
get_partial_effect(
  object,
  names = NULL,
  return_matrix = FALSE,
  which_param = 1,
  newdata = NULL,
   ...
)
```

Arguments

object deepregression object

names string; for partial match with smooth term return_matrix logical; whether to return the design matrix or

which_param integer; which distribution parameter the partial effect (FALSE, default)

newdata data.frame; new data (optional)

... arguments passed to get_weight_by_name

get_processor_name 23

get_processor_name

Extract processor name from term

Description

Extract processor name from term

Usage

```
get_processor_name(term)
```

Arguments

term

term in formula

Value

processor name as string

 $get_special$

Extract terms defined by specials in formula

Description

Extract terms defined by specials in formula

Usage

```
get_special(term, specials, simplify = FALSE)
```

Arguments

term in formula

specials string(s); special name(s)

simplify logical; shortcut for returning only the name of the special in term

Value

specials in formula

24 get_weight_by_name

| | | _ |
|-----|-------|------|
| get | _type | nt c |
| | | |

Function to subset parsed formulas

Description

Function to subset parsed formulas

Usage

```
get_type_pfc(pfc, type = NULL)
```

Arguments

pfc list of parsed formulas

type either NULL (all types of coefficients are returned), "linear" for linear coeffi-

cients or "smooth" for coefficients of

get_weight_by_name

Function to retrieve the weights of a structured layer

Description

Function to retrieve the weights of a structured layer

Usage

```
get_weight_by_name(mod, name, param_nr = 1, postfixes = "")
```

Arguments

mod fitted deepregression object

name of partial effect

param_nr distribution parameter number

postfixes character (vector) appended to layer name

Value

weight matrix

get_weight_by_opname

get_weight_by_opname Function to return

Function to return weight given model and name

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Description

Function to return weight given model and name

Usage

```
get_weight_by_opname(mod, name, partial_match = FALSE)
```

Arguments

mod deepregression model

name character

partial_match logical; whether to also check for a partial match

handle_gam_term

Function to define smoothness and call mgcv's smooth constructor

Description

Function to define smoothness and call mgcv's smooth constructor

Usage

```
handle_gam_term(object, data, controls)
```

Arguments

object character defining the model term

data data.frame or list

controls controls for penalization

Value

constructed smooth term

26 keras_dr

keras_dr

Compile a Deep Distributional Regression Model

Description

Compile a Deep Distributional Regression Model

Usage

```
keras_dr(
  list_pred_param,
  weights = NULL,
  optimizer = tf$keras$optimizers$Adam(),
  model_fun = keras_model,
  monitor_metrics = list(),
  from_preds_to_output = from_preds_to_dist,
  loss = from_dist_to_loss(family = list(...)$family, weights = weights),
  additional_penalty = NULL,
  ...
)
```

Arguments

```
list_pred_param
                  list of input-output(-lists) generated from subnetwork_init
                  vector of positive values; optional (default = 1 for all observations)
weights
optimizer
                  optimizer used. Per default Adam
model_fun
                  which function to use for model building (default keras_model)
monitor_metrics
                  Further metrics to monitor
from_preds_to_output
                  function taking the list_pred_param outputs and transforms it into a single net-
                  work output
loss
                  the model's loss function; per default evaluated based on the arguments family
                  and weights using from_dist_to_loss
additional_penalty
                  a penalty that is added to the negative log-likelihood; must be a function of
                  model$trainable_weights with suitable subsetting
                  arguments passed to from_preds_to_output
```

Value

a list with input tensors and output tensors that can be passed to, e.g., keras_model

layer_add_identity 27

Examples

```
set.seed(24)
n <- 500
x <- runif(n) %>% as.matrix()
z <- runif(n) %>% as.matrix()
y <- x - z
data <- data.frame(x = x, z = z, y = y)
# change loss to mse and adapt
# \code{from_preds_to_output} to work
# only on the first output column
mod <- deepregression(</pre>
 y = y,
 data = data,
 list_of_formulas = list(loc = ~ 1 + x + z, scale = ~ 1),
 list_of_deep_models = NULL,
 family = "normal",
 from_preds_to_output = function(x, ...) x[[1]],
 loss = "mse"
)
```

layer_add_identity

Convenience layer function

Description

Convenience layer function

Usage

