

# Module Interface Specification for Re-ProtGNN

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# 1 Revision History

Date	Version	Notes
Mar 19, 2025	1.0	Initial Draft

## 2 Symbols, Abbreviations and Acronyms

See SRS Documentation at <https://github.com/Yuanqi-X/Re-ProtGNN/blob/main/docs/SRS/SRS.pdf>.

# Contents

<b>1</b>	<b>Revision History</b>	<b>i</b>
<b>2</b>	<b>Symbols, Abbreviations and Acronyms</b>	<b>ii</b>
<b>3</b>	<b>Introduction</b>	<b>1</b>
<b>4</b>	<b>Notation</b>	<b>1</b>
<b>5</b>	<b>Module Decomposition</b>	<b>2</b>
<b>6</b>	<b>MIS of Configuration Module</b>	<b>2</b>
6.1	Module . . . . .	2
6.2	Uses . . . . .	2
6.3	Syntax . . . . .	2
6.3.1	Exported Constants . . . . .	2
6.3.2	Exported Access Programs . . . . .	3
6.4	Semantics . . . . .	3
6.4.1	State Variables . . . . .	3
6.4.2	Environment Variables . . . . .	3
6.4.3	Assumptions . . . . .	3
6.4.4	Access Routine Semantics . . . . .	3
6.4.5	Local Functions . . . . .	3
<b>7</b>	<b>MIS of Input Format Module</b>	<b>3</b>
7.1	Module . . . . .	3
7.2	Uses . . . . .	4
7.3	Syntax . . . . .	4
7.3.1	Exported Constants . . . . .	4
7.3.2	Exported Access Programs . . . . .	4
7.4	Semantics . . . . .	4
7.4.1	State Variables . . . . .	4
7.4.2	Environment Variables . . . . .	4
7.4.3	Assumptions . . . . .	4
7.4.4	Access Routine Semantics . . . . .	4
7.4.5	Local Functions . . . . .	5
<b>8</b>	<b>MIS of Control Module</b>	<b>5</b>
8.1	Module . . . . .	5
8.2	Uses . . . . .	5
8.3	Syntax . . . . .	5
8.3.1	Exported Constants . . . . .	5
8.3.2	Exported Access Programs . . . . .	5

8.4	Semantics . . . . .	5
8.4.1	State Variables . . . . .	5
8.4.2	Environment Variables . . . . .	5
8.4.3	Assumptions . . . . .	6
8.4.4	Access Routine Semantics . . . . .	6
8.4.5	Local Functions . . . . .	6
<b>9</b>	<b>MIS of Training Module</b>	<b>6</b>
9.1	Module . . . . .	6
9.2	Uses . . . . .	6
9.3	Syntax . . . . .	6
9.3.1	Exported Constants . . . . .	6
9.3.2	Exported Access Programs . . . . .	6
9.4	Semantics . . . . .	7
9.4.1	State Variables . . . . .	7
9.4.2	Environment Variables . . . . .	7
9.4.3	Assumptions . . . . .	7
9.4.4	Access Routine Semantics . . . . .	7
9.4.5	Local Functions . . . . .	7
<b>10</b>	<b>MIS of Output Visualization Module</b>	<b>7</b>
10.1	Module . . . . .	7
10.2	Uses . . . . .	8
10.3	Syntax . . . . .	8
10.3.1	Exported Constants . . . . .	8
10.3.2	Exported Access Programs . . . . .	8
10.4	Semantics . . . . .	8
10.4.1	State Variables . . . . .	8
10.4.2	Environment Variables . . . . .	8
10.4.3	Assumptions . . . . .	8
10.4.4	Access Routine Semantics . . . . .	8
10.4.5	Local Functions . . . . .	9
<b>11</b>	<b>MIS of Model Module</b>	<b>9</b>
11.1	Module . . . . .	9
11.2	Uses . . . . .	9
11.3	Syntax . . . . .	9
11.3.1	Exported Constants . . . . .	9
11.3.2	Exported Access Programs . . . . .	9
11.4	Semantics . . . . .	10
11.4.1	State Variables . . . . .	10
11.4.2	Environment Variables . . . . .	10
11.4.3	Assumptions . . . . .	10

