Structure Recognition with Graph Neural Networks

Final Report for the Lab-Course Advanced Projects in Computational Physics 2

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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 them to classification tasks of Bravais lattices.

Contents

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). Results on Bravais lattices can be found in many textbooks. Subsection 1.1 follows [4] and [3]. Introduction to Graph Neural Networks can be found for example in [1] which is also the main reference for section 1.3.

1.1 Bravais lattice

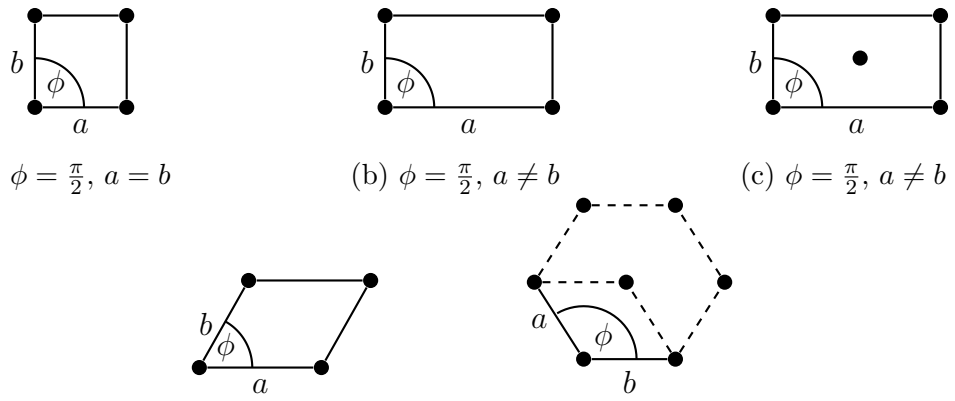
Let $d \in \mathbb{N}$ and $\{b_i\}_{i=1,\dots,d} \subset \mathbb{R}^d$ a basis of $\mathbb{R}^d$. The set

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

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 there exists $g \in GL_n(\mathbb{R})$ such that $G_{\Omega_1} = gG_{\Omega_2}g^{-1}$ and $\Omega_1 = g\Omega_2$. Being of the same Bravais type introduces an equivalence relation on the set of all d-dimensional lattices. We refer to the equivalence classes as Bravais classes. A natural question arising is about the total number of Bravais classes. 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. Roughly speaking, they can be distinguished by the relative lengths of the basis vectors b_i and the angles between them. Visualizations of all Bravais classes for $d = 2$ can be found in figure 1. Visualizations for $d = 3$ and further notes on each Bravais class can be found for example in [2].



(a) $\phi = \frac{\pi}{2}$, $a = b$ (b) $\phi = \frac{\pi}{2}$, $a \neq b$ (c) $\phi = \frac{\pi}{2}$, $a \neq b$

(d) $\phi \neq \frac{\pi}{2}$, $a \neq b$ (e) $\phi = \frac{2\pi}{3}$, $a = b$

Figure 1: All different Bravais classes in two dimensions. They are called (a) square, (b) rectangle, (c) centered rectangle, (d) oblique, (e) hexagonal.

1.2 Introduction to Neural Networks

Stating a precise definition of "Neural Network„ is quite involved. Hence, we will only speak about the most fundamental type of neural networks, the so-called feed forward neural networks. Even for these simple networks, a precise definition is a bit lengthy. We have to introduce some notation first: Let $l \in \mathbb{N}_{\geq 2}$, $n_0, n_1 \ldots, n_l \in \mathbb{N}$ and for each $i \in \mathbb{N}, i \leq l$ choose an affine linear map $T^{(i)} : \mathbb{R}^{n_{i-1}} \to \mathbb{R}^{n_i}$ and a smooth map $a^{(i)} : \mathbb{R} \to \mathbb{R}$. Denoting with $f^{(i)} : \mathbb{R}^{n_i} \to \mathbb{R}^{n_i}$ the function acting element wise by $a^{(i)}$ (i.e $f^{(i)}(x_1, \ldots, x_{n_i}) = (a^{(i)}(x_1), \ldots, a^{(i)}(x_{n_i}))$), we define the composition

$$\tilde{F} \coloneqq T^{(l)} \circ f^{(l-1)} \circ T^{(l-1)} \circ \cdots \circ f^{(2)} \circ T^{(2)} \circ f^{(1)} \circ T^{(1)} : \mathbb{R}^{n_0} \to \mathbb{R}^{n_l}.$$

