Package 'automl'

May 7, 2026

Type Package

Title Deep Learning with Metaheuristic

Version 1.3.2

BugReports https://github.com/aboulaboul/automl/issues

Description Fits from simple regression to highly customizable deep neural networks either with gradient descent or metaheuristic, using automatic hyper parameters tuning and custom cost function.
A mix inspired by the common tricks on Deep Learning and Particle Swarm Optimization.

URL https://aboulaboul.github.io/automl
https://github.com/aboulaboul/automl

License GNU General Public License

Encoding UTF-8

LazyData TRUE

Imports stats, utils, parallel

Suggests datasets

RoxygenNote 6.1.1

NeedsCompilation no

Author Alex Boulangé [aut, cre]

Maintainer Alex Boulangé <aboul@free.fr>

Repository CRAN

Date/Publication 2020-01-16 11:40:09 UTC

Contents

automl_predict *automl_predict*

Description

Predictions function, to apply a trained model on datas

Usage

```
automl_predict(model, X, layoutputnum)
```

Arguments

model	model trained previously with automl_train or automl_train_manual
X	inputs matrix or data.frame (containing numerical values only)
layoutputnum	which layer number to output especially for auto encoding (default 0: no particular layer, the last one)

Examples

```
##REGRESSION (predict Sepal.Length given other parameters)
data(iris)
xmat <- as.matrix(cbind(iris[,2:4], as.numeric(iris$Species)))
ymat <- iris[,1]
amlmodel <- automl_train_manual(Xref = xmat, Yref = ymat,
 hpar = list(modexec = 'trainwpso', verbose = FALSE))
res <- cbind(ymat, automl_predict(model = amlmodel, X = xmat))
colnames(res) <- c('actual', 'predict')
head(res)
#
## Not run:
##CLASSIFICATION (predict Species given other Iris parameters)
data(iris)
xmat = iris[,1:4]
lab2pred <- levels(iris$Species)
lghlab <- length(lab2pred)
iris$Species <- as.numeric(iris$Species)
ymat <- matrix(seq(from = 1, to = lghlab, by = 1), nrow(xmat),
 lghlab, byrow = TRUE)
ymat <- (ymat == as.numeric(iris$Species)) + 0
amlmodel <- automl_train_manual(Xref = xmat, Yref = ymat,
 hpar = list(modexec = 'trainwpso', verbose = FALSE))
res <- cbind(ymat, round(automl_predict(model = amlmodel, X = xmat)))
colnames(res) <- c(paste('act',lab2pred, sep = '_'),
 paste('pred',lab2pred, sep = '_'))
head(res)

## End(Not run)
```

automl_train *automl_train*

Description

The multi deep neural network automatic train function (several deep neural networks are trained with automatic hyperparameters tuning, best model is kept)
This function launches the automl_train_manual function by passing it parameters for each particle at each converging step

Usage

```
automl_train(Xref, Yref, autopar = list(), hpar = list(), mdlref = NULL)
```

Arguments

Xref	inputs matrix or data.frame (containing numerical values only)
Yref	target matrix or data.frame (containing numerical values only)
autopar	list of parameters for hyperparameters optimization, see autopar section Not mandatory (the list is preset and all arguments are initialized with default value) but it is advisable to adjust some important arguments for performance reasons (including processing time)
hpar	list of parameters and hyperparameters for Deep Neural Network, see hpar section Not mandatory (the list is preset and all arguments are initialized with default value) but it is advisable to adjust some important arguments for performance reasons (including processing time)
mdlref	model trained with automl_train to start training with saved hpar and autopar (not the model) nb: manually entered parameters above override loaded ones

Examples

```
## Not run:
##REGRESSION (predict Sepal.Length given other Iris parameters)
data(iris)
xmat <- cbind(iris[,2:4], as.numeric(iris$Species))
ymat <- iris[,1]
amlmodel <- automl_train(Xref = xmat, Yref = ymat)

## End(Not run)
##CLASSIFICATION (predict Species given other Iris parameters)
data(iris)
xmat = iris[,1:4]
lab2pred <- levels(iris$Species)
lghlab <- length(lab2pred)
iris$Species <- as.numeric(iris$Species)
```

```
ymat <- matrix(seq(from = 1, to = lghlab, by = 1), nrow(xmat), lghlab, byrow = TRUE)
ymat <- (ymat == as.numeric(iris$Species)) + 0
#with gradient descent and random hyperparameters sets
amlmodel <- automl_train(Xref = xmat, Yref = ymat,
                         autopar = list(numiterations = 1, psopartpopsize = 1, seed = 11),
                           hpar = list(numiterations = 10))
```

