Rochester Institute of Technology
RIT Digital Institutional Repository

Theses

10-2018

Meta Learning for Graph Neural Networks

Rohan N. Dhamdhere
rnd7528@rit.edu

Follow this and additional works at: https://repository.rit.edu/theses

Recommended Citation
Dhamdhere, Rohan N., "Meta Learning for Graph Neural Networks" (2018). Thesis. Rochester Institute of Technology. Accessed from

This Thesis is brought to you for free and open access by the RIT Libraries. For more information, please contact repository@rit.edu.

Meta Learning for Graph Neural Networks

By

Rohan N. Dhamdhere

October 2018

A Thesis Submitted
in Partial Fulfillment
of the Requirements for the Degree of
Master of Science
in
Computer Engineering

Committee Approval:

Dr. Raymond Ptucha, *Advisor* Date
Assistant Professor

Dr. Andres Kwasinski, *Committee Member* Date
Professor

Dr. Ifeoma Nwogu, *Committee Member* Date
Assistant Professor

R·I·T | KATE GLEASON College of ENGINEERING

Department of Computer Engineering

Acknowledgments

This thesis work is the culmination of an important period of my life. I would like to take this opportunity to thank my advisor Dr. Raymond Ptucha for his continual support and guidance during my master's degree. I am thankful for Dr. Kwasinski and Dr. Nwogu for being in my thesis committee. I would like to give a personal thank you to Miguel Dominguez for getting me involved in the fun research work that is Graph CNNs. I would also like to thank my family and my close friends, without their support this journey would not have been as easy as it was. My time here at RIT was one that I shall remember a long time and would like to thank everyone who made it special.

I dedicate this work to my father, my mother and my sister. For they always supported me in my quest for excellence.

"Somewhere, something incredible is waiting to be known."

- Carl Sagan

Abstract

Deep learning has enabled incredible advances in pattern recognition such as the fields of computer vision and natural language processing. One of the most successful areas of deep learning is Convolutional Neural Networks (CNNs). CNNs have helped improve performance on many difficult video and image understanding tasks but are restricted to dense gridded structures. Further, designing their architectures can be challenging, even for image classification problems. The recently introduced graph CNNs can work on both dense gridded structures as well as generic graphs. Graph CNNs have been performing at par with traditional CNNs on tasks such as point cloud classification and segmentation, protein classification and image classification, while reducing the complexity of the network.

Graph CNNs provide an extra challenge in designing architectures due to more complex weight and filter visualization of generic graphs. Designing neural network architectures, yielding optimal performance, is a laborious and rigorous process. Hyperparameter tuning is essential for achieving state of the art results using specific architectures. Using a rich suite of predefined mutations, evolutionary algorithms have had success in delivering a high-quality population from a low-quality starter population. This thesis research formulates the graph CNN architecture design as an evolutionary search problem to generate a high-quality population of graph CNN model architectures for classification tasks on benchmark datasets.

Contents

Meta Learning for Graph Neural Networks....1
Contents....5
List of Figures....7
List of Tables....9
Acronyms....10
Chapter 1: Introduction....11
1.1 Introduction....11
1.2 Motivation....12
1.3 Contributions....13
Chapter 2: Background....14
2.1 Deep Learning....14
2.2 Convolutional Neural Networks....14
2.3 Graph-Convolutional Neural Networks....15
A. Spectral Approaches....*16*
B. Spatial Approaches....*17*
2.4 Meta Learning for Architecture search....20
Chapter 3: Methodology....23
3.1 Graph Convolutional Neural Networks....23
A. Graph Convolution....*24*
B. Graph Pooling....*27*
3.2 Architecture Search using Evolutionary Algorithm....30
A. Mutations for Evolutionary Algorithm....*31*
B. Fitness Score....*36*
C. Evolutionary Algorithm for Architecture Search....*36*
D. Features of Evolutionary Algorithm....*38*
Chapter 4: Implementation....40
4.1 Datasets....40
A. Enzymes....*40*
B. MUTAG....*40*
4.2 Implementation....41
A. Basic Implementation....*41*

B. Parallel Implementation *42*
C. Saving and Loading Best model *42*
Chapter 5: Results and Analysis 45
5.1 Results 45
A. Comparisons with Other methods *45*
B. Comparisons with Manual method *48*
C. Model Architectures *48*
5.2 Analysis 50
A. Mutation Probability Analysis *50*
B. Weight Loading Analysis *51*
C. Mutation analysis *53*
D. Hyperparameter reduction *55*
Chapter 6: Conclusions and Discussions 57
6.1 Conclusions 57
6.2 Discussions 57
6.3 Future works 58
Bibliography 59

List of Figures

Figure 2.2.1: *A 2D convolution operation [33].* 15

Figure 2.3.1: *The PATCHY-SAN algorithm used to find fixed size vector representations of the graph. [18]* 18

Figure.2.3.2: *Graph CNN proposed by FeaStNet [29], where each node in the input patch is associated in a soft manner to each of the M weight matrices based on its features using the weight $q_m x_i, x_j$. [29]* 19

Figure 2.4.1: *The XOR problem and solutions based on genetic search methods. [10]* 20

Figure 2.4.2: *Evolutionary algorithm proposed by Suganuma et al. [1]* 22

Figure 3.1.1: *An example graph and the corresponding vertex matrix and adjacency matrix.* 24

Figure 3.1.2: *(a) Learnable parameters in 1-hop graph filters. (b) Classical 3×3 convolution filters. (c) Illustration of eight different edge connections combined to form a 3 × 3 filter. [22].* 26

Figure 3.1.3: *(a) and (c) show the original 3D mesh graph of chair. (b) shows the 3Dmesh graph after Lloyd pooling. (d) shows the 3D mesh graph after Graph embed pooling. It can be inferred that graph embed pooling is a dense pooling method. [14]* 30

Figure 3.2.1: *Graph convolution layer mutation.* 31

Figure 3.2.2: *Fully-connected layer mutation.* 31

Figure 3.2.3: *One-by-one graph convolution layer mutation.* 32

Figure 3.2.4: *Graph attention layer mutation.* 33

Figure 3.2.5: *Skip connection mutation.* 33

Figure 3.2.6: *Lloyd pooling mutation.* 33

Figure 3.2.7: *Graph embed pooling mutation.* 34

Figure 3.2.8: *Reduced max pooling mutation.* 34

Figure 3.2.9: *The flow diagram of Test-and-Mutate algorithm.* 37

Figure 3.2.10: *The flow diagram of Test-and-Mutate-with-Probability algorithm.* 38
Figure 4.2.1: *Loss explosion within training of a fold of an architecture.* 43
Figure 5.1.1: *Model evolution over cycles for **(a)** Mutag dataset and **(b)** Enzymes dataset.* 47
Figure 5.1.2: (a) *Best architecture designed manually. **(b)** Best architecture generated by evolution.* 49
Figure 5.1.3: (a)*Best architecture designed manually. **(b)** Top architectures generated by evolution.* 50
Figure 5.2.1: *Top row (Fig. **(a)**, **(b)**) are experiments with no probability associated with mutations (baseline algorithm). Bottom row (Fig. **(c)**, **(d)**) are experiments with probabilities associated with mutations.* 51
Figure 5.2.2: *This figure emphasizes the importance of weight loading. Fig. **(a)** is based on experiment which involved no weight loading, Fig **(b)** is based on experiment with weight loading.* 53
Figure 5.2.3: *Evolution of different mutations' probability over cycles. **(a)** shows the 'add' mutations and their probability change over cycles. **(b)** shows the 'remove' mutations and their probability change over cycles. **(c)** shows the pooling and parameter mutations and their change over cycles. All these figures show the importance of a mutation within the cycle period.* 55

List of Tables

Table 4.1: *Summary of protein datasets to be used in this thesis. 41*
Table 5.1.1: *10-fold cross validation accuracy score comparisons between different methods.. 46*
Table 5.1.2: *Comparison of running times and best accuracy scores between manual and evolutionary approaches. 49*

Acronyms

CNNs

Convolutional Neural networks

Graph-CNNs

Graph Convolutional Neural Networks

MLP

Multi-layer Perceptron

Chapter 1

Introduction

1.1 Introduction

Neural networks can successfully execute challenging tasks when provided with abundant data along with sizable computational resources. Convolutional Neural Networks (CNNs) have broken traditional computer vision barriers and achieved high quality results on image classification and segmentation tasks [7, 8, 19]. CNNs are helping deep learning get embedded into newer fields every day. CNNs have the ability to simultaneously automate the process of feature extraction and classification. This ability of CNNs is helping them beat other machine learning algorithms at several tasks.