Recall that for any affine linear map $L : \mathbb{R}^n \to \mathbb{R}^m$ there exist $b \in \mathbb{R}^m$ and $W \in \mathrm{Mat}(n \times m, \mathbb{R})$ such that $Lx = W^T x + b$ for all $x \in \mathbb{R}^n$ (the transposition is just for our convenience later on). Hence, to each $T^{(i)}$ corresponds a matrix $W^{(i)} \in \mathrm{Mat}(n_{i-1} \times n_i, \mathbb{R})$ called the weight-matrix and a vector $b^{(i)} \in \mathbb{R}^{n_i}$ called bias such that $T^{(i)}x = \left(W^{(i)}\right)^T x + b^{(i)}$. We introduce further notation: Obviously, we can think of $W^{(i)}$ as an element in $\mathbb{R}^{n_{i-1}n_i}$. Let $\theta = (W^{(1)}, b^{(1)}, \ldots, W^{(l)}, b^{(l)}) \in \mathbb{R}^{n_0 n_1} \times \mathbb{R}^{n_0} \times \cdots \times \mathbb{R}^{n_{l-1}n_l} \times \mathbb{R}^l$. Clearly, $\tilde{F}$ depends on the choice of $T^{(l)}$ and hence of the choice of θ. Correspondingly, for each such θ we can build a map $\tilde{F} = F_\theta$. With this notation in mind, we are ready to define what a neural network should be: The map

$$F : \mathbb{R}^{n_0 n_1} \times \mathbb{R}^{n_0} \times \cdots \times \mathbb{R}^{n_{l-1}n_l} \times \mathbb{R}^{n_l} \to C(\mathbb{R}^{n_0}, \mathbb{R}^{n_l}), \quad \theta \mapsto F_\theta$$

is called (feed forward) neural network with l layers and activation function $a^{(i)}$ in layer i.

Though this definition might seem technical, it bears a visual explanation: It is best explained with figure 2. We can view $F_\theta : \mathbb{R}^{n_0} \to \mathbb{R}^{n_l}$ as a graph-like structure. Each coordinate x_i of an input vector $x \in \mathbb{R}^{n_0}$ can be thought if as a node. Applying $f^{(1)} \circ T^{(2)}$ to x yields a new vector $y^1 = f^{(1)} \circ T^{(2)}(x) \in \mathbb{R}^{n_1}$. The coordinates of y^1 can again be interpreted as nodes. All these nodes (coordinates) together constitute the new layer of the network. Applying $f^{(2)} \circ T^{(2)}$ to y^1 yields a new layer y_2 and so on. The last layer $y^{(l)}$ is then given by $F_\theta(x)$. Going from layer $i-1$ to the layer i can be visualized as follows: According to the above definitinos we have

$$\begin{aligned} y_j^i &= a^{(i)}\left(T^{(i)}\left(y^{i-1}\right)\right)_j \\ &= a^{(i)}\left(\sum_{k=1}^{n_{i-1}} \left(W^{(i)}\right)_{jk}^T y_k^{i-1} + b_j^{(i)}\right) \\ &= a^{(i)}\left(\sum_{k=1}^{n_{i-1}} W_{kj}^{(i)} y_k^{i-1} + b_j^{(i)}\right). \end{aligned}$$

Up to application of $a^{(i)}$, the node y_j^i is a weighted sum of all nodes y_k^{i-1} in the previous layer (in addition to a constant bias value $b_j^{(i)}$). The matrix element $W_{kj}^{(i)}$ describes how much the node y_j^i is influenced by node y_k^{i-1}. We picture an edge

