Implement a new Neural Network Regressor The BRAPH 2 Developers September 20, 2023

This is the developer tutorial for implementing a new neural network regressor. In this Tutorial, we will explain how to create the generator file *.gen.m for a new neural network regressor, which can then be compiled by braph2genesis. All kinds of neural network models are (direct or indirect) extensions of the base element NNBase. Here, we will use as examples the neural network regressor NNRegressorMLP (multi-layer perceptron regressor).

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We will start by implementing in detail NNRegressorMLP, which is a direct extension of NNBase. A multi-layer perceptron regressor NNRegressorMLP comprises a multi-layer perceptron regressor model and a given dataset.

Code 1: NNRegressorMLP element header. The header section of the generator code for _NNRegressorMLP.gen.m provides the general information about the NNRegressorMLP element.

```
%% iheader!
2 NNRegressorMLP < NNBase (nn, multi-layer perceptron regressor) comprises a</p>
      multi-layer perceptron regressor model and a given dataset. (1)
4 %% idescription!
5 A neural network multi-layer perceptron regressor (NNRegressorMLP) comprises
       a multi-layer perceptron regressor model and a given dataset.
6 NNRegressorMLP trains the multi-layer perceptron regressor with a formatted
      inputs ("CB", channel and batch) derived from the given dataset.
```

Code 2: NNRegressorMLP element prop update. The props_update section of the generator code for _NNRegressorMLP.gen.m updates the properties of the NNRegressorMLP element. This defines the core properties of the data point.

```
1 %% iprops_update!
3 %% iprop!
4 NAME (constant, string) is the name of the neural network multi-layer
      perceptron regressor.
5 %%% idefault!
6 'NNRegressorMLP'
8 %% iprop!
9 DESCRIPTION (constant, string) is the description of the neural network
       multi-layer perceptron regressor.
10 %%% idefault!
11 'A neural network multi-layer perceptron regressor (NNRegressorMLP)
       comprises a multi-layer perceptron regressor model and a given dataset.
        NNRegressorMLP trains the multi-layer perceptron regressor with a
       formatted inputs ("CB", channel and batch) derived from the given
       dataset.
13 %% iprop!
14 TEMPLATE (parameter, item) is the template of the neural network multi-layer
       perceptron regressor.
15 %%% isettings!
16 'NNRegressorMLP'
18 %% iprop!
19 ID (data, string) is a few-letter code for the neural network multi-layer
      perceptron regressor.
20 %%% idefault!
'NNRegressorMLP ID'
23 %% iprop!
```

(1) defines NNRegressorMLP as a subclass of NNBase. The moniker will be

```
24 LABEL (metadata, string) is an extended label of the neural network multi-
       layer perceptron regressor.
  %%% idefault!
  'NNRegressorMLP label'
28 %% iprop!
29 NOTES (metadata, string) are some specific notes about the neural network
       multi-layer perceptron regressor.
30 %%% idefault!
  'NNRegressorMLP notes'
31
32
33 %% iprop! (1)
_{
m 34} D (data, item) is the dataset to train the neural network model, and its
       data point class DP_CLASS defaults to one of the compatible classes
       within the set of DP_CLASSES.
  %%% isettings!
35
36 'NNDataset'
37 %%% idefault!
NNDataset('DP_CLASS', 'NNDataPoint_CON_REG')
40 %% iprop!
_{\mathtt{41}} DP_CLASSES (parameter, classlist) is the list of compatible data points.
42 %%% idefault! (2)
43 {'NNDataPoint_CON_REG' 'NNDataPoint_CON_FUN_MP_REG' 'NNDataPoint_Graph_REG'
        'NNDataPoint_Measure_REG'}
45 %% iprop!
46 INPUTS (query, cell) constructs the data in the CB (channel-batch) format.
47 %%% icalculate! (3)
48 % inputs = nn.get('inputs', D) returns a cell array with the
_{49} % inputs for all data points in dataset D.
50 if isempty(varargin)
      value = {};
      return
53 end
54 d = varargin{1};
inputs_group = d.get('INPUTS');
56 if isempty(inputs_group)
      value = {};
<sub>58</sub> else
      flattened_inputs_group = [];
59
      for i = 1:1:length(inputs_group)
          inputs_individual = inputs_group{i};
62
           flattened_inputs_individual = [];
           while ~isempty(inputs_individual)
63
               currentData = inputs_individual{end}; % Get the last element
64
       from the stack
               inputs_individual = inputs_individual(1:end-1); % Remove the
       last element
66
               if iscell(currentData)
67
                   % If it's a cell array, add its contents to the stack
68
                   inputs_individual = [inputs_individual currentData{:}];
                   % If it's numeric or other data, append it to the vector
                   flattened_inputs_individual = [currentData(:);
       flattened_inputs_individual];
               end
73
74
           flattened_inputs_group = [flattened_inputs_group;
75
```

(1) defines NNDataset which contains the NNDataPoint to train this regressor.