CNNs are highly successful in tasks involving data represented in discrete gridded structures such as image, videos etc. Unstructured data (e.g.: 3D Point clouds or 3D meshes [26, 27]) or data that cannot be represented in such gridded structures (e.g.: Protein graphs [21, 24, 25]) cannot be filtered by conventional convolution operations, and therefore CNNs have enjoyed very little success in tasks involving such data. Most unstructured data can easily be processed into graphs. This has led to the development of different convolutional operators for graph data and has led to the research field of Graph CNNs [12, 14, 18, 22].

Graph CNNs have shown comparable to state-of-the-art performances on classification tasks of protein graphs, 3D point clouds and images [12, 14]. They have also performed well on image and 3D segmentation tasks [29] as well as classification of functional MRIs of brain [28]. With graph CNNs, Convolutional Neural Networks can now be applied to a wide range of data and applications.

Although CNNs can automatically extract and perform classification of features, they need precise hyperparameters and optimal architectures to achieve high accuracy and precision. Solving for hyperparameters and designing architectures are typically done by a human expert. This is a laborious process and requires high amount of focus and experience. Designing CNN architectures is a tough task even for image data where visualization of weights and filters aid the process of design. Graph CNNs work on unstructured data which are converted to graphs. Visualizations of weights and filters of graph CNNs inform abstract knowledge about the data. Due to the difficulty of weight visualization, the process of designing graph CNNs is extra challenging compared to conventional CNNs.

Research to automate the process of neural network design has been going on for few decades with early work being related to automating Multi-Layer Perceptron (MLP) based neural network design [2, 3, 10, 13]. In recent years, many approaches like reinforcement learning [30, 31], genetic algorithms [6] and evolutionary algorithms [1,17] have been used to automate the process CNN architecture design and hyperparameter search. This process has had some success on standard image datasets like CIFAR [32]. This work attempts automate the process of graph CNN architecture design and hyperparameter search using evolutionary algorithms for the classification of protein graph structures.

1.2 Motivation

Designing of any neural network is laborious process. After designing, tuning of hyperparameters is another time-consuming task. This work is an extension of previous work which was done for classification of protein graphs by designing custom graph CNNs manually. The difficulty of the previous research motivated the automation of various parameters required for graph CNN design. Also, this work is a feasibility check on whether evolutionary algorithms are able to generalize over different datasets and find top performing architectures tailored for specific datasets.

Many other works on automation of CNN architecture design use abundant computing resources. This work attempts to find out if evolutionary search for architecture design can be done in environments with limited computational resources

and what are the modifications required to make the algorithm more computationally efficient. Discovering tangible answers to the above mentioned problems related architecture design is the main motivation for this work.

1.3 Contributions

The main contributions of this thesis work can be summarized as:

- An evolutionary algorithm for graph CNNs based on probabilistic mutation strategy.
- Achieve better than human performance on benchmark protein datasets using same graph CNN method.
- Parallel implementation of cross validation evaluation for evolution of models.
- Selective loading of weights based on layers present in previous architectures.
- Saving and loading of best trained models using training loss for boosting performance.

Chapter 2

Background

2.1 Deep Learning

Deep Learning has provided breakthrough research results in many fields. Deep learning network's ability to extract its own features for classification has provided it an edge over other machine learning techniques. It has especially helped computer vision research by providing better feature descriptors than traditional computer vision features like HoG, SIFT etc. [46, 47]. Also, it has reduced the feature designer's bias introduced in the extracted features. All these merits have resulted in deep neural networks being the method of choice for feature extraction along with MLP classifiers.

2.2 Convolutional Neural Networks

Much of the success achieved by deep learning can be attributed to CNNs. CNN architectures have performed exceptionally well on tasks related to image or video data classification and understanding [7, 8, 19]. CNNs extend the capabilities of MLPs while keeping a similar number of parameters. CNNs make use of localized information by using a common filter over the full input. Parameter sharing over different regions of the input results in sharing of localized features. A CNN layer can be defined as in (2.2.1), where $V^{l}_{(i,j,c)}$ contains pixel information for the layer *l* of the network, for pixel *i, j* at the cth channel, where channel is the third dimension of the image volume. Here, at any layer, image volume ***V*** is convolved with a convolutional filter volume ***W*** to get convolved image volume ***V***.

$$V^{l}_{(i,j,k)} = W_{abc} V^{l-1}_{(\mathrm{i+a,j+b,c})} \tag{2.2.1}$$

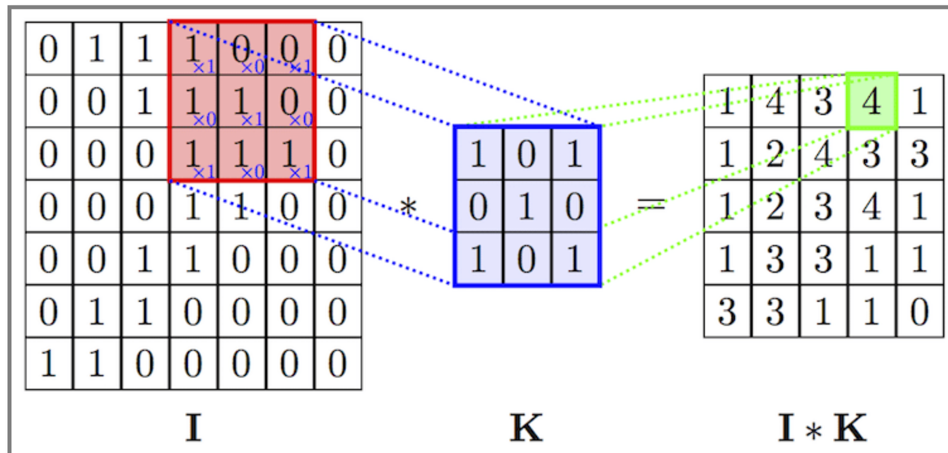


Figure 2.2.1: A 2D convolution operation [33].

Much power of CNNs is derived from the common set of parameters shared over different inputs. Their limitation is that the input needs to be gridded with fixed neighbors. Graph Convolutional Neural Networks (Graph CNNs) remove this limitation using Graph-based Convolution operation.

2.3 Graph-Convolutional Neural Networks

Research to broaden the extent of neural networks to graph structured data has had substantial success in recent times. A graph *G* is represented using a tuple (*V, A*) - vertices *V* and adjacency matrix *A*. The adjacency matrix entries can be defined as in (2.3.1).

$$a_{ij} = \begin{cases} w_{ij}, & if\ there\ is\ an\ edge\ between\ i\ and\ j \\ 0, & otherwise \end{cases} \tag{2.3.1}$$

The scalar w_{ij} is a weight that represents some measure of strength of the edge between vertex *i* and vertex *j*. The research of graph convolutional networks follows two broad general approaches to generalizing CNNs to graph data: spectral and spatial.

