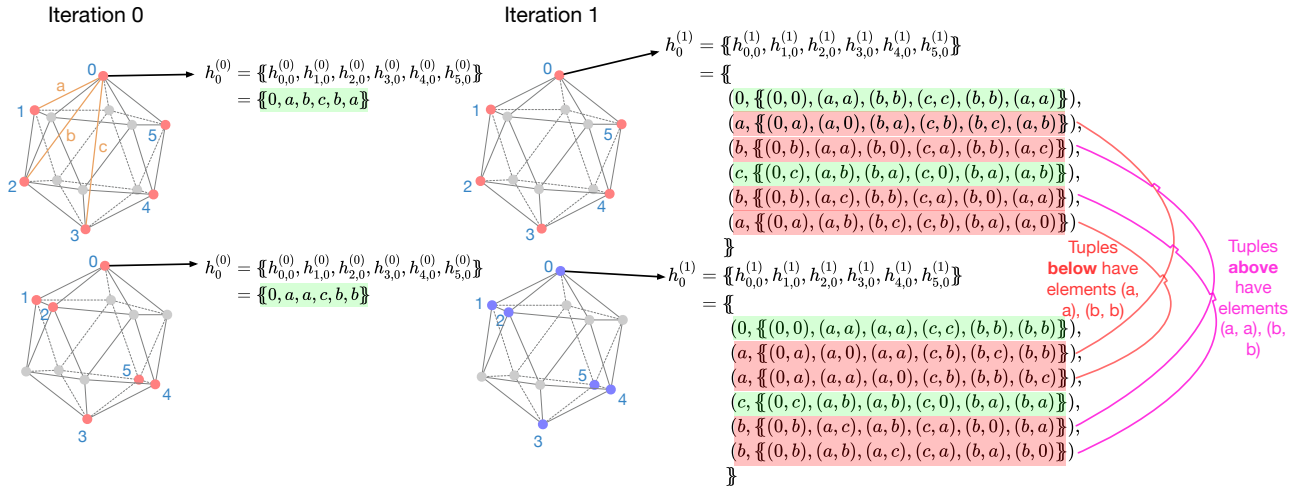

Figure 1. A case showing the explicitly computed node features by GeoNGNN. Only colored nodes belong to the geometric graphs, and the grey nodes and "edges" are for visualization purposes only. The green strips denote identical features, whereas the red strips signify non-identical features. After one iteration, the two graphs are well-seperated.

In Figure 1, we present a simple case that can be distinguished by GeoNGNN. We briefly describe GeoNGNN through the subsequent equations, wherein the initial node attributes are omitted as the point clouds are unlabelled:

$$h_{i,j}^{(0)} = d_{ij}, \tag{20}$$

$$h_{i,j}^{(t)} = (h_{i,j}^{(t-1)}, \{\!\{(h_{k,j}^{(t-1)}, d_{ik}) \mid k \in [N]\}\!\}), \tag{21}$$

where N is the total node number.

We highlight several key points:

- In the case depicted in Figure 1, all nodes within the same graph exhibit identical h, hence we present only one for clarity.
- The graph-level invariant is calculated by $\{\!\{h_i^{(T)} \mid i \in [N]\}\!\}$, which is different for the two graphs in Figure 1 due to difference of their node-level invariants.
- The case illustrated in Figure 1 is easy to distinguish, allowing GeoNGNN to differentiate them after a single iteration. While more complicated geometric graphs may pose a greater challenge for discrimination, GeoNGNN is theoretically guaranteed to differentiate all pairs of geometric graphs **within a maximum of 5 iterations** (Theorem 4.2 in our paper). Other complete models we established are also guaranteed to distinguish all pairings of geometric graphs within a **constant number** (relative to the geometric graph's size, Theorem 4.3 in our paper).
- In practical settings, all representations h are **encoded as vectors** using injective multiset functions (under some parameters) to preserve all information.

