Catalyst Discovery and Optimization using Graph Neural Networks

Charles Fox [1] **Samiha Sharlin** [2]

Abstract

A key goal of catalyst discovery and optimization is to solve the societal and energy challenges, including renewable energy production and its long-term storage. Energy storage needs to execute chemical reactions and use of catalysts drive these conversion processes at higher rates. As we depend more on renewable energy sources, we need solutions that will also scale and are inexpensive. Current catalyst design uses quantum chemical simulations that have a very high computational cost and also scales with the model size. With the use of machine learning, these calculations may be approximated more efficiently, leading to new approaches in finding low-cost and durable catalysts. We plan to design a simple model using graph neural networks (GNN) and the Open Catalyst Project (OC20) dataset that was accumulated to model and discover new catalysts. GNN is a suitable choice for us to explore since the natural representation of chemical structures is through molecular graphs it can be directly used as an input. The performance of our model increased as we consecutively integrated information about atomic positions and radii, and the loss hit a base value which did not improve upon further addition of energy as part of global message.

1. Introduction

Increasing renewable energy is imperative for meeting the world's rising energy demands and reducing the effects of climate change. Solar, wind, and hydro-power provide 17% (Electric Power Monthly, EIA) and 28% (International Energy Outlook, EIA) of the world's electricity, respectively. This is projected to increase significantly in the future, but its expansion presents a major challenge. Unlike traditional power sources, such as coal, natural gas, and nuclear, which provide continuous power, renewable energy provides intermittent power. The transfer of energy from peak periods of generation to peak periods of demand requires effective energy storage solutions.

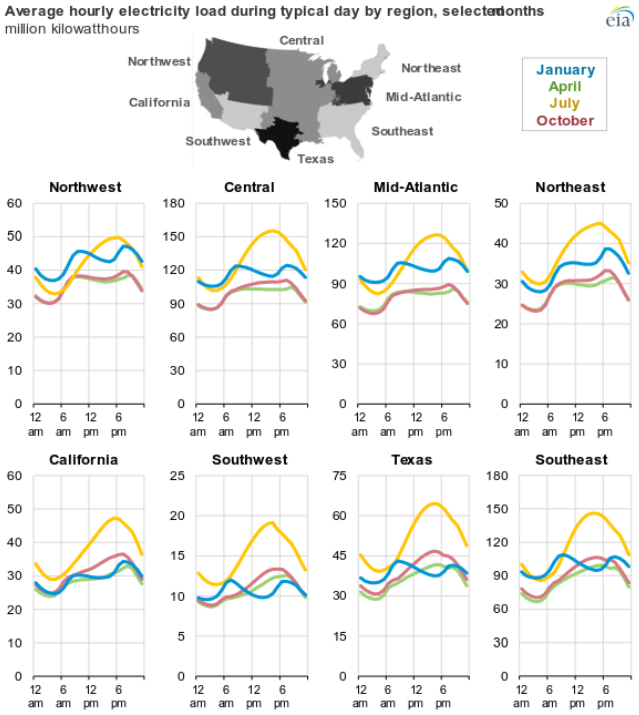

Figure 1. Hourly electricity consumption varies throughout the day and across seasons. (Electric Power Monthly, EIA)

Converting renewable energy into other fuels, such as hydrogen (Ould Amrouche et al., 2016), offers a potential method of scaling up to national grids but this method also needs cost-effective ways to run chemical reactions. Finding low-cost and durable catalysts that can drive these reactions at high rates is an active area of research (Isbrandt et al., 2019). The modern design of catalysts uses computational modeling and simulation to assess the suitability of materials for further exploration. Density Functional Theory (DFT)

[1]Department of Computer Science and Electrical Engineering [2]Department of Chemical, Biochemical and Environmental Engineering. Correspondence to: Charles Fox <charfox1@umbc.edu>, Samiha Sharlin <samiha.sharlin@umbc.edu>.

(Sholl & Steckel, 2009) is often used to compute the atomic interactions. It combines the position of the atoms with quantum mechanics to predict the energy of the structure and compute the forces. The distribution and energy are modified by updating their positions and the iterative process continues until the system's energy reaches a local minimum. The energy of the resulting relaxed structure gives insight into the overall efficiency of a reaction, i.e., how much energy is generated or consumed during the reaction. DFT computation is unfortunately extremely expensive and scales O(n^3) with the number of electrons in the system, which in practice can range from 100 to over 5,000. This leads to computations taking hours or days per relaxation on CPUs with O(10–100) cores (Zitnick et al., 2020). A computationally efficient approximation is required for the large-scale study of new catalysts. Machine learning may be a particularly promising approach if we can train substantial large datasets of DFT calculations to build competent models.