A. Spectral Approaches

Spectral approaches use spectral graph theory. Spectral graph theory works in the spectral domain by constructing a filter based on the eigenvector decomposition of the Graph Laplacian *L* shown in (2.3.2).

$$L = D - A \tag{2.3.2}$$

$$L = I - D^{-1/2} A D^{-1/2} \tag{2.3.3}$$

L can be normalized as shown in (2.3.3), where *A* is the adjacency matrix of the graph, *D* is the diagonal degree matrix and *I* is the identity matrix. *L* can be used to compute an eigenbasis *U*. This eigenbasis *U* is similar to the Discrete Fourier Transform (DFT). A graph signal *x* can be transformed into spectral domain and multiplying each frequency by a filter *h*, to get its filtered output in spectral domain. This is illustrated in (2.3.4), where ⊙ is the elementwise product and '.' represents the matrix multiplication.

$$x * h = U^T . (Ux \odot h) \tag{2.3.4}$$

Thus, the filtering operation in the spectral domain is performed multiplying filter coefficients with spectrally transformed graph signals. Many works propose graph CNN models based on this method of filtering [34, 35, 37]. One of the major practical limitations of spectral domain-based learning of filters is the necessity of input graph samples to be homogenous for converting graphs to Laplacian matrix. This is necessary as the eigenbasis of the Graph Laplacian needs to be solved separately for every unique graph structure. Most spectral works tend to focus on experiments where there is a single graph structure common across all samples, like a single large social network graph. Spatial approaches are advantaged over spectral methods in that they can filter graphs, without the graphs being homogenous.

B. Spatial Approaches

To achieve better generalization across graphs, various works follow a local neighborhood graph filtering strategy. They generally require advanced data preprocessing techniques for learning to process neighborhoods that are different sizes and structures for each vertex. These methods differ in how they find a correspondence between filter weights and nodes in local graph neighborhoods.

Bruna et al. [38] assumed fixed graph structure and does not share weights among neighborhoods. Duvenaud et al. [39] sums the signal over neighboring vertices followed by a weight matrix multiplication, effectively sharing the same weights among all edges. Diffusion Convolutional Neural Networks (DCNNs) [40] arrange vertex features based on sequence of hops from different starting vertices to encode a graph into matrix layers.

Similar to Petroski Such et al. [5], DCNNs use polynomials of the adjacency matrix to define convolutional filters. They also use global vertex mean pooling to obtain a vector representation of the graph. The diffusion process of DCNNs is shown in (2.3.5), where Z_t is the output feature vector for the vertices on the graph G_t , f is the activation function, W_c is a learnable weight-matrix, P_t^* is a degree-normalized polynomial of the adjacency matrix A_t , and X_t is the input feature vector for the vertices on the graph G_t. ($\odot$ is the elementwise product)

$$Z_t = f(W^c \odot P_t^* X_t) \tag{2.3.5}$$

Niepert et al. [18] rely on a heuristic ordering of the nodes, and then apply 1D CNNs. They linearize the graphs using a method called PATCHY-SAN. Using graph search algorithms, PATCHY-SAN attempts to obtain fixed size feature vector representation of the graph. An illustration of PATCHY-SAN is shown in Figure 2.3.1.

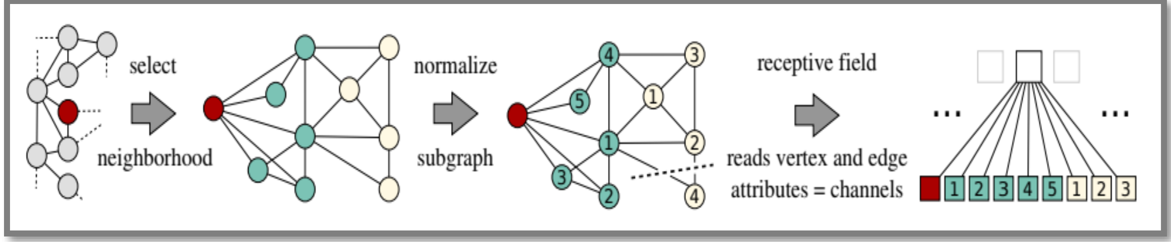


Figure 2.3.1: *The PATCHY-SAN algorithm used to find fixed size vector representations of the graph. [18]*

Simonovsky et al. [12] generate conditioned filter weights for edge labels. These weights are generated dynamically for every input to the graph. This edge conditioned convolution operation is given in (2.3.6), where $X^l(i)$ is the current layer signal to be computed, *N(i)* is the neighborhood of vertex *i*, θ_{ji}^l is the edge-weight matrix, $X^{l-1}(j)$ is the previous layer signal and b^l is the learnable bias. The edge-weights θ_{ji}^l are given as per (2.3.7), where *L(j, i)* is the given class label. F^l is parameterized with learnable network weights w^l. The model parameters w^l and b^l update during training and dynamically generate θ_{ji}^l for an edge label in input graph.

$$X^l(i) = \frac{1}{|N(i)|} \sum_{j \in N(i)} \theta_{ji}^l \, X^{l-1}(j) + b^l \qquad (2.3.6)$$

$$\theta_{ji}^l = F^l(L(j,i); w^l) \qquad (2.3.7)$$

The main challenge in the case of irregular data graphs is to define the correspondence between neighbors and weight matrices. FeaStNet [29] proposes to establish this correspondence in a data-driven manner, using a function over features computed in the preceding layer of the network, and learning the parameters of this function as a part of the network. They propose a similar approach to [12]. Instead of assigning each neighbor *j* of a node *i* to a single weight matrix, we use a soft-assignment $q_m(x_i, x_j)$ of the *j*-th neighbor across all the M weight matrices. The activation $y_i \in \mathbb{R}^E$ of pixel *i* in the output feature map using the soft assignments is defined as in (2.3.8), where *b* ∈ $\mathbb{R}^E$ is the vector of bias terms, $q_m(x_i, x_j)$ is the

assignment of x_i to the *m*-th weight matrix, and $\mathcal{N}_i$ is the set of neighbors of *i* (including *i*), and $|\mathcal{N}_i|$ its cardinal.

$$y_i = b + \sum_{m=1}^{M} \frac{1}{|\mathcal{N}_i|} \sum_{j \in \mathcal{N}_i} q_m(x_i, x_j) W_m x_j \qquad (2.3.8)$$

They use Mahalanolbis distance based soft assignment in feature space to determine local filters dynamically based on previous layers of the network. Their approach is illustrated in Figure 2.3.2.

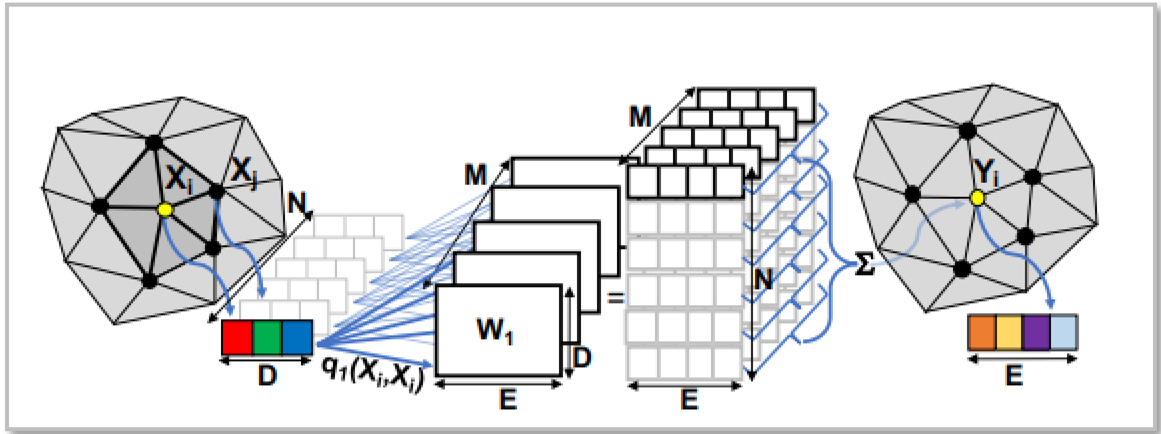


***Figure.2.3.2**: Graph CNN proposed by FeaStNet [29], where each node in the input patch is associated in a soft manner to each of the M weight matrices based on its features using the weight $q_m(x_i, x_j)$. [29]*

Similar to earlier mentioned spatial methods, Such et. al. [22] use local edge features for graph convolution, done by convolving on adjacency matrix of the graph. They introduce vertex graph filters helping to learn on both graph vertex and edges simultaneously. Pooling in traditional CNNs helps to increase the receptive field of the filter and thereby helps to learn higher order features. They introduce pooling for graphs which is further explored by Dominguez et. al [14] to provide deep graph networks for 3D point cloud classification.