11.4.4	Access Routine Semantics . . . . .	10
11.4.5	Local Functions . . . . .	11
<b>12</b>	<b>MIS of Inference Module</b>	<b>11</b>
12.1	Module . . . . .	11
12.2	Uses . . . . .	11
12.3	Syntax . . . . .	11
12.3.1	Exported Constants . . . . .	11
12.3.2	Exported Access Programs . . . . .	11
12.4	Semantics . . . . .	12
12.4.1	State Variables . . . . .	12
12.4.2	Environment Variables . . . . .	12
12.4.3	Assumptions . . . . .	12
12.4.4	Access Routine Semantics . . . . .	12
12.4.5	Local Functions . . . . .	12
<b>13</b>	<b>MIS of Explanation Module</b>	<b>12</b>
13.1	Module . . . . .	12
13.2	Uses . . . . .	12
13.3	Syntax . . . . .	12
13.3.1	Exported Constants . . . . .	12
13.3.2	Exported Access Programs . . . . .	13
13.4	Semantics . . . . .	13
13.4.1	State Variables . . . . .	13
13.4.2	Environment Variables . . . . .	13
13.4.3	Assumptions . . . . .	13
13.4.4	Access Routine Semantics . . . . .	13
13.4.5	Local Functions . . . . .	13

## 3 Introduction

The following document details the Module Interface Specifications for Re-ProtGNN, a re-implementation of an interpretable Graph Neural Network (GNN) Framework.

Complementary documents include the System Requirement Specifications and Module Guide. The full documentation and implementation can be found at <https://github.com/Yuanqi-X/Re-ProtGNN/tree/main>.

## 4 Notation

The structure of the MIS for modules comes from Hoffman and Strooper (1995), with the addition that template modules have been adapted from Ghezzi et al. (2003). The mathematical notation comes from Chapter 3 of Hoffman and Strooper (1995). For instance, the symbol  $:=$  is used for a multiple assignment statement and conditional rules follow the form  $(c_1 \Rightarrow r_1 | c_2 \Rightarrow r_2 | \dots | c_n \Rightarrow r_n)$ .

The following table summarizes the primitive data types used by Re-ProtGNN.

Data Type	Notation	Description
integer	$\mathbb{Z}$	a number without a fractional component in $(-\infty, \infty)$
natural number	$\mathbb{N}$	a number without a fractional component in $[1, \infty)$
real	$\mathbb{R}$	any number in $(-\infty, \infty)$
boolean	<code>bool</code>	Boolean value: either <code>True</code> or <code>False</code>
string	<code>str</code>	A sequence of Unicode characters
tensor	<code>Tensor</code>	A multi-dimensional array object from PyTorch
graph	<code>Data</code>	A graph object from PyTorch Geometric, with node and edge attributes
dataset	<code>Dataset</code>	A collection of graph objects for training or evaluation
dataloader	<code>DataLoader</code>	A PyTorch Geometric data loader for batching graph data
dictionary	<code>dict[K, V]</code>	A mapping from keys of type <code>K</code> to values of type <code>V</code>
list	<code>list[T]</code>	A sequence of elements of type <code>T</code>
function	<code>Customized Function</code>	A self-defined callable function

Re-ProtGNN uses functions, which are defined by the data types of their inputs and outputs. Local functions are described by giving their type signature followed by their specification.

## 5 Module Decomposition

The following table is taken directly from the Module Guide document for this project.

Level 1	Level 2
Hardware-Hiding	
Behaviour-Hiding Module	Configuration Module Input Format Module Control Module Training Module Output Visualization Module
Software Decision Module	Model Module Inference Module Explanation Module

Table 1: Module Hierarchy

## 6 MIS of Configuration Module

### 6.1 Module

Configuration

### 6.2 Uses

Hardware-Hiding Module

### 6.3 Syntax

#### 6.3.1 Exported Constants

- **data\_args**: An instance of **DataParser**, containing dataset-level configuration such as name, directory, splitting strategy, and seed.
- **model\_args**: An instance of **ModelParser**, containing model architecture and prototype-related hyperparameters, including GNN settings.
- **exp\_args**: An instance of **ExpParser**, configuring the algorithm used in explanation, such as rollout number and exploration parameters.
- **reward\_args**: An instance of **RewardParser**, specifying how explanation rewards are calculated.