(2) defines the compatible NNDataPoint classes with this NNRegressorMLP.

(3) is a query that transforms the input data of NNDataPoint to the CB (channelbatch) format by flattening its included cells.

```
flattened_inputs_individual'];
76
       value = {flattened_inputs_group};
77
_{78} end
80 %% iprop!
81 TARGETS (query, cell) constructs the targets in the CB (channel-batch)
       format.
82 % icalculate! (4)
83 % targets = nn.get('PREDICT', D) returns a cell array with the
\mathbf{8_4} % targets for all data points in dataset D.
85 if isempty(varargin)
       value = {};
87
       return
88 end
89 d = varargin{1};
90 targets = d.get('TARGETS');
91 if isempty(targets)
       value = {};
92
93 else
       nn_targets = [];
94
       for i = 1:1:length(targets)
95
           target = cell2mat(targets{i});
96
           nn_targets = [nn_targets; target(:)'];
97
       value = {nn_targets};
100 end
101
102 %% iprop!
103 MODEL (result, net) is a trained neural network model.
104 % icalculate! (5)
inputs = cell2mat(nn.get('INPUTS', nn.get('D'))); (6)
   targets = cell2mat(nn.get('TARGETS', nn.get('D')));
   if isempty(inputs) || isempty(targets)
       value = network();
108
100 else
       number_features = size(inputs, 2);
110
       number_targets = size(targets, 2);
111
       layers = nn.get('LAYERS');(8)
112
113
       nn_architecture = [featureInputLayer(number_features, 'Name', 'Input')];
114
       for i = 1:1:length(layers)
115
           nn_architecture = [nn_architecture
               fullyConnectedLayer(layers(i), 'Name', ['Dense_' num2str(i)])
117
               batchNormalizationLayer('Name', ['BatchNormalization_' num2str(i
118
        )])
               dropoutLayer('Name', ['Dropout_' num2str(i)])
121
       nn_architecture = [nn_architecture
122
           reluLayer('Name', 'Relu_output')
123
           fullyConnectedLayer(number_targets, 'Name', 'Dense_output')
           regressionLayer('Name', 'Output')
125
126
127
       % specify trianing options (9)
128
       options = trainingOptions( ...
           nn.get('SOLVER'), ...
130
           'MiniBatchSize', nn.get('BATCH'), ...
131
           'MaxEpochs', nn.get('EPOCHS'), ...
132
```

(4) is a query that collects all the target values from all data points.

- (5) trains the regressor with the defined dataset by the code under icalculate!.
- (6) and (7) firstly extract the inputs and targets with the corresponding format.
- (8) defines the neural network architecture with user specified number of neurons and number of layers.

(9) defines the neural network training options.

```
'Shuffle', nn.qet('SHUFFLE'), ...
133
            'Plots', nn.get('PLOT_TRAINING'), ...
134
            'Verbose', nn.get('VERBOSE') ...
135
            ):
136
137
       % train the neural network
                                     (10
138
       value = trainNetwork(inputs, targets, nn_architecture, options);
139
   end
```

(10) trains the model with those parameters and the neural network architecture.

Code 3: NNRegressorMLP element props. The props section of generator code for _NNRegressorMLP.gen.m defines the properties to be used in NNRegressorMLP.

```
1 %% iprops!
3 %% iprop! (1)
4 LAYERS (data, rvector) defines the number of layers and their neurons.
5 %%% idefault!
6 [32 32]
7 %%% igui!
8 pr = PanelPropRVectorSmart('EL', nn, 'PROP', NNRegressorMLP.LAYERS, ...
      'MIN', 0, 'MAX', 2000, ...
      'DEFAULT', NNRegressorMLP.getPropDefault('LAYERS'), ...
11
      varargin(:));
13 %% iprop!
14 WAITBAR (gui, logical) detemines whether to show the waitbar.
15 %%% idefault!
16 true
18 %% iprop!
19 INTERRUPTIBLE (gui, scalar) sets whether the comparison computation is
       interruptible for multitasking.
20 %%% idefault!
.001
23 %% iprop! (2)
24 FEATURE_IMPORTANCE (query, cell) evaluates the average significance of each
       feature by iteratively shuffling its values P times and measuring the
       resulting average decrease in model performance.
25 %%% icalculate!
_{26} % fi = nn.get('FEATURE_IMPORTANCE', D) retrieves a cell array containing
27 % the feature importance values for the trained model, as assessed by
_{28} % evaluating it on the input dataset D.
if isempty(varargin)
      value = {};
      return
31
32 end
_{33} d = varargin{1};
_{34} P = varargin{2};
35 seeds = varargin{3};
inputs = cell2mat(nn.get('INPUTS', d));
  if isempty(inputs)
      value = {};
      return
_{41} end
targets = cell2mat(nn.get('TARGETS', d));
43 net = nn.get('MODEL');
```

(1) defines the number of neuron per layer. For example, [32 32] represents two layers, each containing 32 neurons.