In this thesis work, graph convolution and pooling operations introduced in Such et. al. [22] and Dominguez et. al. [14] are used as the base operations for building neural network architectures in the process of architecture search for graph CNNs.

2.4 Meta Learning for Architecture search

CNNs architectures have been able to achieve state-of-the-art performance on a variety of tasks. There are many popular architectures, each of which can be used on a broad variety of data. For example, AlexNet, VggNet, ResNet, DenseNet [7, 9, 41, 42] are popular CNN architectures available for users to develop a neural network based prediction model for the user defined task. Each of these architectures were manually designed by expert humans. These designers leverage their in-depth knowledge about CNN training and optimization to define these architectures.

These popular architectures are flexible and generalize well to a variety of data but often need optimized hyperparameter tuning or custom architecture modifications for good performance. This process of designing neural network architectures is arduous and requires focused human attention. Also, hyperparameter tuning is time consuming and tedious.

Research to automate the design of neural networks has a long but sporadic history. Miller et al. [10] used genetic-search based methods to evolve MLP based neural networks to automate the task of network design. Initially, the evolution was only restricted to only evolving weights of static architectures. They were successful to solve the XOR problem, a big test at the time and Figure 2.3.1 shows some of the evolved architectures for the same.

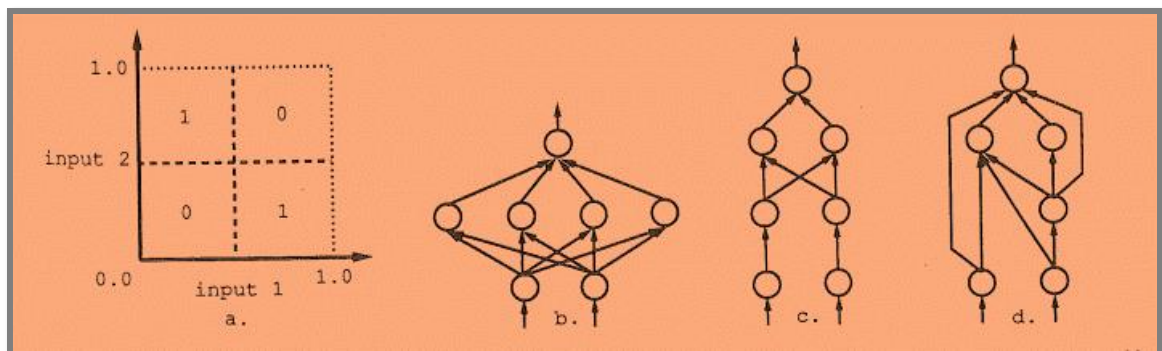


Figure 2.4.1: *The XOR problem and solutions based on genetic search methods. [10]*

“Evolving Neural Networks through Augmenting Topologies” [13] did simultaneous adaption of weights and architectures. They defined basic mutations for evolution:

i. Modify a weight.
ii. Add a connection between existing nodes.
iii. Insert node while splitting existing connection.

These evolutionary algorithms are not sufficient for deep neural networks. Current research directions focus on reinforcement learning and evolutionary strategies for the solving the neural architecture search problem. Both these directions have focused on allowing building of CNN architectures resembling those designed manually by humans.

Reinforcement learning based approaches have been able to achieve more success on real-world image data related classification tasks. Most reinforcement learning based approaches use indirect encoding schemes for network representation. Zoph et al. [31] used reinforcement learning on a deeper fixed-length architecture, adding one layer at a time. Their mutations included addition/removal of skip connections as well as tunable hyperparameters. Baker et al. [30] used Q-learning to discover networks. They made architectures more flexible by allowing the algorithms to decide the number of layers in the network. This allows the network to adapt to the dataset at hand and construct shallow or deep solutions as necessary.

Progressing from earlier works, evolutionary approaches later combined with back-propagation [1, 17, 43] to evolve architectures and tune hyperparameters simultaneously. These approaches introduce architectural mutations and weight back-propagation. More recent approaches [43] added weight inheritance for architectures. Suganuma et al. [1] use a direct encoding type approach using Cartesian Genetic Programming (CGP) [44] for their evolutionary process as shown in Figure 2.3.2. They define functional blocks such as ConvBlock, ResBlock etc. as functional blocks or nodes and do point mutation as in standard CGP.

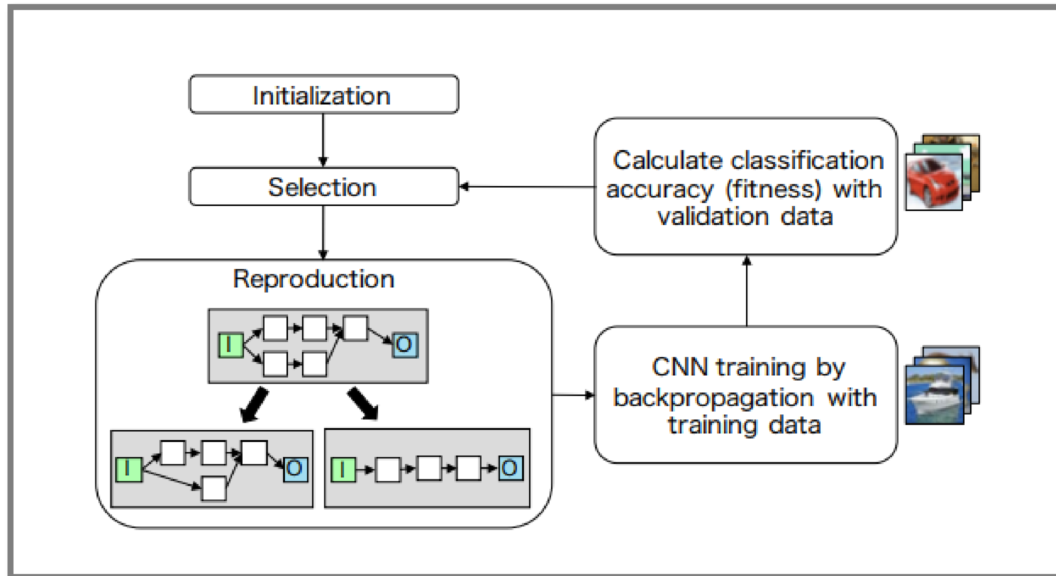


Figure 2.4.2: *Evolutionary algorithm proposed by Suganuma et al. [1]*

This work is uses evolutionary approaches similar to Real et al. [17] and Graph CNN defined by Dominguez et. al. [14] as the base model and built an evolutionary algorithm based approach for architecture search for Graph CNNs.

Chapter 3

Methodology

3.1 Graph Convolutional Neural Networks

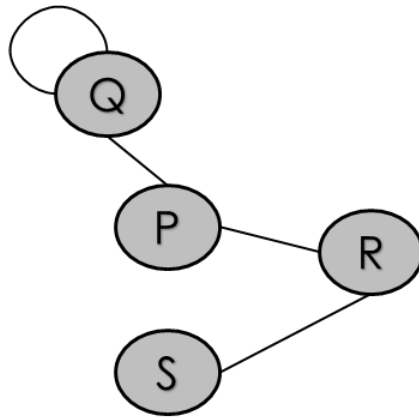
A Graph can be decomposed into two main elements, the graph vertices v_{ij} and graph edges a_{ij}. A graph signal can be represented as a tuple described in (3.1.1)

$$\boldsymbol{G} = (\boldsymbol{V}, \boldsymbol{A}) \tag{3.1.1}$$

where $\boldsymbol{V} \epsilon \mathbb{R}^{N \times f}$ is the vertex signal matrix describing N vertices with f features each. $\boldsymbol{A} \epsilon \mathbb{R}^{N \times N}$ represents the adjacency matrix which encodes the edge information with its elements as defined Chapter 2. Each entry in $\boldsymbol{A}$ is defined as per (3.1.2) previously defined in (2.3.1),

$$a_{ij} = \begin{cases} w_{ij}, & if\ there\ is\ an\ edge\ between\ i\ and\ j \\ 0, & otherwise \end{cases} \tag{3.1.2}$$

An Illustration of the graph and its corresponding vertex matrix ***V*** and adjacency matrix ***A*** is shown in Figure 3.1.1.