---

automl_train_manual *automl_train_manual*

Description

The base deep neural network train function (one deep neural network trained without automatic hyperparameters tuning)

Usage

```
automl_train_manual(Xref, Yref, hpar = list(), mdlref = NULL)
```

Arguments

Xref	inputs matrix or data.frame (containing numerical values only)
Yref	target matrix or data.frame (containing numerical values only)
hpar	list of parameters and hyperparameters for Deep Neural Network, see hpar section Not mandatory (the list is preset and all arguments are initialized with default value) but it is advisable to adjust some important arguments for performance reasons (including processing time)
mdlref	model trained with automl_train or automl_train_manual to start training from a saved model (shape, weights...) for fine tuning nb: manually entered parameters above override loaded ones

Examples

```
##REGRESSION (predict Sepal.Length given other Iris parameters)
data(iris)
xmat <- cbind(iris[,2:4], as.numeric(iris$Species))
ymat <- iris[,1]
#with gradient descent
amlmodel <- automl_train_manual(Xref = xmat, Yref = ymat,
                                hpar = list(learningrate = 0.01,
                                            numiterations = 30,
                                            minibatchsize = 2^2))
## Not run:
#with PSO
amlmodel <- automl_train_manual(Xref = xmat, Yref = ymat,
                                hpar = list(modexec = 'trainwpso',
                                            numiterations = 30,
```

```
                                          psopartpopsize = 50))
#with PSO and custom cost function
f <- 'J=abs((y-yhat)/y)'
f <- c(f, 'J=sum(J[!is.infinite(J)],na.rm=TRUE)')
f <- c(f, 'J=(J/length(y))')
f <- paste(f, collapse = ';')
amlmodel <- automl_train_manual(Xref = xmat, Yref = ymat,
                                hpar = list(modexec = 'trainwpso',
                                            numiterations = 30,
                                            psopartpopsize = 50,
                                            costcustformul = f))

##CLASSIFICATION (predict Species given other Iris parameters)
data(iris)
xmat = iris[,1:4]
lab2pred <- levels(iris$Species)
lghlab <- length(lab2pred)
iris$Species <- as.numeric(iris$Species)
ymat <- matrix(seq(from = 1, to = lghlab, by = 1), nrow(xmat), lghlab, byrow = TRUE)
ymat <- (ymat == as.numeric(iris$Species)) + 0
#with gradient descent and 2 hidden layers
amlmodel <- automl_train_manual(Xref = xmat, Yref = ymat,
                                hpar = list(layersshape = c(10, 10, 0),
                                            layersacttype = c('tanh', 'relu', 'sigmoid'),
                                            layersdropoprob = c(0, 0, 0)))
#with gradient descent and no hidden layer (logistic regression)
amlmodel <- automl_train_manual(Xref = xmat, Yref = ymat,
                                hpar = list(layersshape = c(0),
                                            layersacttype = c('sigmoid'),
                                            layersdropoprob = c(0)))
#with PSO and softmax
amlmodel <- automl_train_manual(Xref = xmat, Yref = ymat,
                                hpar = list(modexec = 'trainwpso',
                                            layersshape = c(10, 0),
                                            layersacttype = c('relu', 'softmax'),
                                            layersdropoprob = c(0, 0),
                                            numiterations = 50,
                                            psopartpopsize = 50))

## End(Not run)
```

`autopar` *parameters for automatic hyperparameters optimization*

Description

List of parameters to allow multi deep neural network automatic hyperparameters tuning with Particle Swarm Optimization
Not mandatory (the list is preset and all arguments are initialized with default value) but it is advisable to adjust some important arguments for performance reasons (including processing time)