- `train_args`: An instance of `TrainParser`, configuring training hyperparameters such as learning rate, epochs, batch size, and prototype projection.

### 6.3.2 Exported Access Programs

None

## 6.4 Semantics

### 6.4.1 State Variables

None

### 6.4.2 Environment Variables

- GPU/CPU environment: used to determine the computing device for training and inference.
- File system: used for checkpoint paths and log saving (e.g., `checkpoint/`, `datasets/`).
- Global random seed: applies to PyTorch, NumPy, and Python's random module for reproducibility.

### 6.4.3 Assumptions

None

### 6.4.4 Access Routine Semantics

None – this module serves as a global container for parameter configurations and does not define any callable functions. Other modules are expected to directly import and access `data_args`, `model_args`, `train_args`, etc.

### 6.4.5 Local Functions

None

## 7 MIS of Input Format Module

### 7.1 Module

Data

## 7.2 Uses

Hardware-Hiding Module

## 7.3 Syntax

### 7.3.1 Exported Constants

None

### 7.3.2 Exported Access Programs

Name	In	Out	Exceptions
get_dataset	dataset_dir: <code>str</code> , dataset_name: <code>str</code>	<code>Dataset</code>	<code>FileNotFoundError</code>
get_dataloader	dataset: <code>Dataset</code> , batch_size: <code>int</code> , data_split_ratio: <code>list[<math>\mathbb{R}</math>]</code>	<code>dict[str → DataLoader]</code>	<code>AssertionError</code>

## 7.4 Semantics

### 7.4.1 State Variables

None

### 7.4.2 Environment Variables

Filesystem: the file system for reading dataset files.

### 7.4.3 Assumptions

None

### 7.4.4 Access Routine Semantics

**get\_dataset(dataset\_dir, dataset\_name):**

- transition: None
- output: A PyTorch Geometric's `Dataset` object containing all graphs in the dataset.
- exception:
  - `FileNotFoundError`: if the dataset directory is invalid.

**get\_dataloader(dataset, batch\_size, data\_split\_ratio):**

- transition: None

- output: A dictionary of PyTorch Geometric’s `DataLoader` objects with keys "train", "eval", and "test".
- exception:
  - `AssertionError`: if a custom split is requested but missing from the dataset.

#### 7.4.5 Local Functions

None

## 8 MIS of Control Module

### 8.1 Module

Main

### 8.2 Uses

Hardware-Hiding Module, Configuration Module (6), Input Format Module (7), Model Module (11), Training Module (9), Inference Module (12), Explanation Module (13), Output Visualization Module (10)

### 8.3 Syntax

#### 8.3.1 Exported Constants

None

#### 8.3.2 Exported Access Programs

Name	In	Out	Exceptions
main	clst: $\mathbb{R}$ , sep: $\mathbb{R}$	-	<code>RuntimeError</code>

### 8.4 Semantics

#### 8.4.1 State Variables

None

#### 8.4.2 Environment Variables

- Filesystem: the file system for loading/saving checkpoints and writing logs/images.
- GPU/CPU hardware for model training and inference.

### 8.4.3 Assumptions

None

### 8.4.4 Access Routine Semantics

**main(clst, sep):**

- **transition:** Loads the dataset and splits it into training, validation, and test sets. Initializes the GNN model and passes it to the **train** function for optimization. After training, the **test** function evaluates the model on the test set. Finally, explanation plots are generated and saved.
- **output:** None
- **exception:**
  - **RuntimeError:** if device mismatch or model loading fails.