V = [P, Q, R, S]

A =

	P	Q	R	S
P	0	1	1	0
Q	1	1	0	0
R	1	0	0	1
S	0	0	1	0

Figure 3.1.1: *An example graph and the corresponding vertex matrix and adjacency matrix.*

A. Graph Convolution

Graph data can succinctly represent information in both vertices and edges. To process and learn the information, the convolution filtering technique for graphs must account for filtering both vertex information and edge information. This work uses the Graph convolution model proposed by Such et al. [22]. This is a spatial approach related graph convolution method following the local neighborhood graph filtering strategy. The graph convolution operation is based on the polynomials of the graph adjacency matrix and is similar to the convolution defined by Sandryhaila et al. [36] as in (3.1.3).

$$H = h_0 I + h_1 A^1 + h_2 A^2 + h_3 A^3 + \cdots + h_k A^k \tag{3.1.3}$$

The filter is defined as the kth-degree polynomial of the graph's adjacency matrix. The exponent of polynomial encodes the number of hops from a given vertex that are being multiplied by the given filter tap. The scalar coefficients h_i control the contribution of the neighbors of a vertex during the convolution operation. The filter matrix thus obtained is $H \in \mathbb{R}^{N \times N}$. To convolve the vertices V with the filter H is a matrix multiplication shown in (3.1.4), where $V_{out}, V_{in} \in \mathbb{R}^{N}$.

$$V_{out} = HV_{in} \tag{3.1.4}$$

Such et al. [22] adjust this model in three ways. First, they avoid the exponentiated ***A*** and simplify the polynomial of adjacency in (3.1.3) to be linear as shown in (3.1.5). This is done because a cascade of filters can effectively approximate the receptive field of a single large filter as shown by VGGNet [41].

$$H \approx h_0 I + h_1 A \tag{3.1.5}$$

Second, they construct an adjacency tensor $\boldsymbol{\mathcal{A}}$. This tensor contains multiple adjacency matrices $\boldsymbol{\mathcal{A}_\ell}$ as the slices of adjacency tensor. Each slice encodes a particular edge feature and thus the linear filter matrix from (3.1.5) is defined as a convex combination of each adjacency matrix as in (3.1.6) and concisely as in (3.1.7).

$$H = h_0 I + h_1 A_1 + h_2 A_2 + \cdots + h_L A_{L-1} \tag{3.1.6}$$

$$H \approx \sum_{\ell=0}^{L} h_\ell A_\ell \tag{3.1.7}$$

Multiple adjacency matrices encode multiple edge features, each encoding a single feature. Also, partitioning the edges into multiple matrices conveys a sense of direction. This is illustrated in Figure 3.1.2. The Figure 3.1.2(a) is an illustration of the

default Graph CNN linear filter in an image application. A given filter tap is applied to all vertices of a given distance, isotropically (no sense of 'direction'). In this case, h_0 is applied to the 0-hop vertex and h_1 is applied to all adjacent vertices. If another border of pixels surrounded this figure, each pixel in that border would be multiplied by a filter tap h_2.

The Figure 3.1.2(c) shows that the adjacency matrix can be partitioned into nine adjacency matrices to form an adjacency tensor. Each partitioned adjacency matrix represents a different relative connection (edge feature) to a given vertex. Now a unique filter is applied to every adjacency matrix and aggregated to perform convolution. This induces a sense of direction into the Graph CNN filter making it anisotropic. This is equivalent to a 3 x 3 FIR filter in conventional CNN applications (Figure 3.1.2(b)).

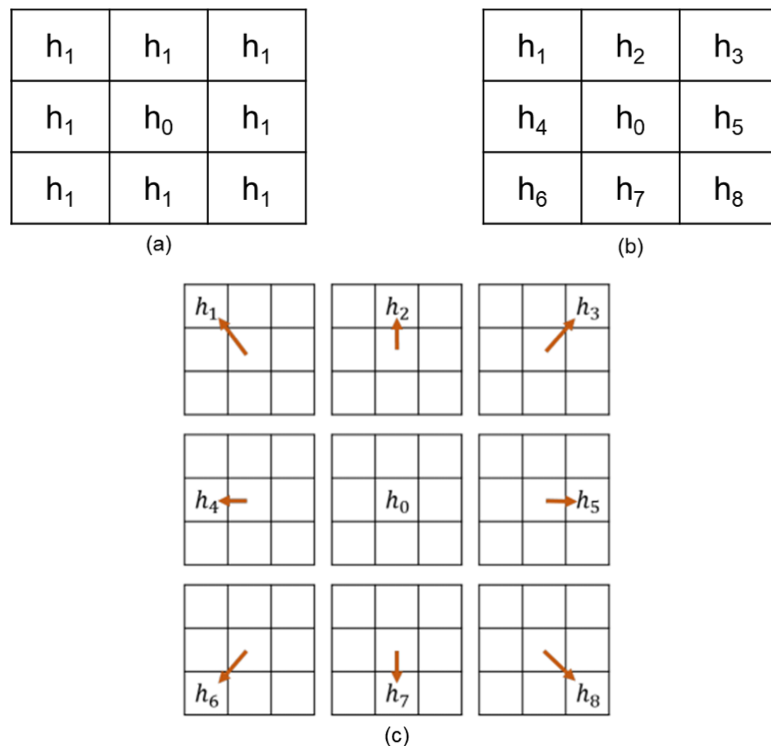


Figure 3.1.2: *(a) Learnable parameters in 1-hop graph filters. (b) Classical 3×3 convolution filters. (c) Illustration of eight different edge connections combined to form a 3 × 3 filter. [22]*

All these filters are described for a single vertex feature. To extend to multiple vertex features, each h_ℓ needs to be in $\mathbb{R}^C$ making ***H*** of dimension $\mathbb{R}^{N \times N \times C}$. Thus, every vertex feature has a *N* * *N* filter matrix ***H***. So (3.1.7) can be modified as in (3.1.8) where $H^{(c)}$ is an *N* * *N* slice of ***H*** and $\boldsymbol{h}^{(c)}$ ` is a scalar corresponding to a given input feature and a given slice of A_ℓ.

$$H^{(c)} \approx \sum_{\ell=0}^{L} h_\ell^{(c)} A_\ell \qquad (3.1.8)$$

The vertex signal is filtered using the $H^{(c)}$ as described in (3.1.9) where $V_{in}^{(c)}$ is the column of V_{in} that only contains vertex feature *c*. We also add a bias *b* ∈ ℝ. This results in $V_{in} \in \mathbb{R}^N$.

$$V_{out} = \sum_{c=1}^{C} H^{(c)} V_{in}^{(c)} + b \qquad (3.1.9)$$

This is how graph convolution is defined on a graph with multiple vertex features and edge features by Such et al. [22]. This approach is used for this thesis work.