```
layer_add_identity(inputs)
layer_concatenate_identity(inputs)
```

Arguments

inputs list of tensors

Details

convenience layers to work with list of inputs where inputs can also have length one

Value

tensor

28 layer_generator

layer_generator

Function that creates layer for each processor

Description

Function that creates layer for each processor

Usage

```
layer_generator(
   term,
   output_dim,
   param_nr,
   controls,
   layer_class = tf$keras$layers$Dense,
   without_layer = tf$identity,
   name = makelayername(term, param_nr),
   further_layer_args = NULL,
   layer_args_names = NULL,
   units = as.integer(output_dim),
   ...
)

int_processor(term, data, output_dim, param_nr, controls)

lin_processor(term, data, output_dim, param_nr, controls)

gam_processor(term, data, output_dim, param_nr, controls)
```

Arguments

character; term in the formula term output_dim integer; number of units in the layer integer; identifier for models with more than one additive predictor param_nr controls list; control arguments which allow to pass further information layer_class a tf or keras layer function without_layer function to be used as layer if controls\$with_layer is FALSE name character; name of layer. if NULL, makelayername will be used to create layer name further_layer_args named list; further arguments passed to the layer layer_args_names character vector; if NULL, default layer args will be used. Needs to be set for layers that do not provide the arguments of a default Dense layer. units integer; number of units for layer

layer_sparse_conv_2d 29

```
other keras layer parametersdatadata frame; the data used in processors
```

Value

a basic processor list structure

```
{\tt layer\_sparse\_conv\_2d} \quad \textit{Sparse 2D Convolutional layer}
```

Description

```
Sparse 2D Convolutional layer
```

Usage

```
layer_sparse_conv_2d(filters, kernel_size, lam = NULL, depth = 2, ...)
```

Arguments

```
filters number of filters
```

kernel_size size of convolutional filter regularization strength

depth depth of weight factorization

arguments passed to TensorFlow layer

Value

layer object

layer_spline

Function to define spline as TensorFlow layer

Description

Function to define spline as TensorFlow layer

Usage

```
layer_spline(
  units = 1L,
  P,
  name,
  trainable = TRUE,
  kernel_initializer = "glorot_uniform"
)
```

log_score

Arguments

units integer; number of output units

P matrix; penalty matrix

name string; string defining the layer's name trainable logical; whether layer is trainable

kernel_initializer

initializer; for basis coefficients

Value

TensorFlow layer

log_score

Function to return the log_score

Description

Function to return the log_score

Usage

```
log_score(
    x,
    data = NULL,
    this_y = NULL,
    ind_fun = function(x) tfd_independent(x),
    convert_fun = as.matrix,
    summary_fun = function(x) x
)
```

Arguments

x the fitted deepregression object

data an optional data set
this_y new y for optional data

ind_fun function indicating the dependency; per default (iid assumption) tfd_independent

is used.

convert_fun function that converts Tensor; per default as.matrix summary_fun function summarizing the output; per default the identity

```
loop_through_pfc_and_call_trafo
```

Function to loop through parsed formulas and apply data trafo

Description

Function to loop through parsed formulas and apply data trafo

Usage

```
loop_through_pfc_and_call_trafo(pfc, newdata = NULL)
```

Arguments

pfc list of processor transformed formulas
newdata list in the same format as the original data

Value

list of matrices or arrays

makeInputs

Convenience layer function

Description

Convenience layer function

Usage

```
makeInputs(pp, param_nr)
```

Arguments

pp processed predictors
param_nr integer for the parameter

Value

input tensors with appropriate names

32 make_folds

| ma | kel | ave | rna | ame |
|----|-----|-----|-----|-----|

Function that takes term and create layer name

Description

Function that takes term and create layer name

Usage

