

| Json template objects | Keyword | Possible values | Default | Constraints | Description |
|-------------------------|------------------------|---|---------|--|---|
| entities* | entities | Array of "entity" objects | - | - | Definition of the entities of the model. |
| entity | name | Dataset variable name | - | - | Define the name of an entity type. |
| | hidden_state_dimension | Natural number | - | - | Dimension of their hidden_states. |
| | features | Array of "feature" objects | - | - | Features to be initialised in the hidden_state. |
| feature | name | Dataset variable name | - | - | Name of a feature. |
| | normalization | main.py function name | None | - | Name of the normalization function defined in the main.py file. |
| message_passing* | num_iterations | Natural number | - | - | Number iterations to repeat the message_passing phase. |
| | stages | Array of "stage" objects | - | The messages are defined in chronological order | Stage of the message passing phase |
| stage | stage_name | String | - | - | Name to identify this stage. |
| | stage_mp | Array of "single_mp" objects | - | - | Pairwise mp forming this stage. |
| single_mp | destination_entity | Entity name | - | - | Entity of the destination nodes. |
| | source_entities | "Source_entity" object | - | - | Defines how a source entity sends messages to the destination_entity |
| | aggregation | "aggregation" object | - | - | Defines how all the source entities aggregate together |
| | update | Operation | - | No input must be defined in the Operation, as it uses the aggregated input and the current hidden_state | Defines how to update the hidden_state given the aggregated information. |
| source_entity | name | Dataset name | - | - | Name of the source entity |
| | adj_vector | Dataset name | - | - | Adjacency list from source to destination nodes |
| | message | Array of "operation" objects | - | We don't allow this operation to use RNN. | Defines how to form the message given the current hidden_state. |
| Operation | type | "recurrent_neural_network", "neural_network", "direct_assignment", "activation" | - | If "recurrent_neural_network" or "neural_network" define "input" and "nn_name". | Defines if a nn is needed to form the message. |
| | input | Array of strings | - | "hs_source" to refer to the source hidden-state. "hs_dest" to refer to the destination hidden-state. "edge_param" to refer to the edge information. Otherwise, match with an "output_name". | Number of parameters that all edges from this source to destination must have. |
| | nn_name | String | - | - | Defines the architecture of the nn. |
| | output_name | String | - | - | The output of the operation can be later referred to using this name. |
| aggregation | type | "sum" / "ordered" / "attention" / "GCN" / "interleave" / "concat" | - | If "interleave", then "interleave_definition" object must be defined. If "concat", then "concat_axis" can be defined. | Defines the type of aggregation |
| | concat_axis | 1 / 2 | 1 | - | If concat_axis = 1, then all the input messages are concatenated to a longer input message list. Otherwise, the messages are concatenated pair-wise to obtain longer messages (e.g message1 is the concat of all the first messages). |
| | interleave_definition | Dataset name | - | - | Defines the interleave sequence to combine together several source entity messages. |
| readout* | readout | Array of "readout_operation" objects | - | - | Definition of the readout model. |

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| readout_operation | type | "predict"/ "pooling" / "neural_network" / "product" / "pooling" / "extend_adjacencies" | - | In all operations, the "input" field must be defined. For "product", also define "type_product" and "output_name". For "pooling", define "type_pooling" and "output_name". For "neural_network", define "nn_name" and "output_name". For "extend_adjacencies", define "adj_list", "output_name_src" and "output_name_dst". For "predict", at least "nn_name" and "label" must be defined. | Defines the readout operation to be applied |
| | input | Entity or previous output _{name} | - | - | Entity of the input hidden_states or previous name of the previous output variables to be used as input. |
| | label | Dataset name | - | - | Labels aimed to predict. |
| | label_normalization | main.py function name | None | - | Normalization function to be applied to the labels. |
| | label_denormalization | main.py function name | None | - | Denormalization function to recover the original labels. |
| | nn_name | String | - | It must match with the name of a neural network | Reference to the architecture of the neural network to use as readout. |
| | type_pooling | "sum"/"max"/"mean" | - | - | Aggregates all the indicated "input" tensors into a single one. To do so, it applies the indicated operation position-wise. |
| | type_product | "element_wise"/"dot_product" | - | - | Applies the product operation to the two inputs defined. |
| | adj_list | Dataset name | - | - | Defines the adj_list to use for extending. |
| | output_name_src | String | - | - | Defines the name where the source extended values are stored. |
| | output_name_dst | String | - | - | Defines the name where the dst extended values are stored. |
| | output_name | String | - | - | Defines the name where the output is stored. |
| neural_networks* | neural_networks | Array of "neural_network" objects | - | - | Definition of the necessary feed-forward and recurrent models of the GNN model. |
| neural_network | nn_name | String | - | - | Identifier of the neural network |
| | nn_type | "feed_forward"/"recurrent" | - | If "feed_forward", define the "nn_architecture". Otherwise, define at least the "recurrent_type" as well as any additional Keras parameter. | Indicates the types of NN aimed to define. |
| | nn_architecture | Array of "layer" objects | - | - | Architecture of the feed-forward neural network |
| | recurrent_type | Recurrent cell name (Keras documentation). | - | - | Recurrent Neural Network model definition |
| | (Keras parameter name) | Parameter value (Keras docu) | - | - | We can add any parameter accepted by Keras library model of the type defined |
| layer | type | Layer type (Keras docu) | - | - | Type of layer |
| | (Keras parameter name) | Parameter value (Keras docu) | - | - | We can add any parameter accepted by Keras library model of the type defined |
| learning_options* | loss | Function name (Keras docu) | - | - | Define the loss function to be used |
| | optimizer | "Optimizer" object | - | - | Define the optimizer options |
| optimizer | type | Name of the optimizer (Keras docu) | - | - | Define the name of the optimizer to be used |
| | (Keras parameter name) | Parameter values (Keras docu) | - | - | We can add any parameter accepted by Keras library to costume the optimizer strategy. |
| | schedule | "schedule object" | None | - | - |
| schedule | type | Name of the schedule (Keras docu) | - | - | Define the name of the schedule strategy |
| | (Keras parameter name) | Parameter values (Keras docu) | - | - | We can add any parameter accepted by Keras library to costume the schedule strategy |