### 8.4.5 Local Functions

None

## 9 MIS of Training Module

### 9.1 Module

Train

### 9.2 Uses

Hardware-Hiding Module, Configuration Module (6), Model Module (11), Explanation Module (10), Output Visualization Module (10)

### 9.3 Syntax

#### 9.3.1 Exported Constants

None

#### 9.3.2 Exported Access Programs

Name	In	Out	Exceptions
train	model: <code>GnnNets</code> , dataset: <code>Dataset</code> , dataloader: <code>dict[str → <code>DataLoader</code>]</code> , clst: $\mathbb{R}$ , sep: $\mathbb{R}$	-	<code>FileNotFoundError</code>

## 9.4 Semantics

### 9.4.1 State Variables

None

### 9.4.2 Environment Variables

Filesystem: the file system for saving model checkpoints.

### 9.4.3 Assumptions

None

### 9.4.4 Access Routine Semantics

`train(model, dataset, dataloader, clst, sep):`

- transition: Trains the model using the provided data and hyperparameters. Projects prototypes periodically. Monitors evaluation accuracy, saves the best-performing model to disk.
- output: None
- exception:
  - `FileNotFoundError`: if the dataset path or checkpoint directory is invalid

### 9.4.5 Local Functions

`evaluate(loader: DataLoader, model: GnnNets, criterion: Customized Function) → dict[str → float]`

- transition: None
- output: A dictionary containing the average loss and accuracy over the input dataset split. Specifically:
  - `"loss"`: average loss (float)
  - `"acc"`: classification accuracy (float)
- exception: None

## 10 MIS of Output Visualization Module

### 10.1 Module

OutputVisualize

## 10.2 Uses

Hardware-Hiding Module

## 10.3 Syntax

### 10.3.1 Exported Constants

None

### 10.3.2 Exported Access Programs

Name	In	Out	Exceptions
PlotUtils	dataset_name: <b>str</b>	PlotUtils instance	-
plot	graph: <b>Data</b> , nodelist: <b>list[int]</b> , figname: <b>str</b> , kwargs: <b>dict</b>	-	-
append_record	info: <b>str</b>	-	FileNotFoundError

## 10.4 Semantics

### 10.4.1 State Variables

None

### 10.4.2 Environment Variables

- Filesystem: the file system for saving log files and outputting explanation images.

### 10.4.3 Assumptions

None

### 10.4.4 Access Routine Semantics

**PlotUtils(dataset\_name):**

- transition: None
- output: A **PlotUtils** object with methods for graph visualization.
- exception: None

**plot(graph, nodelist, figname, kwargs):**

- transition: Generates explanation images and saves them to the specified path.

- output: None
- exception: None

#### **append\_record(info):**

- transition: Appends the `info` string to the log file located in the given log directory.
- output: None
- exception:
  - `FileNotFoundError`: if the directory does not exist.

### **10.4.5 Local Functions**

None

## **11 MIS of Model Module**

### **11.1 Module**

GnnNets

### **11.2 Uses**

None

### **11.3 Syntax**

#### **11.3.1 Exported Constants**

None

#### **11.3.2 Exported Access Programs**

<b>Name</b>	<b>In</b>	<b>Out</b>	<b>Exceptions</b>
GnnNets	input_dim: int, output_dim: int, model_args: dict	GnnNets	NotImplementedError
forward	data: Data, prot- gnn_plus: bool, similar- ity: Tensor	logits: Tensor, - prob: Tensor, emb1: Tensor, emb2: Tensor, min_distances: Tensor	-
update_state_dict	state_dict: dict	-	-
to_device	-	-	-

## 11.4 Semantics

### 11.4.1 State Variables

- `self.model`: the internal GNN encoder consisting of learnable layers.
- `self.prototype_vectors`: a tensor containing learnable prototype embeddings, where each prototype represents a latent concept tied to a specific class.
- `self.device`: the computing device (e.g., 'cpu' or 'cuda') on which the model is running.

### 11.4.2 Environment Variables

GPU/CPU hardware for model training and inference.

### 11.4.3 Assumptions

None

### 11.4.4 Access Routine Semantics

**GnnNets(input\_dim, output\_dim, model\_args):**

- transition: None
- output: Returns an instance of the **GnnNets** class with specified input/output dimensions and model hyperparameters.
- exception:
  - `NotImplementedError`: if the specified model name in `model_args` is unsupported.