```
makelayername(term, param_nr, truncate = 60)
```

Arguments

term in formula

param_nr integer; defining number of the distribution's parameter truncate integer; value from which on names are truncated

Value

name (string) for layer

make_folds

Generate folds for CV out of one hot encoded matrix

Description

Generate folds for CV out of one hot encoded matrix

Usage

```
make_folds(mat, val_train = 0, val_test = 1)
```

Arguments

matrix with columns corresponding to folds and entries corresponding to a one

hot encoding

val_train the value corresponding to train, per default 0 val_test the value corresponding to test, per default 1

Details

val_train and val_test can both be a set of value

make_generator 33

make_generator

creates a generator for training

Description

creates a generator for training

Usage

```
make_generator(
  input_x,
  input_y = NULL,
  batch_size,
  sizes,
  shuffle = TRUE,
  seed = 42L
)
```

Arguments

```
input_x list of matrices
input_y list of matrix
batch_size integer
```

sizes sizes of the image including colour channel

shuffle logical for shuffling data

seed seed for shuffling in generators

Value

```
generator for all x and y
```

```
{\tt make\_generator\_from\_matrix}
```

Make a DataGenerator from a data.frame or matrix

Description

Creates a Python Class that internally iterates over the data.

make_tfd_dist

Usage

```
make_generator_from_matrix(
    x,
    y = NULL,
    generator = image_data_generator(),
    batch_size = 32L,
    shuffle = TRUE,
    seed = 1L
)
```

Arguments

x matrix;y vector;

generator as e.g. obtained from 'keras::image_data_generator'. Used for con-

sistent train-test splits.

batch_size integer

shuffle logical; Should data be shuffled? seed integer; seed for shuffling data.

make_tfd_dist

Families for deepregression

Description

Families for deepregression

Usage

```
make_tfd_dist(family, add_const = 1e-08, output_dim = 1L, trafo_list = NULL)
```

Arguments

family character vector

add_const small positive constant to stabilize calculations

output_dim number of output dimensions of the response (larger 1 for multivariate case)

trafo_list list of transformations for each distribution parameter. Per default the transfor-

mation listed in details is applied.

make_tfd_dist 35

Details

To specify a custom distribution, define the a function as follows function(x) do.call(your_tfd_dist, lapply(1:ncol(x)[[1]], function(i) your_trafo_list_on_inputs[[i]](x[,i,drop=FALSE]))) and pass it to deepregression via the dist_fun argument. Currently the following distributions are supported with parameters (and corresponding inverse link function in brackets):

- "normal": normal distribution with location (identity), scale (exp)
- "bernoulli": bernoulli distribution with logits (identity)
- "bernoulli_prob": bernoulli distribution with probabilities (sigmoid)
- "beta": beta with concentration 1 = alpha (exp) and concentration 0 = beta (exp)
- "betar": beta with mean (sigmoid) and scale (sigmoid)
- "cauchy": location (identity), scale (exp)
- "chi2": cauchy with df (exp)
- "chi": cauchy with df (exp)
- "exponential": exponential with lambda (exp)
- "gamma": gamma with concentration (exp) and rate (exp)
- "gammar": gamma with location (exp) and scale (exp), following gamlss.dist::GA, which
 implies that the expectation is the location, and the variance of the distribution is the location^2
 scale^2
- "gumbel": gumbel with location (identity), scale (exp)
- "half_cauchy": half cauchy with location (identity), scale (exp)
- "half_normal": half normal with scale (exp)
- "horseshoe": horseshoe with scale (exp)
- "inverse_gamma": inverse gamma with concentation (exp) and rate (exp)
- "inverse gamma ls": inverse gamma with location (exp) and variance (1/exp)
- "inverse_gaussian": inverse Gaussian with location (exp) and concentation (exp)
- "laplace": Laplace with location (identity) and scale (exp)
- "log_normal": Log-normal with location (identity) and scale (exp) of underlying normal distribution
- "logistic": logistic with location (identity) and scale (exp)
- "negbinom": neg. binomial with count (exp) and prob (sigmoid)
- "negbinom_ls": neg. binomail with mean (exp) and clutter factor (exp)
- "pareto": Pareto with concentration (exp) and scale (1/exp)
- "pareto_ls": Pareto location scale version with mean (exp) and scale (exp), which corresponds to a Pareto distribution with parameters scale = mean and concentration = 1/sigma, where sigma is the scale in the pareto_ls version
- "poisson": poisson with rate (exp)
- "poisson_lograte": poisson with lograte (identity))
- "student_t": Student's t with df (exp)

names_families

- "student_t_ls": Student's t with df (exp), location (identity) and scale (exp)
- "uniform": uniform with upper and lower (both identity)
- "zinb": Zero-inflated negative binomial with mean (exp), variance (exp) and prob (sigmoid)
- "zip": Zero-inflated poisson distribution with mean (exp) and prob (sigmoid)

multioptimizer

Function to define an optimizer combining multiple optimizers

Description

Function to define an optimizer combining multiple optimizers

Usage