Arguments

psopartpopsize	number of particles in swarm, the main argument that should be tuned (default value 8, which is quite low) #tuning priority 1
psoxxx	see pso for other PSO specific arguments details
numiterations	number of convergence steps between particles (hyperparameters), default value 3) #tuning priority 1
auto_modexec	if 'TRUE' the type of Neural Net optimization will be randomly choosen between 'trainwgrad' and 'trainwpso' for each particle default value is 'FALSE' (so default value of argument 'modexec' in automl_train_manual function, actually 'trainwgrad' as default is more suited to large data volume) the value can be forced if defined in hpar list
auto_runtype	if '2steps' the 2 following steps will be run automatically (default value is 'normal'): 1st overfitting, the goal is performance 2nd regularization, the goal is generalization nb: 'overfitting' or 'regularization' may be directly specified to avoid the 2 steps
auto_minibatchsize	see below
auto_minibatchsize_min	see below
auto_minibatchsize_max	'auto_minibatch' default value 'TRUE' for automatic adjustment of 'minibatchsize' argument in automl_train_manual function the minimum and maximum value for 'minibatchsize' corespond to 2 to the power value (default 0 for 'auto_minibatchsize_min' and 9 for 'auto_minibatchsize_max')
auto_learningrate	see below
auto_learningrate_min	see below
auto_learningrate_max	'auto_learningrate' default value 'TRUE' for automatic adjustment of 'learningrate' argument in automl_train_manual function the minimum and maximum value for 'learningrate' correspond to 10 to the power negative value (default -5 for 'auto_learningrate_min' and -2 for 'auto_learningrate_max')
auto_beta1	see below
auto_beta2	'auto_beta1' and 'auto_beta2' default value 'TRUE' for automatic adjustment of 'beta1' and 'beta2' argument in automl_train_manual function
auto_psopartpopsize	see below
auto_psopartpopsize_min	see below

`auto_psopartpopsize_max`
: 'auto_psopartpopsize' default value 'TRUE' for automatic adjustment of 'psopartpopsize' argument in automl_train_manual function (concern only 'modexec' set to 'trainwpso')
the minimum and maximum value for 'psopartpopsize' ; default 2 for 'auto_psopartpopsize_min' and 50 for 'auto_psopartpopsize_max')

`auto_lambda`
: see below

`auto_lambda_min`
: see below

`auto_lambda_max`
: 'auto_lambda' default value 'FALSE' for automatic adjustment of 'lambda' regularization argument in automl_train_manual function
the minimum and maximum value for 'lambda' correspond to 10 to the power value (default -2) for 'auto_lambda_min' and (default 4) for 'auto_lambda_max')

`auto_psovelocitymaxratio`
: see below

`auto_psovelocitymaxratio_min`
: see below

`auto_psovelocitymaxratio_max`
: 'auto_psovelocitymaxratio' default value 'TRUE' for automatic adjustment of 'psovelocitymaxratio' PSO velocity max ratio argument in automl_train_manual function
the minimum and maximum value for 'psovelocitymaxratio'; default 0.01 for 'auto_psovelocitymaxratio_min' and 0.5 for 'auto_psovelocitymaxratio_max'

`auto_layers`
: see below ('auto_layers' default value 'TRUE' for automatic adjustment of layers shape in automl_train_manual function)

`auto_layers_min`
: (linked to 'auto_layers' above, set hpar 'layersshape' and 'layersacttype') the minimum number of hidden layers (default 1 no hidden layer)

`auto_layers_max`
: (linked to 'auto_layers' above, set hpar 'layersshape' and 'layersacttype') the maximum number of hidden layers (default 2)

`auto_layersnodes_min`
: (linked to 'auto_layers' above, set hpar 'layersshape' and 'layersacttype') the minimum number of nodes per layer (default 3)

`auto_layersnodes_max`
: (linked to 'auto_layers' above, set hpar 'layersshape' and 'layersacttype') the maximum number of nodes per layer (default 33)

`auto_layersdropo`
: see below

`auto_layersdropoprob_min`
: see below

`auto_layersdropoprob_max`
: 'auto_layersdropo' default value 'FALSE' for automatic adjustment of hpar 'layersdropoprob' in automl_train_manual function)
the minimum and maximum value for 'layersdropoprob'; default 0.05 for 'auto_layersdropoprob_min' and 0.75 for 'auto_layersdropoprob_max'

seed	seed for reproductibility (default 4)
nbcores	number of cores used to parallelize particles optimization, not available on Windows (default 1, automatically reduced if not enough cores)
verbose	to display or not the costs at each iteration for each particle (default TRUE)
subtimelimit	time limit in seconds for sub modelizations to avoid waiting too long for a specific particle to finish its modelization (default 3600)

back to automl_train

---

hpar *Deep Neural Net parameters and hyperparameters*

Description

List of Neural Network parameters and hyperparameters to train with gradient descent or particle swarm optimization
Not mandatory (the list is preset and all arguments are initialized with default value) but it is advisable to adjust some important arguments for performance reasons (including processing time)

Arguments

modexec	'trainwgrad' (the default value) to train with gradient descent (suitable for all volume of data) 'trainwpso' to train using Particle Swarm Optimization, each particle represents a set of neural network weights (CAUTION: suitable for low volume of data, time consuming for medium to large volume of data)