**forward(data, protgnn\_plus, similarity):**

- transition: Moves graph data to the correct device and performs a forward pass through the model.
- output:
  - `logits`: raw output scores for each class.
  - `prob`: predicted class probabilities for each input graph, obtained by applying softmax to logits.
  - `emb1`: intermediate representation from an early layer of the model.
  - `emb2`: deeper-level embedding capturing higher-level graph features after additional processing layers.



- `min_distances`: for each input graph, the minimum distance to each prototype vector.

- exception: None

**update\_state\_dict(state\_dict):**

- transition: Loads and updates model parameters from a dictionary of saved weights.
- output: None
- exception: None

**to\_device():**

- transition: Moves all model components to the device.
- output: None
- exception: None

#### 11.4.5 Local Functions

None

## 12 MIS of Inference Module

### 12.1 Module

Test

### 12.2 Uses

Model Module ([11](#)), Output Visualization Module ([10](#))

### 12.3 Syntax

#### 12.3.1 Exported Constants

None

#### 12.3.2 Exported Access Programs

Name	In	Out	Exceptions
test	model: GnnNets, DataLoader	dataloader: -	RuntimeError

## 12.4 Semantics

### 12.4.1 State Variables

None

### 12.4.2 Environment Variables

None

### 12.4.3 Assumptions

The model has been trained and its best checkpoint has been loaded.

### 12.4.4 Access Routine Semantics

test(model, dataloader):

- transition: Evaluates the trained model on the test set. Computes loss and accuracy, and uses the Output Visualization Module to log results.
- output: None
- exception:
  - `RuntimeError`: if inference fails due to an invalid model state or shape mismatch

### 12.4.5 Local Functions

None

## 13 MIS of Explanation Module

### 13.1 Module

Explanation

### 13.2 Uses

Configuration Module ([6](#))

### 13.3 Syntax

#### 13.3.1 Exported Constants

None

### 13.3.2 Exported Access Programs

Name	In	Out	Exceptions
get_explanation	data: Data, GnnNets, Tensor	gnnNet: coalition: list[int], P: $\mathbb{R}$ , prototype: embedding: Tensor	-

## 13.4 Semantics

### 13.4.1 State Variables

None

### 13.4.2 Environment Variables

None

### 13.4.3 Assumptions

None

### 13.4.4 Access Routine Semantics

get\_explanation(data, gnnNet, prototype):

- transition: None
- output:
  - coalition: list of node indices forming the explanation.
  - P: float score indicating similarity to the prototype.
  - embedding: matrix of floats representing the masked subgraph embedding.
- exception: None

### 13.4.5 Local Functions

MCTSNode(coalition: list[int], data: Data, ori\_graph: networkx.Graph, c\_puct:  $\mathbb{R}$ , W:  $\mathbb{R}$ , N:  $\mathbb{R}$ , P:  $\mathbb{R}$ )  $\rightarrow$  MCTSNode

- transition: None
- output: A node object representing a state in the search tree.
- exception: None

**mcts\_rollout**(tree\_node: MCTSNode, state\_map: dict, data: Data, graph: networkx.Graph, score\_func: Customized Function)  $\rightarrow \mathbb{R}$

- transition: None
- output: Scalar value representing the reward from this rollout.
- exception: None

**child\_scores**(score\_func: Customized Function, children: list[MCTSNode])  $\rightarrow \text{list}[\mathbb{R}]$

- transition: None
- output: List of float scores, one for each child.
- exception: None

**prot\_score**(coalition: list[int], data: Data, gnnNet: GnnNets, prototype: Tensor)  $\rightarrow \mathbb{R}$

- transition: None
- output: A float similarity score (higher = more aligned with prototype).
- exception: None

## References

- Carlo Ghezzi, Mehdi Jazayeri, and Dino Mandrioli. *Fundamentals of Software Engineering*. Prentice Hall, Upper Saddle River, NJ, USA, 2nd edition, 2003.
- Daniel M. Hoffman and Paul A. Strooper. *Software Design, Automated Testing, and Maintenance: A Practical Approach*. International Thomson Computer Press, New York, NY, USA, 1995. URL <http://citeseer.ist.psu.edu/428727.html>.