Structure Recognition with Graph Neural Networks - Intermediate Report

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Abstract

The project lies at the intersection of Machine Learning and solid-state physics. A common task in solid-state physics is the classification of atomic structures, for example in crystals. Machine Learning on the other hand is well known for its ability in classification tasks. Combining these two worlds provides a powerful tool for classifying different crystal-structures. As crystal structures are described by the so called Bravais lattices, which closely relate to graphs, we will need machine learning tools capable of properly handling graph-like data. Fortunately, in the last few years, a new type of neural networks, exactly designed for this kind of data, emerged: Graph-Neural-Networks. The overall goal of this project is to get familiar with GNNs and apply to them to classification tasks of Bravais lattices.

1 Background

This introductory section lays the theoretical foundation of Bravais lattices and GNNs. We start with a short recap of lattice structures in 2d and 3d and then continue with the most fundamental background of Graph-Neural Networks (GNN). Bravais lattice can be found in many textbooks. Subsection 1.1 follows [1]. Introduction to Graph Neural Networks can be found for example in [**zw**] which is also the main reference for section 1.2.

1.1 Bravais lattice

Let $d \in \mathbb{N}$ and $\{b_i\}_{i=1,\ldots,d} \subset \mathbb{R}^d$ a basis of $\mathbb{R}^d$. The set

$$\Omega \coloneqq \left\{ \sum_{i=1}^{d} z_i b_i : z_i \in \mathbb{Z}\, \forall i \in \{1, \ldots, d\} \right\}$$

is called a d-dimensional lattice. Given any subset $S \subset \mathbb{R}^d$ we define its point group G_S to be

$$G_S \coloneqq \{M \in O(d) : MS = S\} \subset O(d).$$

G_S is obviously a subgroup of $O(d)$. We say that two d-dimensional lattices $\Omega_1, \Omega_2 \subset \mathbb{R}^d$ are of the same Bravais type if their exists $g \in GL(n, \mathbb{Z})$ such that $G_{\Omega_1} = gG_{\Omega_2}g^{-1}$. Being of the same Bravais type introduces and equivalence

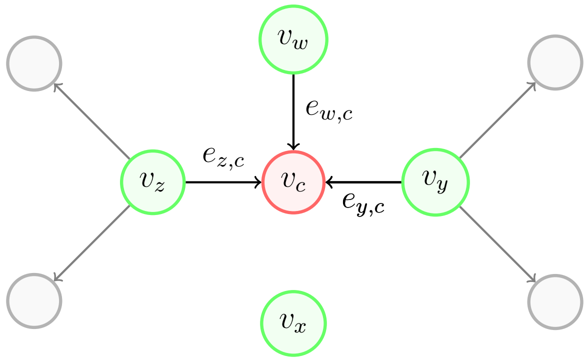

Figure 1: caption

relation on the set of all d-dimensional lattices. We call the equivalences classes Bravais classes. A natural question is, how many equivalence Bravais classes there are. Despite being a very interesting and challenging problem, we will leave this question to the mathematicians. For us, the result is more important than the actual proof. One obtains the following result: For $d = 2$ there are 5 Bravais classes and for $d = 3$ there are 14 Bravais classes.

Maybe add a picture

1.2 Fundamentals of GNNs

To talk about graphs, we first have to agree on some notation: Let V be a set and $E \subset V \times V$. The tuple $G = (V, E)$ is called a graph. Furthermore, we call an element $x \in V$ a node and a tuple $(x, y) \in E$ a directed edge from x to y. In case $(x, y) \in E$ implies $(y, x) \in E$ we speak of an undirected graph. In that case, we call G an undirected graph, and we can think of elements in E as unordered tuples x, y instead of ordered ones. We still call x, y an edge between x and y. For working with GNNs we have to assign to each node $x \in V$ a vector $v_x \in \mathbb{R}^n$ called node feature and to each edge $(x, y) \in E$ a vector $e_{x,y} \in \mathbb{R}^m$ called edge feature. Roughly, a GNN takes a graph with all its nodes and edge features as an input and manipulates these feature in each step produces. More than that, a GNN can transform the structure of the graph itself, e.g. by introducing new nodes or edges. However, we will not go into detail about this possibility and stick to the more simple case of manipulating node and edge-features. Lets write this in a bit more formal way: xplain a bit what gnns are, how they work (message passing class, message, update, aggregate) differs from an ordinary or undirected graph, in that the latter is defined in terms of unordered pairs of vertices, which are usually called edges, links or lines.

2 Project Goals

The project can be split into two parts. The goal of the first part is to build a GNN that is capabale of assigning a 2- or 3-dimentional lattices its Bravais class. For this instance, different lattices needs to be created programmatically. Furthermore, they have to be labeled so that they can serve as training data. Once we have a good amount of training data at hand we need to determine the optimal structure of the GNN. This amounts to finding the right functions ϕ, ψ in equation xy and to determine which edge-/node-features do best. In the second part of the project, we will take a look at more complex structures. getting familiar with basic gnn techniques jonas nach neuer aufgabe fragen

3 Schedule

The first goal mentioned in the previous section has already been achieved. The 2d and 3d lattice-generation is finished and some different GNN structures have already been tested and evaluated. Both, in 2d and in 3d, an accuracy of about 90% have been achieved but probably with further testing, the accuracy can be increased even more. Until end of December further experiments with the network structure is planned. The second goal mentioned in the previous section has not yet been achieved. The code for this is planned to be finished until begin of January. The final results are then expected until mid January so that the final report can be written in the last two weeks of January.

References

[1] Willard Miller. *Symmetry Groups and Their Applications.* Academic Press, 1972.