Below specific arguments to 'trainwgrad' execution mode

learningrate	learningrate alpha (default value 0.001) #tuning priority 1
beta1	see below
beta2	'Momentum' if beta1 different from 0 and beta2 equal 0) 'RMSprop' if beta1 equal 0 and beta2 different from 0 'adam optimization' if beta1 different from 0 and beta2 different from 0 (default) (default value beta1 equal 0.9 and beta2 equal 0.999) #tuning priority 2
lrdecayrate	learning rate decay value (default value 0, no learning rate decay, 1e-6 should be a good value to start with) #tuning priority 4
chkgradevery	epoch interval to run gradient check function (default value 0, for debug only)
chkgradepsilon	epsilon value for derivative calculations and threshold test in gradient check function (default 0.0000001)

Below specific arguments to 'trainwpso' execution mode

`psoxxx` see pso for PSO specific arguments details

`costcustformul` custom cost formula (default '', no custom cost function)
standard input variables: yhat (prediction), y (target actual value)
custom input variables: any variable declared in hpar may be used via alias mydl (ie: hpar(list = (foo = 1.5)) will be used in custom cost formula as mydl$foo))
result: J
see 'automl_train_manual' example using Mean Average Percentage Error cost function
nb: X and Y matrices used as input into automl_train_manual or automl_train_manual functions are transposed (features in rows and cases in columns)

Below arguments for both execution modes

`numiterations` number of training epochs (default value 50))
#tuning priority 1

`seed` seed for reproductibility (default 4)

`minibatchsize` mini batch size, 2 to the power 0 for stochastic gradient descent (default 2 to the power 5) #tuning priority 3

`layersshape` number of nodes per layer, each nodes number initialize a hidden layer
output layer nodes number, may be left to 0 it will be automatically set by Y matrix shape
default value one hidden layer with 10 nodes: c(10, 0)
#tuning priority 4

`layersacttype` activation function for each layer; 'linear' for no activation or 'sigmoid', 'relu' or 'reluleaky' or 'tanh' or 'softmax' (softmax for output layer only supported in trainwpso exec mode)
output layer activation function may be left to '', default value 'linear' for regression, 'sigmoid' for classification
nb: layersacttype parameter vector must have same length as layersshape parameter vector
default value c('relu', '')
#tuning priority 4

`layersdropoprob`
drop out probability for each layer, continuous value from 0 to less than 1 (give the percentage of matrix weight values to drop out randomly)
nb: layersdropoprob parameter vector must have same length as layersshape parameter vector
default value no drop out: c(0, 0)
#tuning priority for regularization

`printcostevery` epoch interval to test and print costs (train and cross validation cost: default value 10, for 1 test every 10 epochs)

`testcvsize` size of cross validation sample, 0 for no cross validation sample (default 10, for 10 percent)

`testgainunder`	threshold to stop the training if the gain between last train or cross validation cost is smaller than the threshold, 0 for no stop test (default 0.000001)
`costtype`	cost type function name 'mse' or 'crossentropy' or 'custom' 'mse' for Mean Squared Error, set automatically for continuous target type ('mape' Mean Absolute Percentage Error may be specified) 'crossentropy' set automatically for binary target type 'custom' set automatically if 'costcustformul' different from ''
`lambda`	regularization term added to cost function (default value 0, no regularization)
`batchnor_mom`	batch normalization momentum for j and B (default 0, no batch normalization, may be set to 0.9 for deep neural net)
`epsil`	epsilon the low value to avoid dividing by 0 or log(0) in cost function, etc ... (default value 1e-12)
`verbose`	to display or not the costs and the shapes (default TRUE)

back to automl_train, automl_train_manual

See Also

Deep Learning specialization from Andrew NG on Coursera

`pso` *PSO parameters and hyperparameters*

Description

List of parameters and hyperparameters for Particle Swarm Optimization

Arguments

All PSO parameters and hyperparameters are preset with default value

`psopartpopsize`	number of particles in swarm (discrete value) ('autopar' context: default value 8, which means that 8 different neural net hyperparameters sets will be tested ('hpar' context: default value 50, which means that 50 neural net weights sets will be tested #tuning priority 1

(impact on memory consumption)

CAUTION: you should only change the values below if you know what you are doing

`psovarvalmin`	Minimum value for particles positions (default value -10)

`psovarvalmax` maximum value for particles positions (default value 10)

`psovelocitymaxratio`
ratio applied to limit velocities (continuous value between 0 and 1, default value 0.2)

`psoinertiadampratio`
inertia damp ratio (continuous value between 0 and 1, default value 1 equivalent to OFF)

`psokappa` kappa (default value 1)

`psophi1` Phi 1 (default value 2.05)

`psophi2` Phi 2 (default value 2.05)

back to autopar, hpar

See Also

PSO video tutorial from Yarpiz

Index