| Json template objects | Keyword | Possible values | Default | Constraints | Description |
|-----------------------|----------------------------------|---|---------|--|---|
| entities* | entities | Array of "entity" objects | Delauit | Constraints | Definition of the entities of the model. |
| endles. | name | Dataset variable name | - | - | Define the name of an entity type. |
| entity | hidden state dimension | Natural number | - | - | Dimension of their hidden_states. |
| catty | | | | | Features to be initialised |
| | features | Array of "feature" objects | - | - - | in the hidden_state. |
| | name | Dataset variable name | - | - | Name of a feature. |
| feature | normalization | main my function name | None | | Name of the normalization function |
| | normanzation | main.py function name | None | | defined in the main.py file. |
| | num_iterations | Natural number | - | _ | Number iterations to repeat the |
| message_passing* | | | | 77 | message_passing phase. |
| | architecture | Array of "time_step" objects | - | The messages are defined in chronological order | Steps of the message passing phase |
| time_step | step_name | String | - | - | Name to identify this step. |
| time_step | mp_step | Array of "single_mp" objects | - | - | Pairwise mp forming this step. |
| | | "single_source" / | | If "multi_source", then | If "single_source", then a destination doesn't |
| single_mp | type | "multi_source" | - | "combined_mp_options" | have sending sources from multiple entities. |
| | source entity | Entity name | _ | object must be defined. | Entity of the sending nodes. |
| | destination_entity | Entity name | - | - | Entity of the destination nodes. |
| | _ , | • | | - | Adjacency list from source |
| | adj_vector | Dataset name | - | - | to destination nodes |
| | | Array of "operation" | | We don't allow this operation to use RNN. | Defines how to form the message |
| | message | objects | | we don't allow this operation to use KNN. | given the current hidden_state. |
| | aggregation | "sum"/"ordered"/"GAT"/ | _ | _ | Defines how to aggregate all the |
| | | "GCN"/"combined" | | | messages received. |
| | update | Operation | _ | No input must be defined in the Operation, as it uses | Defines how to update the hidden_state |
| | • | "recurrent_neural_network", "neural_network", | | the aggregated input and the current hidden_state If "recurrent_neural_network" or "neural_network" | given the aggregated information. Defines if a nn is needed to |
| Operation | type | "direct_assignation", "activation" | - | define "input" and "nn_name". | form the message. |
| | | unce_assignation , activation | | "hs_source" to refer to the source hidden-state. | form the message. |
| | input | Array of strings | - | "hs_dest" to refer to the destination hidden-state. | Number of parameters that all edges from |
| | | | | "edge_param" to refer to the edge information. | this source to destination must have. |
| | | | | Otherwise, match with an "output_name". | |
| | nn_name | String | - | <u>-</u> | Defines the architecture of the nn. |
| | output_name | String | _ | - | The output of the operation can be later |
| | | | | | referred to using this name. |
| combined_mp_options | combined_message_passing_options | Array of "combined_mp" objects | - | - | Each of these defines how a destination entity treats multiple-source messages at one step. |
| | step | Step name of all its message_passings | - | - | Time step when the coalition exists. |
| combined_mp | destination_entity | Entity name | _ | _ | Destination entity of the |
| comonica_mp | occanianon_cara, | Lance, mane | | 16 19 10 10 | multiple-source messages. |
| | massage ac-biti | "interleave" / "concat" | | If "interleave", then | Interleave defines a costume sequence |
| | message_combination | | - | "interleave_definition" object must be defined. | from the input messages. Concat simply concatenates them together. |
| | interleave_definition | Dataset name | _ | object must be defined. | Definition of the costume interleave pattern. |
| | | | | No input must be defined in the "Operation", as it uses | Defines how to update the hidden_state |
| | update | "Operation" object | - | all the aggregated inputs and the current hidden_state | given the all the aggregated information. |
| | | | | | 00 0 |

| Json template objects | Keyword | Possible values | Default | Constraints | Description |
|-----------------------|------------------------|--|---------|--|---|
| readout* | readout | Array of "readout_operation" objects | - | - | Definition of the readout model. |
| | type | "predict"/ "pooling" | - | If "Predict", then at least "input", "label" and "nn_name" must be defined. If "Pooling", then at least "type_pooling", "input" and "output_name" must be defined. | "Predict" defines a NN to predict the final label. "Pooling" transforms a set of input arrays into a new single representation. |
| readout_operation | 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" | 1 | - | Aggregates all the indicated "input" tensors into a single one. To do so, it applies the indicated operation position-wise. |
| neural_networks* | neural_networks | Array of "neural_network" objects | 1 | - | Definition of the necessary feed-forward and recurrent models of the GNN model. |
| | nn_name | String | - | - | Identifier of the neural network |
| neural_network | nn_type | "feed_forward"/"recurrent" | 1 | 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) | 1 | - | We can add any parameter accepted by Keras library model of the type defined |
| layer | type | Layer type (Keras docu) | 1 | - | Type of layer |
| | (Keras parameter name) | Parameter value (Keras docu) | i | - | We can add any parameter accepted by Keras library model of the type defined |
| learning options* | loss | Function name (Keras docu) | i | - | Define the loss function to be used |
| | optimizer | "Optimizer" object | - | - | Define the optimizer options |
| | schedule | "Schedule"object | - | - | Define the schedule options if any |
| 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 | type | Name of the schedule (Keras docu) | ı | - | 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 |