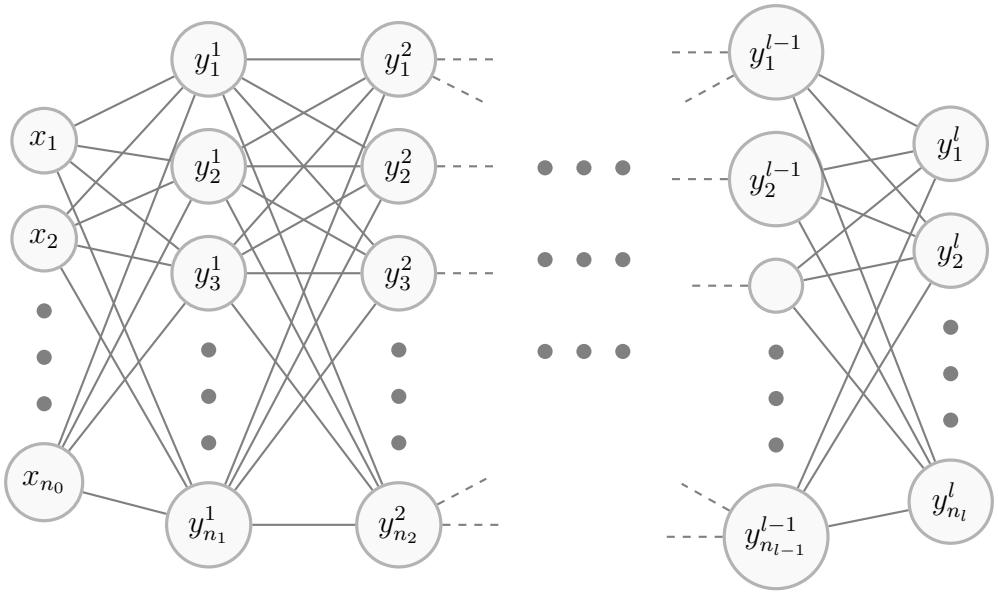


Figure 2: Visualization of a feed forward neural network. [warum können nicht einfach alle nodes gleich groß sein?!]

from node y_k^{i-1} to node y_j^i which has the weight $W_{kj}^{(i)}$. Consequently, the matrix $W^{(i)}$ is called weight-matrix.

With the visuals in mind, we can explain what neural networks are used for and how they are being used. The purpose of neural network lies in the approximation of unknown functions. Suppose we were given a function $G : \mathbb{R}^n \to \mathbb{R}^m$ from which we only know the values at D-many ($D \in \mathbb{N}$) points $x_1, \dots, x_D \in \mathbb{R}^n$, i.e. only the values $y_1 = G(x_1), \dots, y_D = G(x_D)$ are known. Choose $l \in \mathbb{N}$, set $n_0 = n$, $n_l = m$ and consider the neural network

$$F : \mathbb{R}^{n_0 n_1} \times \mathbb{R}^{n_0} \times \cdots \times \mathbb{R}^{n_{l-1} n_l} \times \mathbb{R}^{n_l} \to C(\mathbb{R}^{n_0}, \mathbb{R}^{n_l}), \quad \theta \mapsto F_\theta.$$

We can then try to find an „optimal“ θ such that $F_\theta \approx G$. To do so, we have to introduce a measure for how much F_θ differs from G. This is commonly called a cost functions, i.e. a function $C : \mathbb{R}^m \times \mathbb{R}^m \to \mathbb{R}$, that maps to a pair $(F_\theta(x_i), y_i)$ a real value $C(F_\theta(x_i), y_i)$ that can be interpreted as a distance between the true value y_i and the predicted value $F_\theta(x_i)$. Finding an optimal θ is achieved by minimizing the map $\theta \to C(F_\theta(x_i), y_i)$ for all $i = 1, \dots, D$. This optimization is called „training the neural network“. There is a whole theory about optimization of real valued functions. A common way to do this by means of the gradient descent method. Roughly speaking, the idea is the following: Calculate the gradient of the map $\theta \mapsto C(F_\theta(x_i), y_i)$ for a fixed $i = 1, \dots, D$, and then change θ slightly in the opposite direction of the gradient. As F_θ is a large composition, computing basically comes down to repeated application of the chain rule. An efficient algorithm that does exactly this and is widely used is called backpropagation. We can repeat this step until we found a θ such that $C(F\theta(x_i), y_i)$ is sufficiently small for all $i = 1, \dots, d$.