1.1. Proposed method

Machine learning methods, specifically deep learning via neural networks, have been used to great effect in more complex classification and regression tasks. In the past decade these methods have demonstrated remarkable success in understanding and translating natural languages (Lupu, 2017), audio signals (Almeida et al., 2019), and inferring features from images and videos (Wang et al., 2018). Additionally, they are becoming a standard tool in chemical and materials sciences by accelerating quantum calculations to the point of DFT level accuracies (Ramakrishnan & von Lilienfeld, 2017). A challenge to the application of deep learning in chemistry is the appropriate selection and computation of molecular descriptors (Collins & Raghavachari, 2020). Graph neural networks (GNNs) are a class of deep learning networks that provide a way around by allowing us to take a molecule directly as input.

A graph G is a set of nodes (V) and edges (E) that shows relations between them. We can store information in each piece of the graph. In our context, nodes are atoms which can contain information about their positions, identity, valency etc. and edges can show the bond order (single bonds/ double bonds) or distance between two atoms.

The two defining attributes of GNN are 1.) Its input and output is a graph and 2.) It is permutation invariant which means it does not matter how we order our nodes. We might also sometimes want the GNN output to be *permutation equivariant*, i.e., when the GNN output is per-node features, so if we switch the input order, we expect our per-node output to change. This is important with respect to applications in chemistry to carefully distinguish between node features that might be element identifiers from those that specify

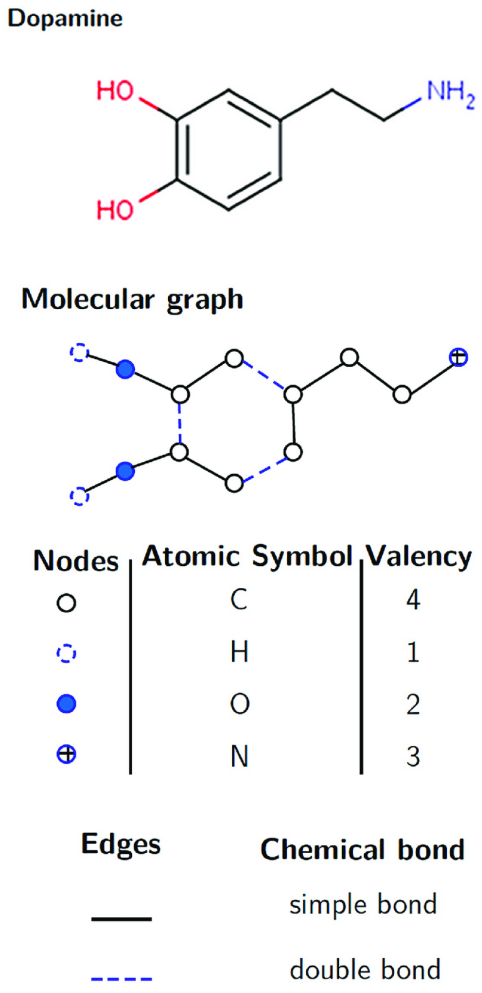

Figure 2. Dopamine and its molecular graph (Nouleho Ilemo et al., 2019)

their position (White, 2021). They are referred to as point clouds data, which contain a set of cartesian coordinates (X, Y, Z) for each point position and are generally produced by 3D scanners (Wand et al., 2009) or photogrammetry (Baqersad et al., 2012).

Operations into GNNs can be broadly divided to three categories: graph-level, node-level, and edge-level. A graph-level problem could be classifying a molecule type or its energy in global-context. A node-level problem could be predicting positions or charges of atoms and an edge-level task could be predicting presence/absence of connections between atoms. As mentioned before, information in graph can be stored in both nodes and edges, in edges-only or in nodes-only or as global information like initial energy. We might need to use the information on edges to make predictions on nodes or vice-versa. Pooling operation is used that allows us to gather information in each of their embedding and concatenate them into a matrix by sum, mean or max.