```
multioptimizer(optimizers_and_layers)
```

Arguments

```
optimizers_and_layers
a list if tuples of optimizer and respective layers
```

Value

an optimizer

names_families

Returns the parameter names for a given family

Description

Returns the parameter names for a given family

Usage

```
names_families(family)
```

Arguments

family

character specifying the family as defined by deepregression

Value

vector of parameter names

orthog_control 37

orthog_control

Options for orthogonalization

Description

Options for orthogonalization

Usage

```
orthog_control(
  split_fun = split_model,
  orthog_type = c("tf", "manual"),
  orthogonalize = options()$orthogonalize,
  identify_intercept = options()$identify_intercept,
  deep_top = NULL,
  orthog_fun = NULL,
  deactivate_oz_at_test = TRUE
)
```

Arguments

split_fun a function separating the deep neural network in two parts so that the orthog-

onalization can be applied to the first part before applying the second network part; per default, the function <code>split_model</code> is used which assumes a dense layer as penultimate layer and separates the network into a first part without this last layer and a second part only consisting of a single dense layer that is fed into the

output layer

orthog_type one of two options; If "manual", the QR decomposition is calculated before

model fitting, otherwise ("tf") a QR is calculated in each batch iteration via TF. The first only works well for larger batch sizes or ideally batch_size ==

NROW(y).

orthogonalize logical; if set to TRUE, automatic orthogonalization is activated

identify_intercept

whether to orthogonalize the deep network w.r.t. the intercept to make the inter-

cept identifiable

deep_top function; optional function to put on top of the deep network instead of splitting

the function using split_fun

orthog_fun function; for custom orthogonaliuation. if NULL, orthog_type is used to de-

fine the function that computes the orthogonalization

deactivate_oz_at_test

logical; whether to deactive the orthogonalization cell at test time when using

orthog_tf for orthog_fun (the default).

Value

Returns a list with options

38 orthog_post_fitting

orthog_P

Function to compute adjusted penalty when orthogonalizing

Description

Function to compute adjusted penalty when orthogonalizing

Usage

```
orthog_P(P, Z)
```

Arguments

P matrix; original penalty matrix
Z matrix; constraint matrix

Value

adjusted penalty matrix

orthog_post_fitting

Orthogonalize a Semi-Structured Model Post-hoc

Description

Orthogonalize a Semi-Structured Model Post-hoc

Usage

```
orthog_post_fitting(mod, name_penult, param_nr = 1)
```

Arguments

mod deepregression model

 ${\tt name_penult} \qquad {\tt character} \ {\tt name} \ {\tt of} \ {\tt the} \ {\tt penultimate} \ {\tt layer} \ {\tt of} \ {\tt the} \ {\tt deep} \ {\tt part} \ {\tt part}$

param_nr integer; number of the parameter to be returned

Value

a deepregression object with weights frozen and deep part specified by name_penult orthogonalized

```
orthog\_structured\_smooths\_Z
```

Orthogonalize structured term by another matrix

Description

Orthogonalize structured term by another matrix

Usage