1.3 Fundamentals of Graphs and Graph Neural Networks

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, and we say that x is a neighbor of y. In case $(x, y) \in E$ implies $(y, x) \in E$, we speak of an undirected graph. In that case, 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 $y \in V$ we define the neighborhood N_y of y to be the set of all neighbors, i.e.

$$N_y := \{x \in V : (x, y) \in E\} \subset V. \tag{1}$$

Furthermore, we 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 features in each step. 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 simpler case of manipulating only node and edge-features. Furthermore, we restrict ourselves to the case where the GNN does not alter the edge features. Let us make these ideas

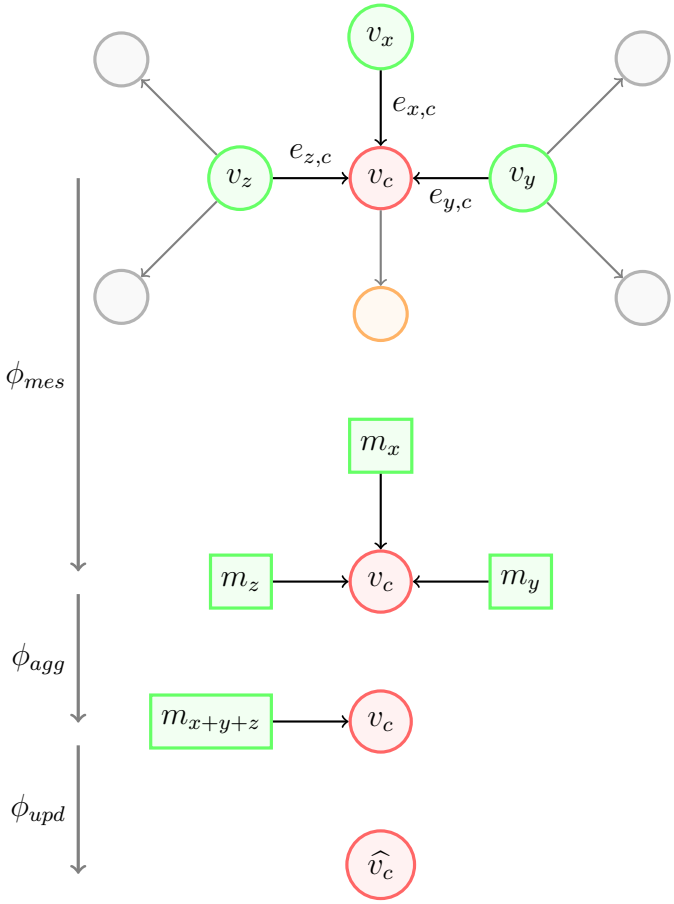


Figure 3: Illustration of the message passing procedure according to equation (2). The neighbors of node c (red) are the nodes x, y, z (green). Attention: According to equation (1) the orange node is not regarded as a neighbor of c as the edge points in the wrong direction. For each neighbor (x, y, z), ϕ_{mes} computes messages (m_x, m_y, m_z) which are sent to c. Then, ϕ_{agg} aggregates these three messages and outputs one overall message m_{x+y+z} that is sent to c. In the last step, ϕ_{upd} updates the node value v_c to a new value $\widehat{v_c}$.