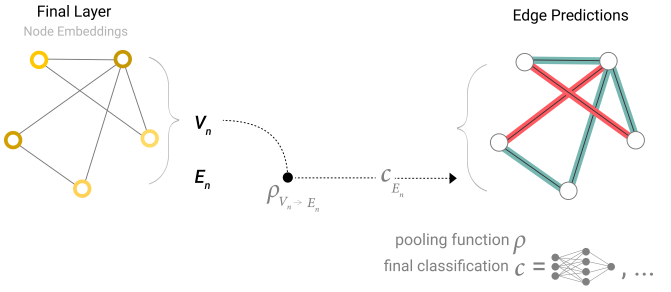

Figure 3. Node-level features to predict edge-level information (Sanchez-Lengeling et al., 2021)

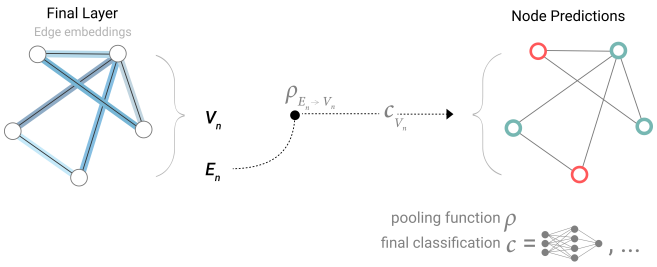

Figure 4. Edge-level features to predict node information (Sanchez-Lengeling et al., 2021)

As we can see, we are not using the whole graph connectivity inside the GNN layer in this simplest formulation. Each node and each edge, as well as the global context, are processed independently.

This basic model allows communication between a node and its immediate neighbors. In the context of chemistry, this is not enough. We can stack multiple layers and do message passing by making our learned embeddings aware of a wider aspect of graph, for instance a two layer will have one node's neighbors' neighbors' information. This allows passing messages between further parts of the graph and with more elaborate message passing in GNN layers, we can develop models with greater expressiveness.

These networks have the drawback that nodes located far apart in the graph may not be able to transfer information efficiently to each other. By using the global representation of the graph (U) which is sometimes called a master node connected to all other nodes, we can build up a representation of the whole graph by passing information between them. The result is a richer and more complex representation than could ordinarily be obtained by learning.

With graph data all around us, we are seeing applications of GNNs in areas such as the discovery of antibiotic (Stokes et al., 2020), the detection of fake news (Song et al., 2021), the prediction of traffic (Jiang & Luo, 2021) and the systems

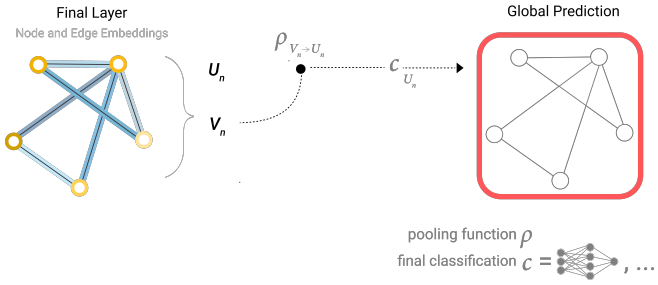

Figure 5. Node-level features to predict global property (Sanchez-Lengeling et al., 2021)

recommendation (Guo & Wang, 2021).

1.2. Dataset

Though much effort has been expended by the catalysis community to apply machine learning models to the computational catalyst discovery process, it remains a challenge to build models that can generalize across both adsorbate compositions and elemental compositions of surfaces. To address this issue, the Open Catalyst Project (OC20) released a FAIR (Wilkinson et al., 2016) dataset containing 1.2 million molecular relaxations from over 250 million DFT calculations for a wide range of materials, surfaces, and adsorbates (nitrogen, carbon, and oxygen) (Chanussot et al., 2021). The Open Catalyst Project is a collective research effort between Facebook AI Research and Department of Chemical Engineering at Carnegie Mellon to address the design of new cost-effective catalysts for renewable energy storage.