For other counterexamples, it is tedious to show all node features, and hence we here only present the separation of node features in Figure 2:

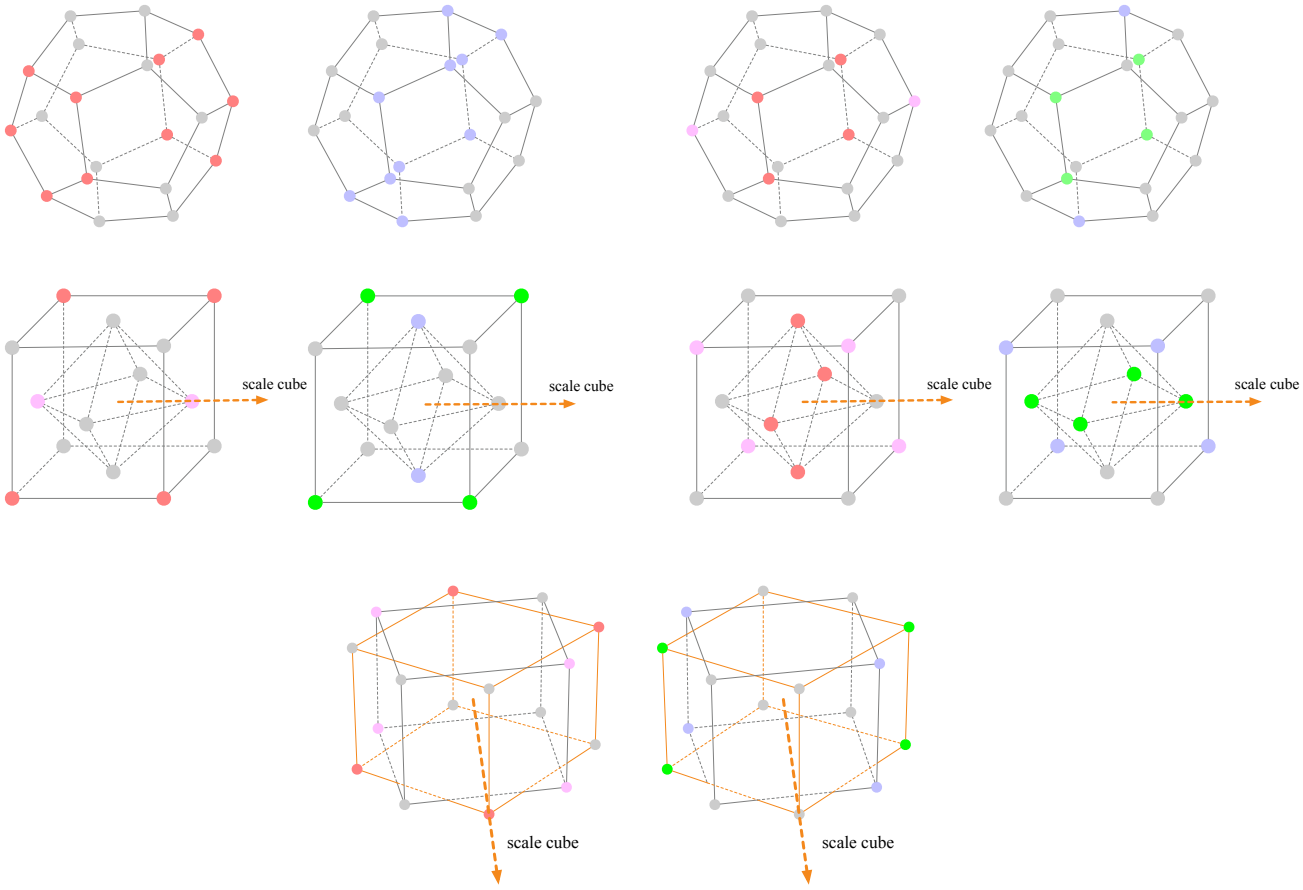

Figure 2. Several cases showing the separation of node features by GeoNGNN (more than 5 iterations). Only colored nodes belong to the geometric graphs, and the grey nodes and "edges" are for visualization purposes only. Different colors denote different node features.