a bit more rigorous (see figure 1.3 for an illustration): Let (V, E) be a graph with node features $\{v_x \in \mathbb{R}^n : x \in V\}$ and edge features $\{e_{x,y} \in \mathbb{R}^m : (x, y) \in E\}$. For each $c \in V$ a new node feature $\widehat{v_c}$ is calculated according to the following rule

$$\widehat{v_c} = \phi_{upd}\left(v_c, \phi_{agg}\left(\{\phi_{mes}\left(v_y, v_c, e_{y,c}\right) : y \in N_c\}\right)\right), \tag{2}$$

where $\phi_{upd}, \phi_{agg}, \phi_{mes}$ denote differentiable functions. These three functions are commonly interpreted as follows: ϕ_{mes} takes as inputs the node value v_c and the node value v_y of one neighbor y of c as well as the value $e_{y,c}$ of the edge (y, c). Depending on these inputs, it then computes a value, which can be thought of as a message originating from node y which is sent to node c. ϕ_{agg} collects all these messages to node c and aggregates them in some way, so that the output can be thought of as one overall message to node c. ϕ_{upd} takes this overall message as well as the value of node c and computes, how the value of node c is altered. Unsurprisingly, this scheme is called Message-Passing-Layer. Given a specific problem, that is required to be solved by a GNN, the challenge is to make appropriate choices for $\phi_{upd}, \phi_{agg}, \phi_{mes}$ that suit the problem at hand. Furthermore, one has to decide how many iterations of the above procedure are suitable.

1.4 Percolation

Besides Bravais classes, neural networks and graph neural networks, the fourth ingredient for this report is a percolation. We start with an undirected graph $G = (V, E)$ and want to define what paths and cycles are. Pick two nodes $n_1, n_2 \in V$. We say that n_1 and n_2 are connected if there are nodes $m_0, m_1, \ldots, m_N \in V$ such that $m_0 = n_1$, $m_N = n_2$ and for each $i \in \{0, \ldots, N-1\}$ there is an edge $\{m_i, m_{i+1}\} \in E$. In this case, the tuple $(m_0, m_1, ..., m_N)$ is called a path of length N from n_1 to n_2. A path is $(m_0, m_1, ..., m_N)$ is called a cycle if $m_i \neq m_j$ for $i \neq j$ (i.e. no node is visited twice).

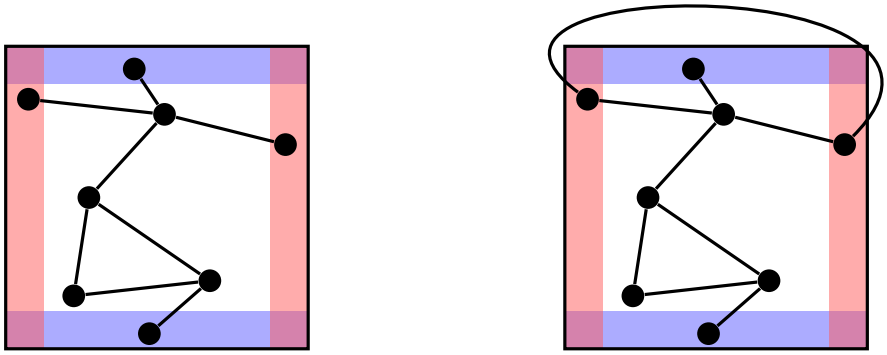
Knowing what paths and cycles are, everything is set up to introduce percolating graph. Suppose $G = (V, E)$ is an undirected graph, where each node $n \in V$ has a position $p_n = (n_x, n_y) \in [0, 1] \times [0, 1]$. Visually, we think of G as a graph inside the unit square. Fix $\frac{1}{2} > r > 0$. The graph is called percolating, if there are nodes $n, m \in V$ such that

1. there is a cycle containing n and m,
2. $\{n, m\} \in E$ and
3. either $n_x < r$ and $m_x > 1 - r$ or $n_y < r$ and $m_y > 1 - r$.

Figure 4 gives an example of percolating and non-percolating graphs. Properties 1. and 2. are easily understood. It is worth mentioning, that 1. and 2. imply, that there is a cycle containing n,m as well as the edge $\{n, m\}$. Property 3. needs a bit more explanation: We can picture small trips of width r at the sides of the unit square (see figure 4 where the strips are colored red and blue), Requiring $n_x < r$ and $m_x > 1 - r$ means that n is located on the left side of the unit square while m is located on the right side. Accordingly, $n_y < r$ and $m_y > 1 - r$ requires n to be on the bottom and m to be on the top of the unit square. In any of these two cases, n and m are in strips of the same color but on opposite sites. The restriction to $r < \frac{1}{2}$ guarantees that strips of the same color do not overlap.