```
orthog_structured_smooths_Z(S, L)
```

Arguments

S matrix; matrix to orthogonalize

L matrix; matrix which defines the projection and its orthogonal complement, in

which S is projected

Value

constraint matrix

penalty_control

Options for penalty setup in the pre-processing

Description

Options for penalty setup in the pre-processing

Arguments

defaultSmoothing

function applied to all s-terms, per default (NULL) the minimum df of all possible terms is used. Must be a function the smooth term from mgcv's smoothCon

and an argument df.

df degrees of freedom for all non-linear structural terms (default = 7); either one

common value or a list of the same length as number of parameters; if different df values need to be assigned to different smooth terms, use df as an argument

for s(), te() or ti()

null_space_penalty

logical value; if TRUE, the null space will also be penalized for smooth effects.

Per default, this is equal to the value give in variational.

absorb_cons logical; adds identifiability constraint to the basis. See ?mgcv::smoothCon for

more details.

anisotropic whether or not use anisotropic smoothing (default is TRUE)

zero_constraint_for_smooths

logical; the same as absorb_cons, but done explicitly. If true a constraint is put on each smooth to have zero mean. Can be a vector of length(list_of_formulas)

for each distribution parameter.

no_linear_trend_for_smooths

logical; see zero_constraint_for_smooths, but this removes the linear trend

from splines

hat1 logical; if TRUE, the smoothing parameter is defined by the trace of the hat

matrix sum(diag(H)), else sum(diag(2*H-HH))

sp_scale function of response; for scaling the penalty (1/n per default)

Value

Returns a list with options

plot.deepregression Generic functions for deepregression models

Description

Generic functions for deepregression models

Predict based on a deepregression object

Function to extract fitted distribution

Fit a deepregression model (pendant to fit for keras)

Extract layer weights / coefficients from model

Print function for deepregression model

Cross-validation for deepgression objects

mean of model fit

Standard deviation of fit distribution

Calculate the distribution quantiles

```
## S3 method for class 'deepregression'
plot(
  Х,
 which = NULL,
  which_param = 1,
  only_data = FALSE,
  grid_length = 40,
  main_multiple = NULL,
  type = "b",
  get_weight_fun = get_weight_by_name,
)
## S3 method for class 'deepregression'
predict(
  object,
  newdata = NULL,
  batch_size = NULL,
  apply_fun = tfd_mean,
  convert_fun = as.matrix,
)
## S3 method for class 'deepregression'
fitted(object, apply_fun = tfd_mean, ...)
## S3 method for class 'deepregression'
fit(
  object,
  batch_size = 32,
  epochs = 10,
  early_stopping = FALSE,
  early_stopping_metric = "val_loss",
  verbose = TRUE,
  view_metrics = FALSE,
  patience = 20,
  save_weights = FALSE,
  validation_data = NULL,
  validation_split = ifelse(is.null(validation_data), 0.1, 0),
  callbacks = list(),
  convertfun = function(x) tf$constant(x, dtype = "float32"),
```

