`graph_energy` Overview

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Summary

The goal of this project is to predict the energy distrubution of a group of microstates from their topological parameters.

Motivation

Approach

Data Description

Methodology

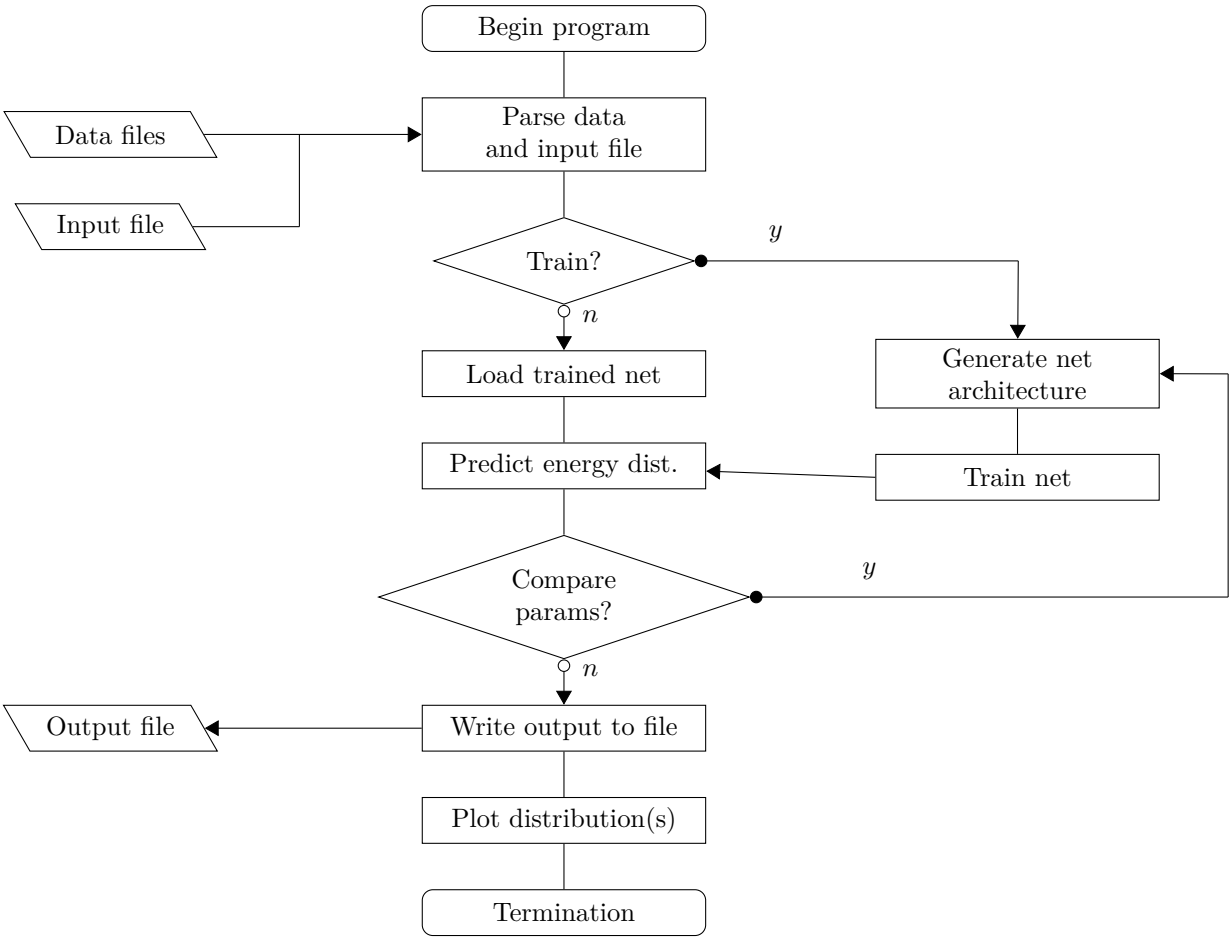
Software Design

Use Cases

The `graph_energy` package has four main use cases:

1. Train a neural net to reproduce the energy distribution of a set of microstates, given graph topological parameters that define the microstate, temperature, and population of the microstate at that temperature.
2. Evaluate the accuracy of nets trained on different sets of topological parameters at capturing the energy distribution.
3. Use previously trained neural nets to predict the energy distribution of microstates whose energy distribution was previously unknown.
4. Visualize the predicted energy distribution and, if available, contrast it with the known energy distribution.

Software flow



Component specification