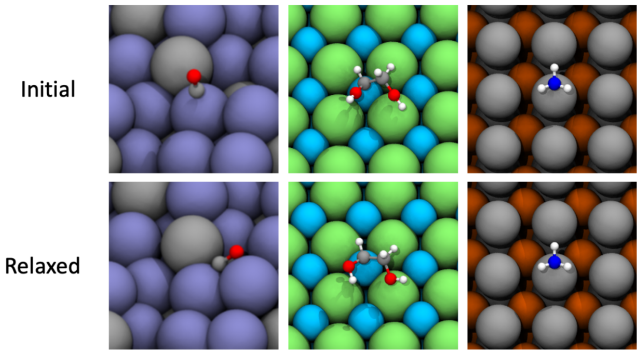

Figure 6. Example initial and relaxed structures from the OC20 dataset. Changes from initial to relaxed structures can appear to be quite small, however the changes in energy can be significant. (Chanussot et al., 2021)

We planned to implement our model using a small subset of this data and build a model to predict the energy and position

of relaxed structure given initial positions using PyTorch (Paszke et al., 2019) and the PyG (PyTorch Geometric (Fey & Lenssen, 2019)) library.

2. Experiments

2.1. Baseline Models

There are many successful models based on GNN for modeling catalysis that use advanced architectures that incorporate current machine learning algorithms and use chemical structures as inputs to predict energy, force, and position (Zitnick et al., 2020). In order to make a simple GNN model for the project, we studied two model architectures that are summarized in the following section.

CGCNN: Crystal Graph Convolutional Neural Networks for an Accurate and Interpretable Prediction of Material Properties (Xie & Grossman, 2018)
A convolutional neural network is constructed using atomic positions in crystals as nodes and bond lengths as edges on top of an undirected multigraph structure to extract representations that are optimum for predicting target properties by training on DFT calculated data. The crystal graph differs from normal graphs in that it allows multiple edges between adjacent end nodes, a characteristic of crystal graphs due to their periodicity, in contrast to molecular graphs. There are two fully connected hidden layers in addition to the convolutional and pooling layers to identify the underlying relationships between structure and property. For simplicity, they have used a normalized summation as the pooling function. Computer vision (Krizhevsky et al., 2012) and natural language processing (Collobert & Weston, 2008) also use similar architectures of GNN.

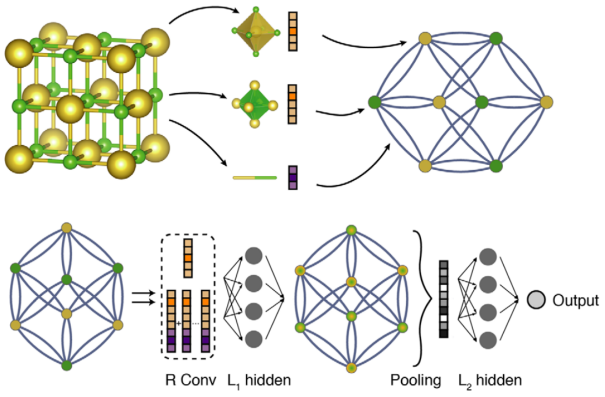

Figure 7. CGCNN model architecture (Xie & Grossman, 2018)

SchNet: A continuous-filter convolutional neural network for modeling quantum interactions
(Schütt et al., 2017)
As a means of moving beyond grid-bound data sets such as images and audio towards modeling objects with random positions such as astronomical observations or atoms in molecules and materials, SchNet proposes continuous-filter convolutional layers for deep neural networks. By making rotationally invariant force predictions as well as rotationally invariant energy predictions, this architecture specifically caters to quantum chemical constraints. Each layer represents a molecule atom-by-atom, like pixels in an image. Interactions between atoms are modeled by three interaction blocks using atom-wise layers that recombines as feature maps. The interaction blocks update the atomic representations based on the molecular geometry. In the final prediction, the feature representation is updated atom-wise atom, and energies are pooled similarly.

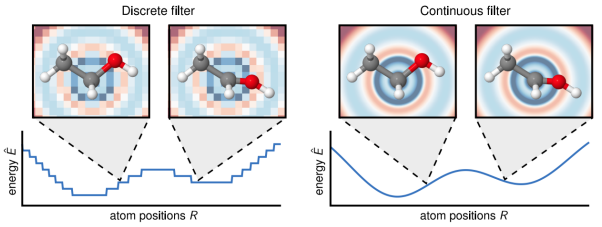

Figure 8. Discrete filter (left) is not able to capture subtle positional changes of atoms resulting in discontinuous energy predictions (bottom left). Continuous filter in SchNet captures these changes and yields smooth energy predictions (bottom right). (Schütt et al., 2017)

