Package 'spinner'

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Title An Implementation of Graph Net Architecture Based on 'torch'
Version 1.1.1
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Description Proposes a 'torch' implementation of Graph Net architecture allowing different options for message passing and feature embedding.
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Description

Spinner is an implementation of Graph Nets based on torch. Graph Nets are a family of neural network architectures designed for processing graphs and other structured data. They consist of a set of message-passing operations, which propagate information between nodes and edges in the graph, and a set of update functions, which compute new node and edge features based on the received messages.

Proposes a 'torch' implementation of Graph Net architecture allowing different options for message passing and feature embedding.

Usage

```
spinner(
 graph,
  target,
  node_labels = NA,
  edge_labels = NA,
  context_labels = NA,
  direction = "from_head",
  sampling = NA,
  threshold = 0.01,
 method = "null",
  node_embedding_size = 5,
  edge_embedding_size = 5,
  context_embedding_size = 5,
  update_order = "enc",
  n_{\text{layers}} = 3,
  skip_shortcut = FALSE,
  forward_layer = 32,
  forward_activation = "relu",
  forward\_drop = 0.3,
 mode = "sum",
 optimization = "adam",
  epochs = 100,
  lr = 0.01,
  patience = 30,
 weight_decay = 0.001,
  reps = 1,
  folds = 3,
  holdout = 0.2,
  verbose = TRUE,
  seed = 42
)
```

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Arguments

graph A graph in igraph format (without name index for nodes).
target String. Predicted dimension. Options are: "node", "edge".

node_labels String. Character vector with labels of node features. In case of absent features,

default to NA (automatic node embedding with selected method).

edge_labels String. Character vector with labels of edge features. In case of absent features,

default to NA (automatic edge embedding with selected method).

context_labels String. Character vector with labels of context features. In case of absent fea-

tures, default to NA (automatic context embedding with selected method).

direction String. Direction of message propagation. Options are: "from_head", "from_tail".

Default to: "from_head".

sampling Positive numeric or integer. In case of huge graph, you can opt for a subgraph.

Sampling dimension expressed in absolute value or percentage. Default: NA

(no sampling).

threshold Numeric. Below this threshold (calculated on edge density), sampling is done

on edges, otherwise on nodes. Default: 0.01.

method String. Embedding method in case of absent features. Options are: "null" (ze-

roed tensor), "laplacian", "adjacency". Default: "null".

node_embedding_size

Integer. Size for node embedding. Default: 5.

edge_embedding_size

Integer. Size for edge embedding. Default: 5.

 ${\tt context_embedding_size}$

Integer. Size for node embedding. Default: 5.

update_order String. The order of message passing through nodes (n), edges (e) and context

(c) for updating information. Available options are: "enc", "nec", "cen", "ecn",

"nce", "cne". Default: "enc".

n_layers Integer. Number of graph net variant layers. Default: 1.

skip_shortcut Logical. Flag for applying skip shortcut after the graph net variant layers. De-

fault: FALSE.

forward_layer Integer. Single integer vector with size for forward net layer. Default: 32 (layers

with 32 nodes).

forward_activation

String. Single character vector with activation for forward net layer. Available options are: "linear", "relu", "mish", "leaky_relu", "celu", "elu", "gelu", "selu",

"bent", "softmax", "softmin", "softsign", "sigmoid", "tanh". Default: "relu".

forward_drop Numeric. Single numeric vector with drop out for forward net layer. Default:

0.3

mode String. Aggregation method for message passing. Options are: "sum", "mean",

"max". Default: "sum".

optimization String. Optimization method. Options are: "adadelta", "adagrad", "rmsprop",

"rprop", "sgd", "asgd", "adam".

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epochs Positive integer. Default: 100.

1r Positive numeric. Learning rate. Default: 0.01.

patience Positive integer. Waiting time (in epochs) before evaluating the overfit perfor-

mance. Default: 30.

weight_decay Positive numeric. L2-Regularization weight. Default: 0.001.

reps Positive integer. Number of repeated measures. Default: 1.

folds Positive integer. Number of folds for each repetition. Default: 3.

holdout Positive numeric. Percentage of nodes for testing (edges are computed accord-

ingly). Default: 0.2.

verbose Logical. Default: TRUE seed Random seed. Default: 42.

Value

This function returns a list including:

• graph: analyzed graph is returned (original graph or sampled subgraph).

• model_description: general model description.

• model_summary: summary for each torch module.

• pred_fun: function to predict on new graph data (you need to add new nodes/edges to the original graph respecting the directionality).

• cv_error: cross-validation error for each repetition and each fold. The error is a weighted normalized loss based on mse and binary cross-entropy (depending on the nature of each specific feature).