B. Graph Pooling

The pooling operation can be dissected in two parts: the coarsening of structure and the reduction of signal on that structure. In grid structures such as images, the coarsening of structure is implicitly understood. But for graphs, such as protein structures, every sample can have a unique structure. Dominguez et al. [14] defined various pooling frameworks for graphs. These will be described here in succession. The first method they proposed is Lloyd Algebraic graph pooling on graphs that can do both signal reduction and graph coarsening.

a. <u>Lloyd Algebraic graph pooling:</u>

In this, a coarsening operator ***P*** is defined to reduce the Graph ***G = (V,A)*** with N_1 vertices to $\boldsymbol{G^{reduced}} = (\boldsymbol{V^{reduced}}, \boldsymbol{A^{reduced}})$ with N_2 vertices. ***P*** is a $N_1 \times N_2$ matrix with its elements defined as in (3.1.10).

$$\boldsymbol{P_{ij}} = \begin{cases} C, & if\ i^{th}\ vertex\ of\ \boldsymbol{G}\ is\ used\ to \\ & define\ the\ j^{th} of\ \boldsymbol{G^{reduced}}. \\ 0, & otherwise \end{cases} \tag{3.1.10}$$

C is determined by mapping the graph clustering method used in mapping “fine” vertices to the “coarsen” vertices. Distances are calculated by finding the shortest path on a graph using the Bellman Ford algorithm. Using the coarsening operator ***P***, $\boldsymbol{A^{reduced}}$ is defined using (3.1.11) and $\boldsymbol{V^{reduced}}$ is defined using (3.1.12) through (3.1.14). Sum, average, and max pooling are defined using (3.1.12), (3.1.13), and (3.1.14) respectively.

$$A^{reduced} = P^T A P \tag{3.1.11}$$

$$V_{sum}^{reduced} = P^T(V) \tag{3.1.12}$$

$$V_{avg}^{reduced} = P^{\wedge T}(V) \tag{3.1.13}$$

$$V_{max}^{reduced} = \phi_P(V) \tag{3.1.14}$$

Element $\boldsymbol{A_{i,j}^{reduced}}$ can be thought of as the aggregation of all the weights of edges while coarsening the graph *G to* $\boldsymbol{G^{reduced}}$. $\boldsymbol{P^{\wedge T}}$ is the column-sum normalized version of P. Also, ϕ_P is a non-linear max pooling function. Here in this work we used only max pooling. Thus, the graph structure is reduced by (3.1.11) and the graph signal is reduced by (3.1.14).

b. <u>Graph Embed Pooling:</u>

Such et al. [5, 22] introduced graph embed pooling for graphs. It is a dense pooling method but fits the structure of Algebraic pooling. Graph embed pooling learns a fully connected layer whose output is treated as an embedding matrix that produces a fixed size output. To produce a pooled graph reduced to a fixed *N'* vertices, the learned filter taps from this pooling layer produce an embedding matrix $V_{emb} \in \mathbb{R}^{N \times N'}$. Like in (3.1.9), a filter tensor $H_{emb} \in \mathbb{R}^{N \times N \times C \times N'}$ is learned and multiplied by the vertices to produce a filtered output as shown in (3.1.15).

$$V_{emb}^{(n')} = \sum_{c=1}^{C} H_{emb}^{(c,n')} V_{in}^{(c)} + b \quad (3.1.15)$$

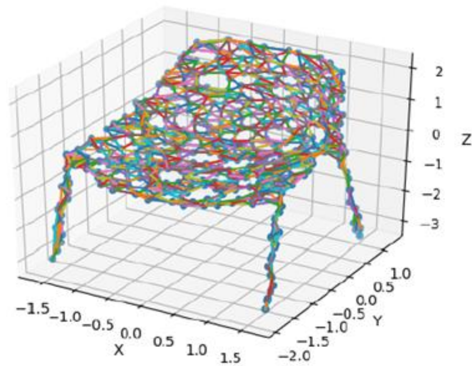
$V_{emb}^{(n')}$ is column wise stacked up to form the matrix V_{emb}. Softmax function is used for normalization of values of V_{emb} as in (3.1.16). Equations (3.1.17) and (3.1.18) show how V_{emb} pools the graph data.

$$V_{emb}^{*} = \sigma(V_{emb}) \quad (3.1.16)$$

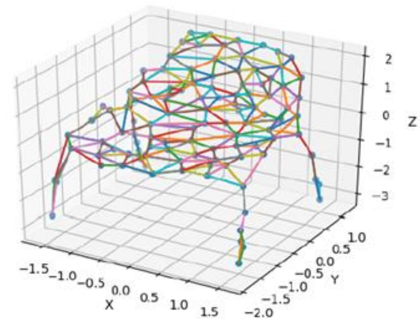
$$V_{out} = V_{emb}^{*T} V_{in} \quad (3.1.17)$$

$$A_{out} = V_{emb}^{*T} A_{in} V_{emb}^{*} \quad (3.1.18)$$

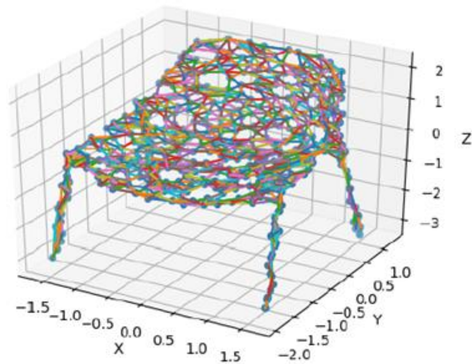
The above equations represent the graph embed pooling defined by Such et al. [22] and Dominguez et al. [14]. Figure 3.1.3 illustrates both the graph pooling methods used as mutations in architecture selection task.



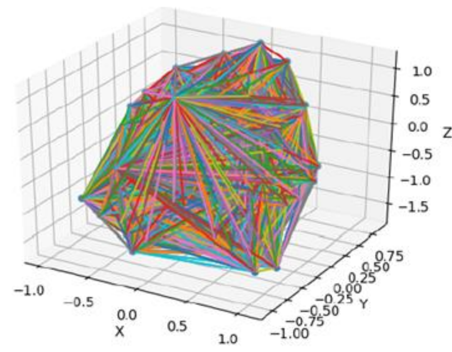
(a) Original



(b) Lloyd



(c) Original



(d) Graph embed

Figure 3.1.3: *(a) and (c) show the original 3D mesh graph of chair. (b) shows the 3Dmesh graph after Lloyd pooling. (d) shows the 3D mesh graph after Graph embed pooling. It can be inferred that graph embed pooling is a dense pooling method. [14]*

3.2 Architecture Search using Evolutionary Algorithm

This work uses evolutionary algorithms for searching architectures in graph convolution neural networks. A set of mutations are defined which the architectures can choose to improve their fitness scores and maximize the fitness function. Added features of the evolutionary algorithm help in speeding up the architecture search while achieving good fitness scores. This section explains in detail the evolutionary algorithm and the its features.

A. Mutations for Evolutionary Algorithm

For architecture search using evolutionary methods, it is important to define mutations that can find improved architectures or hyperparameters that would raise the fitness score of the architecture. There are 3 types of mutations:

a. Architectural change mutations:

These mutations change the architecture of the network by adding or removing layers from the previous architecture. These mutations are as follows:

i. Adding / Removing a graph convolution layer:

In this mutation a graph convolution layer is added to or removed from a randomly chosen position in the current network architecture. While adding, the number of output filters of the new convolution layer are randomly chosen from [128, 256, 512]. An example mutation is shown in Figure 3.2.1.

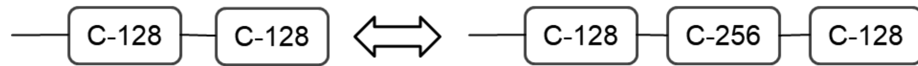


Figure 3.2.1: *Graph convolution layer mutation.*

ii. Adding / Removing a fully-connected layer:

In this mutation a fully-connected layer is added to or removed from a randomly chosen position in the current network architecture. While adding, the number of units of the new fully-connected layer is a randomly chosen value x, where $x \in$ (output_classes,500]. This mutation is shown in Figure 3.2.2.