2.2. Our Model

The Basic Graph Convolutional Model: The first model we designed simply used the prebuilt GCNConv layer which implements a convolution over neighboring nodes for each node in a graph. That is, for each node, the data from each of the nodes connected to it by an edge is collected and pooled by some pooling function (sum, mean or max). The result is then used by some neural network layer(s) (in our case one or two linear layers) to find the updated data vector for the node. For our model specifically, because we wanted to predict the position for each atom once the whole system had relaxed, we only used the starting positions as data for each node (atom). One major issue with this method is that it utilizes very little information. In the best case, each node will learn the average position of all its neighbors and might be able to make a reasonable guess as to where it should move, but this is the most optimistic scenario. Furthermore, because we were initially using ReLU as our

activation function, values had a tendency to go to zero, meaning node positions would tend towards zero as well (we eventually started using leaky ReLU which does not set negative values to zero) . Unfortunately, a bad but easy to reach local minima is sending all nodes to (0,0,0) and this model almost always ends up at this point.

The Basic Message Passing Model: Once we knew we could make a basic GNN and that it could train properly (although not well), we determined that we would need to include more data such as bond length (distance across an edge), and atomic number, and that these attributes would be better suited to the structure message passing model. Our model uses a custom message passing layer which we implemented with another PyTorch-Geometric class which inherits from the base message passing layer. Our layer takes the atomic number embedding for two nodes connected by an edge and bond length of that edge and uses two linear layers with leaky ReLU activation to form the messages that the second node will receive. With this structure and subset of data, each node receives messages which incorporate what element it and it's neighbors are and how far away they are, leading to much more well-informed prediction.

The first message passing model performed reasonably well when compared to the previous graph convolutional model but overall it was not very accurate. While the predicted positions of the atoms were not all at the origin, they were far from where they should have been, which in most cases was very near their starting locations. We quickly realized that although we had very informative messages, we had forgotten to include the starting positions! This meant that while the atoms knew well how they should move, they had no idea where they were moving from. With this context, the performance of our first message passing model becomes much more impressive. Furthermore, once we added the initial positions as an input to the final sub model which uses the pooled messages to compute the predicted final position, the loss dropped dramatically. Now, instead of all atoms at one point or in a blob somewhat averaging their distances from each other, they were now all almost where they needed to be (which, again, is not far from where they start for most).

Embeddings and Added Information: One tool used in the CGCNN model is a set of precomputed embeddings for each atomic number. Specifically, each element has a corresponding vector of 96 1s and 0s which supposedly contains more detailed information about how they relate to each other. The CGCNN model uses a few fully connected layers to convert this large embedding (which is similar to a one-hot encoding) to an arbitrary (usually smaller) size before using the data in the message passing layers of the model. We followed the structure of the CGCNN model closely for this portion because it seemed to be a simple and effective way of giving the model more detailed information about how atoms may behave near each other. Another file provided in the GitHub for the OCP dataset that we eventually leveraged is the list of atomic radii. Again, we hoped this information would allow the message passing layers to better predict how different atoms would behave across the number of forces between them.

Global/Graph-level Data and Prediction: The task we chose from the dataset IS2RS (Initial State to Relaxed State) is closely tied to another task, IS2RE (Initial State to Relaxed Energy) and thus, our model is structured in a reasonable way to work with that task as well. Specifically, instead of (or in conjunction with) predicting the final position of each atom in a given graph once it is relaxed, one can also predict the total energy of the graph which will correspondingly be minimized if the graph is in its most relaxed state. To help with predicting final energy values, the dataset includes initial energy along with the initial positions of the atoms. We realized that our model may be more effective if we used this initial energy and took advantage of the global state of the graph to pass data over larger distances than would be reasonable with message passing (Sanchez-Lengeling et al., 2021). The final, and most complex iteration of our model takes energy information into account and is able to predict the global energy at the relaxed state.

3. Results

As briefly discussed in the previous section, we had some issues initially with training/designing our models to be accurate on the atoms that don't move at the very least. Our first model, which just used graph convolution layers (shown below) was barely able to keep atoms apart and tended to move them all to the average of their initial positions. This makes sense given that it had no other information or complex way of passing messages.