2 Goals and Implementation

The project can be split into two parts. The goal of the first part is to build a GNN that is capable of assigning a 2- or 3-dimensional lattice its Bravais class. For this



(a) non-percolating graph (b) percolating graph

Figure 4: Illustration of percolating and non-percolating graphs.

instance, different lattices need 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 $\phi_{upd}, \phi_{mes}, \phi_{agg}$ in equation 2 and to determine which edge-/node-features do best. In the second part of the project, we will build upon the results in the first part and take a look at more complex structures. The goal is to distinguish between percolating and non-percolating structures.

2.1 Lattice Creation

To be precise, we will not create lattice according to the definition given in sectio 1.1, as this would require the creation of sets with infinite elements. Clearly, a GNN can only deal with finitely many nodes. Hence, we will only create finite subsets of lattice but, for sake of simplicity, we will still call them lattices.

Let us start with the creation of two-dimensional lattices. Choose $a, b \in \mathbb{R}_+$, $\phi \in (0, \pi)$ and set $e_x = (0, a)^T$, $e_y = (b\cos(\phi), b\sin(\phi))^T$. Then, the set $\tilde{\Omega} = \mathbb{Z}e_x \times \mathbb{Z}e_y \subset \mathbb{R}^2$ is a two-dimensional lattice. As mentioned, we only work with finite subsets of Ω. Hence, we choose $N_x, N_y \in \mathbb{N}$ and set $\Omega = \mathbb{N}_{\leq N_x}e_x \times \mathbb{N}_{\leq N_y}e_y \subset \tilde{\Omega}$. This lattice now has N_xN_y elements. Next, we add some noise to the elements in Ω and restrict their coordinates to a certain range. For this instance, let $\mu, \sigma, s \in \mathbb{R}_+$ and draw random samples from a normal distribution with mean value μ and standard deviation σ. Secondly, we scale these random numbers by the factor s and add the scaled noise to all elements in Ω (component-wise, i.e. add noise to the first coordinate of the elements in Ω as well as to the second coordinate). Restricting all coordinates to a certain range is simply done. Let $x_{max}, y_{max} \in \mathbb{R}_+$ and replace each $(x, y) \in \Omega$ with $(x \mod x_{max}, y \mod y_{max})$ [modular arithmetic with non-integers values: stupid!]. Next, we want to turn our lattice Ω into a graph (V, E). Obviously, we can set $V = \Omega$ and what remains is the choice of edges. For this, we take $r \in \mathbb{R}_+$ and set

$$E = \{(v, w) \in V \times V : \|v - w\| < r\},$$

where $\|\cdot\|$ denotes the standard norm in R^d [not quite, actually I used the 3-norm]. Lastly, we choose $p_n, p_e \in [0, 1]$ and randomly delete nodes with probability p_n (and

(a) 2d (b) 3d

Figure 5: Examples of lattices created by the procedure described in section 2.1. [TODO]

edges with probability p_e respectively).

The creation of three-dimensional lattices is completely analogously. The only difference is that we have to pick three basis vectors e_x, e_y, e_z which have length $a, b, c \in \mathbb{R}_+$ and enclose angles $\phi = \angle(e_x, e_y)$, $\psi = \angle(e_x, e_z)$, $\chi = \angle(e_y, e_z)$.

Figure 5 shows two different lattices created by the above procedure.

2.2 Implementing the GNN

2.3 On the Problem of Percolation

3 Results and Discussion

This chapter presents the results of the problems mentioned in chapter 2. Furthermore, we are going to analyze these results. As in chapter 2 we start by looking at the classification tasks and after that, we will proceed with the percolation problem.

3.1 Classifying Graphs into Bravais Classes

3.2 On the Problem of Percolation

4 Conclusion and Outlook

References

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