```
)
## S3 method for class 'deepregression'
coef(object, which_param = 1, type = NULL, ...)
## S3 method for class 'deepregression'
print(x, ...)
## S3 method for class 'deepregression'
cv(
 х,
 verbose = FALSE,
 patience = 20,
 plot = TRUE,
 print_folds = TRUE,
  cv_folds = 5,
  stop_if_nan = TRUE,
 mylapply = lapply,
 save_weights = FALSE,
  callbacks = list(),
 save_fun = NULL,
)
## S3 method for class 'deepregression'
mean(x, data = NULL, ...)
## S3 method for class 'deepregression'
stddev(x, data = NULL, ...)
## S3 method for class 'deepregression'
quant(x, data = NULL, probs, ...)
```

Arguments

| x | a deepregression object |
|---------------------------|---|
| which | character vector or number(s) identifying the effect to plot; default plots all effects $ \\$ |
| which_param | integer, indicating for which distribution parameter coefficients should be returned (default is first parameter) |
| only_data | logical, if TRUE, only the data for plotting is returned |
| grid_length | the length of an equidistant grid at which a two-dimensional function is evaluated for plotting. |
| main_multiple | vector of strings; plot main titles if multiple plots are selected |
| type | either NULL (all types of coefficients are returned), "linear" for linear coefficients or "smooth" for coefficients of smooth terms $\frac{1}{2}$ |
| <pre>get_weight_fun</pre> | function to extract weight from model given x, a name and param_nr |

... arguments passed to the predict function

object a deepregression model

newdata optional new data, either data.frame or list

batch_size integer, the batch size used for mini-batch training

apply_fun function applied to fitted distribution, per default tfd_mean

convert_fun how should the resulting tensor be converted, per default as.matrix

epochs integer, the number of epochs to fit the model

early_stopping logical, whether early stopping should be user.

early_stopping_metric

character, based on which metric should early stopping be trigged (default:

"val_loss")

verbose whether to print training in each fold

view_metrics logical, whether to trigger the Viewer in RStudio / Browser.

patience number of patience for early stopping

save_weights logical, whether to save weights in each epoch.

validation_data

optional specified validation data

validation_split

float in [0,1] defining the amount of data used for validation

callbacks a list of callbacks used for fitting

convertfun function to convert R into Tensor object

plot whether to plot the resulting losses in each fold

print_folds whether to print the current fold

cv_folds an integer; can also be a list of lists with train and test data sets per fold

stop_if_nan logical; whether to stop CV if NaN values occur mylapply lapply function to be used; defaults to lapply

save_fun function applied to the model in each fold to be stored in the final result

data either NULL or a new data set

probs the quantile value(s)

Value

Returns an object drCV, a list, one list element for each fold containing the model fit and the weighthistory.

44 precalc_gam

plot_cv

Plot CV results from deepregression

Description

Plot CV results from deepregression

Usage

```
plot_cv(x, what = c("loss", "weight"), ...)
```

Arguments

x drCV object returned by cv.deepregression

what character indicating what to plot (currently supported 'loss' or 'weights')

... further arguments passed to matplot

precalc_gam

Pre-calculate all gam parts from the list of formulas

Description

Pre-calculate all gam parts from the list of formulas

Usage

```
precalc_gam(lof, data, controls)
```

Arguments

lof list of formulas data the data list

controls controls from deepregression

Value

a list of length 2 with a matching table to link every unique gam term to formula entries and the respective data transformation functions

predict_gen 45

predict_gen

Generator function for deepregression objects

Description

Generator function for deepregression objects

Usage

```
predict_gen(
  object,
  newdata = NULL,
  batch_size = NULL,
  apply_fun = tfd_mean,
  convert_fun = as.matrix,
  ret_dist = FALSE
)
```

Arguments

object deepregression model;

newdata data.frame or list; for (optional) new data
batch_size integer; NULL will use the default (20)
apply_fun see ?predict.deepregression
convert_fun see ?predict.deepregression

ret_dist logical; whether to return the whole distribution or only the (mean) prediction

Value

matrix or list of distributions

prepare_data

Function to prepare data based on parsed formulas

Description

Function to prepare data based on parsed formulas

```
prepare_data(pfc, gamdata = NULL)
```

process_terms

Arguments

pfc list of processor transformed formulas

gamdata processor for gam part

Value

list of matrices or arrays

prepare_newdata

Function to prepare new data based on parsed formulas

Description

Function to prepare new data based on parsed formulas

Usage

```
prepare_newdata(pfc, newdata, gamdata = NULL)
```

Arguments

pfc list of processor transformed formulas

newdata list in the same format as the original data

gamdata processor for gam part

Value

list of matrices or arrays

process_terms

Control function to define the processor for terms in the formula

Description

Control function to define the processor for terms in the formula

quant 47

Usage

```
process_terms(
   form,
   data,
   controls,
   output_dim,
   param_nr,
   parsing_options,
   specials_to_oz = c(),
   automatic_oz_check = TRUE,
   identify_intercept = FALSE,
   ...
)
```

Arguments

form the formula to be processed

data the data for the terms in the formula

controls controls for gam terms

output_dim the output dimension of the response

param_nr integer; identifier for the distribution parameter

parsing_options

options

specials_to_oz specials that should be automatically checked for

automatic_oz_check

logical; whether to automatically check for DNNs to be orthogonalized

identify_intercept

logical; whether to make the intercept automatically identifiable

.. further processors

Value

returns a processor function

quant

Generic quantile function

Description

Generic quantile function