Adding embeddings of elemental information as well as the atomic radii to the most basic message passing model we made allowed it to quickly reach a base loss of about 180 which even our best model was not able to move much past. At this loss it seems that all atoms that barely move stay in their correct place, and the adsorbant molecule moves somewhat towards its correct location but again does not move much. This shows that despite the huge improvement over our more simple models, we still are not correctly predicting the most important nodes in the model.

Although there was significant increase in computational load per epoch with the addition of global energy as part of messages and as something to be predicted, our most complex model still ran into roughly the same plateau as the previous few (at around 175-180 loss). Furthermore,

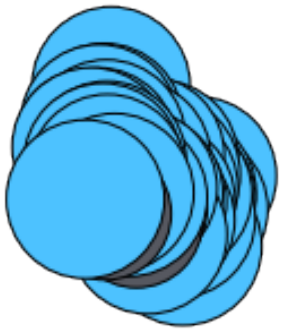

Figure 9. Predicted positions from the most simple model we designed, which only used initial positions of atoms to predict their relaxed positions.

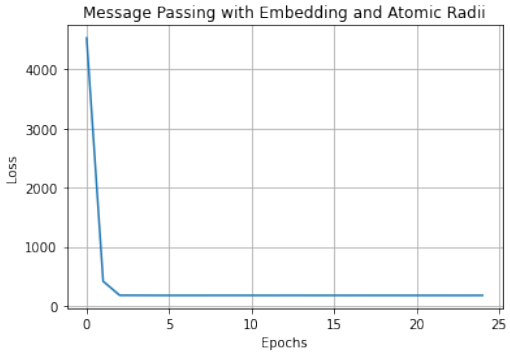

Figure 10. The loss over time of our second most complex model which included information about atomic radii but did not energy.

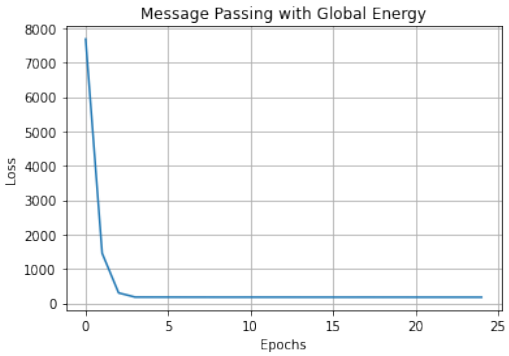

Figure 11. The loss over time of the most complex and capable model we designed which predicted global energy in the relaxed state as well as relaxed positions.

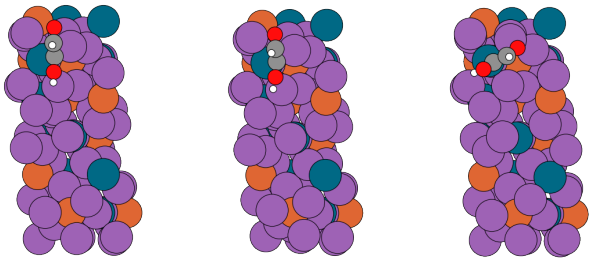

Figure 12. Initial state, predicted relaxed state, and true relaxed state generated by our second most complex model which includes information about atomic radii but does not examine or predict the energy of the system.

although there was little improvement in the loss for atom positions, we were unable to get the global energy prediction to be accurate at all. This seems to indicate that while the structure of the problem is similar between IS2RS and IS2RE, the actual final prediction task for energy might still be significantly difficult and/or predicting a global value is just a more difficult task.

As mentioned previously, the best our models could achieve in terms of positional accuracy was learning to keep most atoms in almost the same spot and only slightly moving the adsorbent molecule (typically less than needed). The plot below shows how small the difference between initial and final positions are and how, while our models were accurate for the vast majority of atoms, just a few atoms are truly important and difficult to predict.

4. Discussion

Our experiments and results show that both having access to the right data and the structure of a model play a large role in its effectiveness. The consecutive addition of messages demonstrates how the output functions are better at predicting molecular properties when we pass in the appropriate message and update. Besides, far-off interactions between nodes in the graph through a global/master node showed little impact on the overall output. It makes sense as in chemical simulations we also use a cut-off and avoid computing interactions beyond a certain distance to reduce the computational cost which later is corrected using some approximate functions.

Acknowledgements

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Code hosted here: https://github.com/CharFox1/CMSC678Project

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