• summary_errors: final summary of error during cross-validation and testing.

history: plot with loss for final training and testing.

• time_log: computation time.

Author(s)

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See Also

Useful links:

• https://rpubs.com/giancarlo_vercellino/spinner

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```
spinner_random_search
```

Description

spinner_random_search is a function for fine-tuning using random search on the hyper-parameter space of spinner (predefined or custom).

Usage

```
spinner_random_search(
  n_samp,
 graph,
  target,
  node_labels = NA,
  edge_labels = NA,
  context_labels = NA,
  direction = NULL,
  sampling = NA,
  threshold = 0.01,
 method = NULL,
  node_embedding_size = NULL,
  edge_embedding_size = NULL,
  context_embedding_size = NULL,
  update_order = NULL,
  n_layers = NULL,
  skip_shortcut = NULL,
  forward_layer = NULL,
  forward_activation = NULL,
  forward_drop = NULL,
 mode = NULL,
  optimization = NULL,
  epochs = 100,
  1r = NULL,
  patience = 30,
 weight_decay = NULL,
  reps = 1,
  folds = 2,
  holdout = 0.2,
  verbose = TRUE,
  seed = 42,
 keep = FALSE
)
```

Arguments

n_samp

Positive integer. Number of models to be randomly generated sampling the hyper-parameter space.

graph A graph in igraph format (without name index for nodes).
target String. Predicted dimension. Options are: "node", "edge".

node_labels String. Character vector with labels of node features. In case of absent features,

default to NA (automatic node embedding with selected method).

edge_labels String. Character vector with labels of edge features. In case of absent features,

default to NA (automatic edge embedding with selected method).

context_labels String. Character vector with labels of context features. In case of absent fea-

tures, default to NA (automatic context embedding with selected method).

direction String. Direction of message propagation. Options are: "from_head", "from_tail".

Default to: "from_head".

sampling Positive numeric or integer. In case of huge graph, you can opt for a subgraph.

Sampling dimension expressed in absolute value or percentage. Default: NA

(no sampling).

threshold Numeric. Below this threshold (calculated on edge density), sampling is done

on edges, otherwise on nodes. Default: 0.01.

method String. Embedding method in case of absent features. Options are: "null" (ze-

roed tensor), "laplacian", "adjacency". Default: "null".

node_embedding_size

Integer. Size for node embedding. Default: 5.

edge_embedding_size

Integer. Size for edge embedding. Default: 5.

context_embedding_size

Integer. Size for node embedding. Default: 5.

update_order String. The order of message passing through nodes (n), edges (e) and context

(c) for updating information. Available options are: "enc", "nec", "cen", "ecn",

"nce", "cne". Default: "enc".

n_layers Integer. Number of graph net variant layers. Default: 1.

skip_shortcut Logical. Flag for applying skip shortcut after the graph net variant layers. De-

fault: FALSE.

forward_layer Integer. Single integer vector with size for forward net layer. Default: 32 (layers

with 32 nodes).

forward_activation

String. Single character vector with activation for forward net layer. Available options are: "linear", "relu", "mish", "leaky relu", "celu", "elu", "gelu", "selu",

"bent", "softmax", "softmin", "softsign", "sigmoid", "tanh". Default: "relu".

forward_drop Numeric. Single numeric vector with drop out for forward net layer. Default:

0.3.

mode String. Aggregation method for message passing. Options are: "sum", "mean",

"max". Default: "sum".

optimization String. Optimization method. Options are: "adadelta", "adagrad", "rmsprop",

"rprop", "sgd", "asgd", "adam".

epochs Positive integer. Default: 100.

1r Positive numeric. Learning rate. Default: 0.01.

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patience Positive integer. Waiting time (in epochs) before evaluating the overfit perfor-

mance. Default: 30.

weight_decay Positive numeric. L2-Regularization weight. Default: 0.001.
reps Positive integer. Number of repeated measures. Default: 1.

folds Positive integer. Number of folds for each repetition. Default: 3.

holdout Positive numeric. Percentage of nodes for testing (edges are computed accord-

ingly). Default: 0.2.

verbose Logical. Default: TRUE seed Random seed. Default: 42.

keep Logical. Flag to TRUE to keep all the explored models. Default: FALSE.

Value

This function returns a list including:

• random_search: summary of the sampled hyper-parameters and average error metrics.

- best: best model according to overall ranking on all average error metrics (for negative metrics, absolute value is considered).
- time_log: computation time.
- all_models: list with all generated models (if keep flagged to TRUE).

Author(s)

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References

https://rpubs.com/giancarlo_vercellino/spinner

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