```
quant(x, ...)
```

Arguments

x object

... further arguments passed to the class-specific function

reinit_weights

Genereic function to re-intialize model weights

Description

Genereic function to re-intialize model weights

Usage

```
reinit_weights(object, seed)
```

Arguments

object model to re-initialize seed seed for reproducibility

reinit_weights.deepregression

Method to re-initialize weights of a "deepregression" model

Description

Method to re-initialize weights of a "deepregression" model

Usage

```
## S3 method for class 'deepregression'
reinit_weights(object, seed)
```

Arguments

object of class "deepregression"

seed seed for reproducibility

Value

invisible NULL

separate_define_relation

```
separate_define_relation
```

Function to define orthogonalization connections in the formula

Description

Function to define orthogonalization connections in the formula

Usage

```
separate_define_relation(
  form,
  specials,
  specials_to_oz,
  automatic_oz_check = TRUE,
  identify_intercept = FALSE,
  simplify = FALSE
)
```

Arguments

```
form a formula for one distribution parameter
specials specials in formula to handle separately
specials_to_oz parts of the formula to orthogonalize
automatic_oz_check
logical; automatically check if terms must be orthogonalized
identify_intercept
logical; whether to make the intercept identifiable
simplify logical; if FALSE, formulas are parsed more carefully.
```

Value

Returns a list of formula components with ids and assignments for orthogonalization

stddev

Generic sd function

Description

Generic sd function

```
stddev(x, ...)
```

subnetwork_init

Arguments

```
x object... further arguments passed to the class-specific function
```

stop_iter_cv_result Function to get the stoppting iteration from CV

Description

Function to get the stoppting iteration from CV

Usage

```
stop_iter_cv_result(
  res,
  thisFUN = mean,
  loss = "validloss",
  whichFUN = which.min
)
```

Arguments

res result of cv call

thisFUN aggregating function applied over folds

loss which loss to use for decision whichFUN which function to use for decision

subnetwork_init

Initializes a Subnetwork based on the Processed Additive Predictor

Description

Initializes a Subnetwork based on the Processed Additive Predictor

```
subnetwork_init(
  pp,
  deep_top = NULL,
  orthog_fun = orthog_tf,
  split_fun = split_model,
  shared_layers = NULL,
  param_nr = 1,
  selectfun_in = function(pp) pp[[param_nr]],
```

tfd_mse 51

```
selectfun_lay = function(pp) pp[[param_nr]],
gaminputs,
summary_layer = layer_add_identity
)
```

Arguments

pp list of processed predictor lists from processor

deep_top keras layer if the top part of the deep network after orthogonalization is different

to the one extracted from the provided network

orthog_fun function used for orthogonalization

split_fun function to split the network to extract head

shared_layers list defining shared weights within one predictor; each list item is a vector of

characters of terms as given in the parameter formula

param_nr integer number for the distribution parameter

selectfun_in, selectfun_lay

functions defining which subset of pp to take as inputs and layers for this sub-

network; per default the param_nr's entry

gaminputs input tensors for gam terms

summary_layer keras layer that combines inputs (typically adding or concatenating)

Value

returns a list of input and output for this additive predictor

tfd_mse

For using mean squared error via TFP

Description

For using mean squared error via TFP

Usage

```
tfd_mse(mean)
```

Arguments

mean parameter for the mean

Details

deepregression allows to train based on the MSE by using loss = "mse" as argument to deepregression. This tfd function just provides a dummy family

Value

a TFP distribution

52 tf_repeat

tfd_zinb

Implementation of a zero-inflated negbinom distribution for TFP

Description

Implementation of a zero-inflated negbinom distribution for TFP

Usage

```
tfd_zinb(mu, r, probs)
```

Arguments

| mu, r | parameter of the negbin_ls distribution | |
|---------|---|--|
| probs | vector of probabilites of length 2 (probability for poisson and probability for 0s) | |
| tfd_zip | Implementation of a zero-inflated poisson distribution for TFP | |

Description

Implementation of a zero-inflated poisson distribution for TFP

Usage