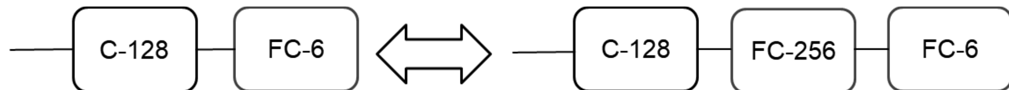


Figure 3.2.2: *Fully-connected layer mutation.*

iii. Adding / Removing a one-by-one graph convolution layer:

One-by-one convolution were proposed by Lin et al. [48]. These are used to alter the size of the channel dimension c of the convolution filters. They also require less parameters to change the channel size when compared to the 3×3 filter. One-by-one graph convolution is same as the one-by-one normal convolution. In this mutation a one-by-one graph convolution layer is added to or removed from a randomly chosen position in the current network architecture. One-by-one convolution helps in reducing dimensionality in filter dimension. While adding, the number of output filters of the new one-by-one layer are randomly chosen from [128, 256, 512]. This mutation is shown in Figure 3.2.3.

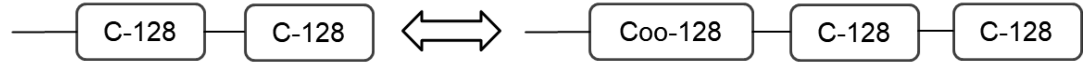


Figure 3.2.3: *One-by-one graph convolution layer mutation.*

iv. Adding / Removing a graph attention layer:

In this mutation, a graph attention layer is added to or removed from a randomly chosen position in the current network architecture. This attention layer is a soft attention. It learns attention over the vertices by weighing the vertex features. The attention is given by (3.2.1) and applied on the vertices as given in (3.2.2), where $V$is the vertex graph signal, w is the vertex feature, α is the attention vector and $V \in \mathbb{R}^{B\times N\times F}, w \in \mathbb{R}^{F}, \alpha \in \mathbb{R}^{N}$

$$\alpha = \mathrm{softmax}(Vw) \tag{3.2.1}$$

$$V_{out}^{(n)} = \alpha_n V^{(n)} \tag{3.2.2}$$

While adding, the number of output filters of the new attention layer are randomly chosen from [128, 256, 512]. This mutation is shown in Figure 3.2.4.

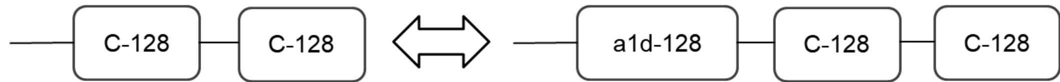


Figure 3.2.4: *Graph attention layer mutation.*

v. Adding / Removing a skip connection:

In this mutation, a skip connection path is added or removed between randomly chosen graph convolution layers in the current network architecture. This mutation is shown in Figure 3.2.5.

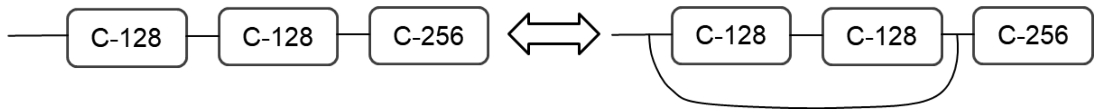


Figure 3.2.5: *Skip connection mutation.*

b. <u>Graph structure change mutation:</u>

These mutations are responsible for changing the graph structure to increase the receptive field of the filters applied on them. These help in understanding high level features in the graphs. These mutations are as follows:

i. Pooling mutation:

In this mutation, the graph structure is changed using max pooling defined in (3.1.11) and (3.1.12). The pooling ratio is a randomly chosen value x where $x \in (0,1]$. The pooling layer is added at a randomly chosen position in the current network. This mutation is shown in Figure 3.2.6.

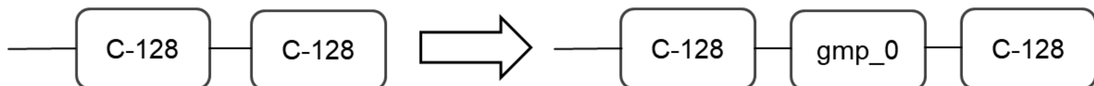


Figure 3.2.6: *Lloyd pooling mutation.*

ii. Graph embed pooling mutation:

In this mutation, the graph structure is changed using graph embed pooling defined in (3.1.15) and (3.1.16). The pooled number of vertices is randomly chosen from [16,32,64]. The pooling layer is added at a randomly chosen position in the current network. This mutation is shown in Figure 3.2.7.

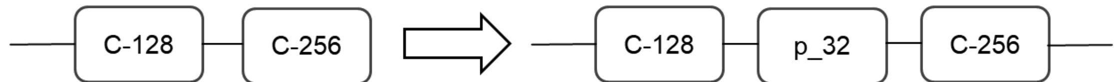


Figure 3.2.7: *Graph embed pooling mutation.*

iii. Reduced max layer:

Reduce max operation for a matrix/tensor reduces the matrix/tensor to a single dimension vector, where each element of the vector is maximum value along other dimensions of the matrix/tensor. The reduce max mutation changes the graph structure to a linear feature vector. The reduce max layer is added at the position before the first fully-connected layer in the current network. There can be at max. one reduced-max layer in the network. This mutation is shown in Figure 3.2.8.

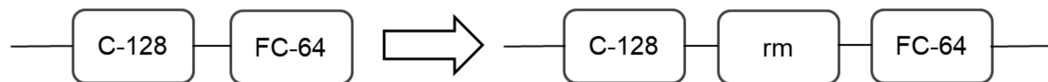


Figure 3.2.8: *Reduced max pooling mutation.*

c. <u>Hyperparameter mutations:</u>

These mutations change some of the different hyperparameters needed to tune the architecture. These mutations are as follows:

i. Learning rate mutations:

These mutations change the learning rate parameter in different ways. There are three types of learning rate mutations. When the learning rate mutation is chosen, a random number of these mutations are chosen and applied to the current architecture. They are:

- Changing starter learning rate:
  Starter learning rate is the parameter which decides the learning rate of the model at the beginning of a model training cycle. In this mutation, the starter learning rate is changed from an old value to a value randomly chosen from [0.5×old value, 2×old value]
- Changing learning rate step:
  Learning rate step is the parameter which decides the iteration steps of the model training cycle at which learning rate value is decreased. A model starts its training cycles with the starter learning rate and after every learning rate step cycles, the learning rate value is decreased. In this mutation, the learning rate step is changed from the old value old value to a value randomly chosen from [0.5×old value, 2×old value]
- Changing learning rate exponential:
  Learning rate exponential decides the factor by which the learning rate value is decreased at the learning rate step in a model training cycle. In this mutation, the learning rate exponential is changed from the old value to a value randomly chosen from [0.5×old value, 2×old value]

ii. Regularization mutations:

These mutations change the learning rate parameter in different ways. There are two types of regularization mutations. When the regularization mutation is chosen, a random number of these mutations are chosen and applied to the current architecture. They are:

- L1 regularization: In this mutation, the L1 regularization is changed from the old value old value to a value randomly chosen from [0.5×old value, 2×old value]
- L2 regularization: In this mutation, the L2 regularization is changed from the old value old value to a value randomly chosen from [0.5×old value, 2×old value]

B. Fitness Score

For evaluating the success of a mutation, it is important to define a good metric as the fitness score. In the case of architecture search of graph CNNs for classification tasks, the accuracy of the network is a good measure to evaluate the performance of the architecture. But this accuracy score must be on unforeseen data. Hence, in this case, this work uses validation accuracy score as fitness score metric for architecture search.

C. Evolutionary Algorithm for Architecture Search

Architecture design is a laborious and resource intensive process. Evolutionary algorithms used for its automatic discovery must increase its efficiency of resource usage and improve the time taken for reaching optimal performance compared to manual architecture design. For this task, this research defines a baseline evolutionary algorithm model and then introduces an improved evolutionary algorithm model which reduces the training time and converges to better solutions faster.

a. Test-and-Mutate Algorithm (Baseline):

In this algorithm, all the N models in the pool are trained for the first cycle and for every next cycle two random models are chosen and compared based on their validation accuracy scores. The best model from the chosen two are mutated. Mutation is selected randomly from all the available mutations. Mutated model is trained, and its validation accuracy is compared with the two chosen models. If it is better than either of the two chosen models, the worst model is replaced with the mutated model in the pool of models. The flow of this algorithm is shown in the Figure 3.2.9.