(2) is a query that calculates the permuation feature importance. Note that, other neural network architectures, such as convolutional neural network, have other techniques to obtain feature importance.

```
45 number_features = size(inputs, 2);
46 original_loss = crossentropy(net.predict(inputs), targets);
48 wb = braph2waitbar(nn.get('WAITBAR'), 0, ['Feature importance permutation
50 start = tic;
_{51} for i = 1:1:P (4)
      rng(seeds(i), 'twister')
      parfor j = 1:1:number_features (5)
53
          scrambled_inputs = inputs;
54
          permuted_value = squeeze(normrnd(mean(inputs(:, j)), std(inputs(:, j
       )), squeeze(size(inputs(:, j))))) + squeeze(randn(size(inputs(:, j))))
       + mean(inputs(:, j));
          scrambled_inputs(:, j) = permuted_value;
          scrambled_loss = crossentropy(net.predict(scrambled_inputs), targets
57
       );
           feature_importance(j) = scrambled_loss;
58
59
      feature_importance_all_permutations{i} = feature_importance /
       original_loss;
      braph2waitbar(wb, i / P, ['Feature importance permutation ' num2str(i) '
63
        of ' num2str(P) ' - ' int2str(toc(start)) '.' int2str(mod(toc(start),
       1) * 10) 's ...'])
      if nn.get('VERBOSE')
64
          disp(['** PERMUTATION FEATURE IMPORTANCE - sampling #' int2str(i) '/
       ' int2str(P) ' - ' int2str(toc(start)) '.' int2str(mod(toc(start), 1) *
       10) 's'])
      if nn.get('INTERRUPTIBLE')
          pause(nn.get('INTERRUPTIBLE'))
      end
70 end
praph2waitbar(wb, 'close')
74 value = feature_importance_all_permutations;
```

(4) and (5) iteratively shuffle the feature values from any given dataset P times and measuring the resulting average decrease in model performance. Code 4: NNRegressprMLP element tests. The tests section from the element generator _NNRegressprMLP.gen.m. A test for creating example files should be prepared to test the properties of the data point. Furthermore, an additional test should be prepared for validating the value of input and target for the data point.

```
1 %% itests!
3 %% itest!
4 %%% iname!
5 train the regressor with example data
6 %%% icode!
8 % ensure the example data is generated
9 if ~isfile([fileparts(which('NNDataPoint_CON_REG')) filesep 'Example data NN
        REG CON XLS' filesep 'atlas.xlsx'])
      test_NNDataPoint_CON_REG % create example files
11 end
13 % Load BrainAtlas
im_ba = ImporterBrainAtlasXLS( ...
      'FILE', [fileparts(which('NNDataPoint_CON_REG')) filesep 'Example data
       NN REG CON XLS' filesep 'atlas.xlsx'], ...
      'WAITBAR', true ...
      );
19 ba = im_ba.get('BA');
21 % Load Groups of SubjectCON
im_gr = ImporterGroupSubjectCON_XLS( ...
      'DIRECTORY', [fileparts(which('NNDataPoint_CON_REG')) filesep 'Example
       data NN REG CON XLS' filesep 'CON_Group_XLS'], ...
      'BA', ba, ...
      'WAITBAR', true ...
      );
26
28 gr = im_gr.get('GR');
30 % create a item list of NNDataPoint_CON_REG
31 it_list = cellfun(@(x) NNDataPoint_CON_REG( ...
      'ID', x.get('ID'), ...
32
      'SUB', x, ...
33
      'TARGET_IDS', x.get('VOI_DICT').get('KEYS')), ...
      gr.get('SUB_DICT').get('IT_LIST'), ...
35
      'UniformOutput', false);
38 % create a NNDataPoint_CON_REG DICT
39 dp_list = IndexedDictionary(...
          'IT_CLASS', 'NNDataPoint_CON_REG', ...
          'IT_LIST', it_list ...
41
42
44 % create a NNData containing the NNDataPoint_CON_REG DICT
45 d = NNDataset( ...
      'DP_CLASS', 'NNDataPoint_CON_REG', ...
46
      'DP_DICT', dp_list ...
47
50 nn = NNRegressorMLP('D', d, 'LAYERS', [20 20]);
51 trained_model = nn.get('MODEL');
```

```
53 % Check whether the number of fully-connected layers matches (excluding
       Dense_output layer) (1)
54 assert(length(nn.get('LAYERS')) == sum(contains({trained_model.Layers.Name},
      'Dense')) - 1, ...
[BRAPH2.STR ':NNRegressorMLP:' BRAPH2.FAIL_TEST], ...
       'NNRegressorMLP does not construct the layers correctly. The number of
       the inputs should be the same as the length of dense layers the
       property.' ...
```

(1) checks whether the number of layers from the trained model is correctly set.