```
tfd_zip(lambda, probs)
```

Arguments

| lambda | scalar value for rate of poisson distribution |
|--------|---|
| probs | vector of probabilites of length 2 (probability for poisson and probability for 0s) |
| | |

tf_repeat

TensorFlow repeat function which is not available for TF 2.0

Description

TensorFlow repeat function which is not available for TF 2.0

Usage

```
tf_repeat(a, dim)
```

Arguments

a tensor

dim dimension for repeating

tf_row_tensor 53

tf_row_tensor

Row-wise tensor product using TensorFlow

Description

Row-wise tensor product using TensorFlow

Usage

```
tf_row_tensor(a, b, ...)
```

Arguments

a, b tensor

... arguments passed to TensorFlow layer

Value

a TensorFlow layer

tf_split_multiple

Split tensor in multiple parts

Description

Split tensor in multiple parts

Usage

```
tf_split_multiple(A, len)
```

Arguments

A tensor

len integer; defines the split lengths

Value

list of tensors

tf_stride_cols

Function to index tensors columns

Description

Function to index tensors columns

Usage

```
tf_stride_cols(A, start, end = NULL)
```

Arguments

A tensor start first index

end last index (equals start index if NULL)

Value

sliced tensor

```
tf_stride_last_dim_tensor
```

Function to index tensors last dimension

Description

Function to index tensors last dimension

Usage

```
tf_stride_last_dim_tensor(A, start, end = NULL)
```

Arguments

A tensor start first index

end last index (equals start index if NULL)

Value

sliced tensor

tib_layer 55

tib_layer

Hadamard-type layers

Description

Hadamard-type layers

Usage

```
tib_layer(units, la, ...)
simplyconnected_layer(la, ...)
inverse_group_lasso_pen(la)
regularizer_group_lasso(la, group_idx)
tibgroup_layer(units, group_idx, la, ...)
layer_hadamard(units = 1, la = 0, depth = 3, ...)
layer_group_hadamard(units, la, group_idx, depth, ...)
layer_hadamard_diff(
   units,
   la,
   initu = "glorot_uniform",
   initv = "glorot_uniform",
   ...
)
layer_hadamard(units = 1, la = 0, depth = 3, ...)
```

Arguments

```
units integer; number of units

la numeric; regularization value (> 0)

... arguments passed to TensorFlow layer group_idx list of group indices

depth integer; depth of weight factorization initu, initv initializers for parameters
```

Value

layer object

56 weight_control

```
update_miniconda_deepregression
```

Function to update miniconda and packages

Description

Function to update miniconda and packages

Usage

```
update_miniconda_deepregression(
  python = VERSIONPY,
  uninstall = TRUE,
  also_packages = TRUE
)
```

Arguments

python string; version of python

uninstall logical; whether to uninstall previous conda env also_packages logical; whether to install also all required packages

weight_control

Options for weights of layers

Description

Options for weights of layers

```
weight_control(
   specific_weight_options = NULL,
   general_weight_options = list(activation = NULL, use_bias = FALSE, trainable = TRUE,
   kernel_initializer = "glorot_uniform", bias_initializer = "zeros", kernel_regularizer
   = NULL, bias_regularizer = NULL, activity_regularizer = NULL, kernel_constraint =
        NULL, bias_constraint = NULL),
   warmstart_weights = NULL,
   shared_layers = NULL
)
```

weight_control 57

Arguments

specific_weight_options

specific options for certain weight terms; must be a list of length length(list_of_formulas) and each element in turn a named list (names are term names as in the formula)

with specific options in a list

general_weight_options

default options for layers

 $warmstart_weights$

While all keras layer options are availabe, the user can further specify a list for each distribution parameter with list elements corresponding to term names with values as vectors corresponding to start weights of the respective weights

list for each distribution parameter; each list item can be again a list of character shared_layers

vectors specifying terms which share layers

Value

Returns a list with options

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