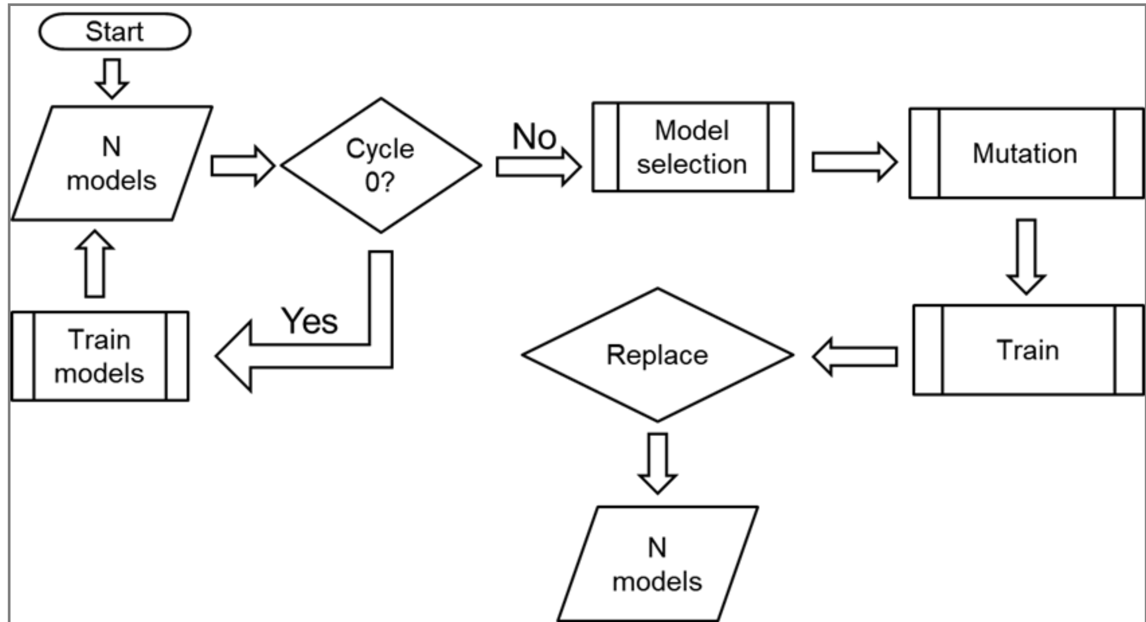


Figure 3.2.9: *The flow diagram of Test-and-Mutate algorithm.*

b. <u>Test-and-Mutate-with-Probability Algorithm:</u>

This algorithm is an improvement over the baseline Test-and-Mutate baseline algorithm described above. The model training and selection process remains same as in the baseline algorithm. The mutation process is improved. In the First cycle, all mutations are assigned equal selection probabilities. Based on the helpfulness of the mutation a constant reward is added or subtracted from the mutation's selection probability. The changed mutation selection probabilities are applied to the mutation selection process after every *p* cycles. The flow of this algorithm is shown in the Figure 3.2.10.

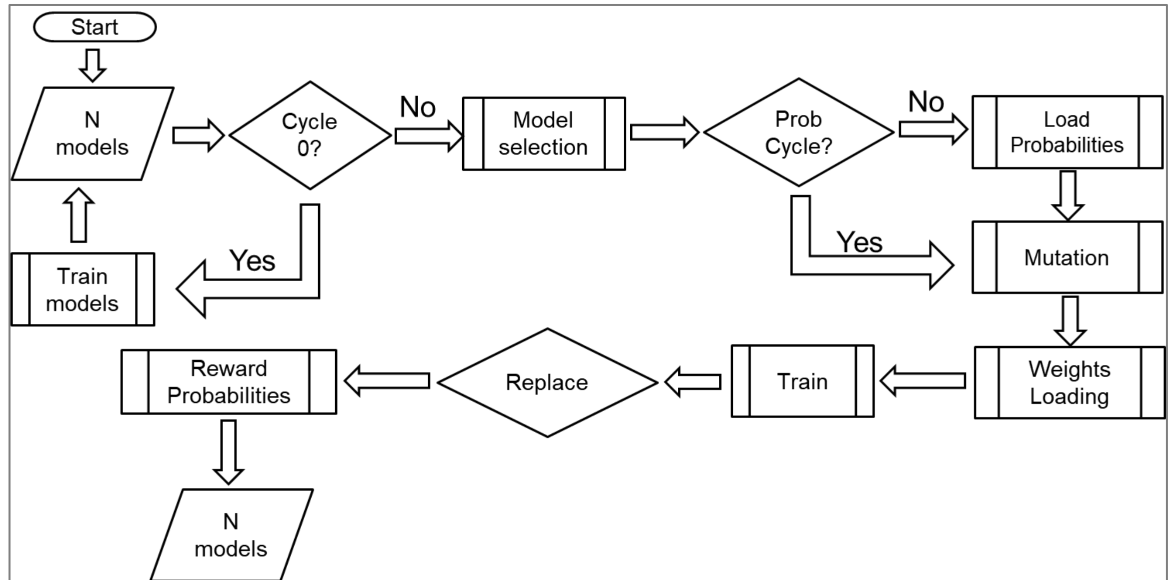


Figure 3.2.10: *The flow diagram of Test-and-Mutate-with-Probability algorithm.*

D. Features of Evolutionary Algorithm

The improved evolutionary algorithm Test-and-Mutate-with-Probability has some salient features that helps the algorithm converge to better graph CNNs architectures. These salient features are as follows:

a. <u>Mutation probability:</u>

   In this algorithm, every mutation is assigned a selection probability. All the mutations are assigned equal selection probabilities at the training cycle. This selection probability changes every cycle a model is replaced with a better model architecture.

b. <u>Mutation probability reward:</u>

   Every mutation selection probability is changed by a factor of the mutation probability reward. The Mutation probability reward is set value between (0,1). If the mutation was successful in replacing an architecture, the mutation probability

is multiplied by a factor of (1.0 + reward). If the mutation is unsuccessful in replacing an architecture, the mutation probability is multiplied by a factor of (1.0 – reward).

c. <u>Mutation probability cycle:</u>

The mutation selection probability value is changed and stored after every cycle based on the replacement of the model architecture. The mutation probability cycle decides the update cycle, when the most current mutation selection probabilities are used for the process of model selection. The mutation probability cycle is a set number to update probabilities in recurring manner. This gives an account for history of mutations which have helped in replacing model architecture.

d. <u>Weights loading:</u>

Loading weights of a model from a similar model trained previously often aids in model convergence. It is particularly important in this evolutionary algorithm. In this algorithm, the difference between the previous model and mutated model architecture is no more than one layer different. Thus, loading the weights of all the unchanged layers would help the model in learning faster. The weights are loaded according to the type of mutation:

i. Architectural change mutations:

These mutations add or remove a layer in the architecture keeping the graph structure unchanged. In these types of mutations, all the layer weights except the added or mutated layer are loaded from the previous model architecture. In the case of layer removal, all the layer weights except the layer before and after removed layer are loaded.

ii. Graph structure change mutations:

These mutations are pooling type mutations. In these types of mutations, all the layer weights before the added pooling layer are loaded from the previous model architecture.

iii. Hyperparameter mutations:

These mutations just change the hyperparameters without changing either the architecture or the graph structure. Hence all the weights from the previous model architecture are loaded.

Chapter 4

Implementation

4.1 Datasets

The Weisfeiler-Lehman Graph Kernel proteins datasets [25] are standard datasets for graph classification. These are small protein classification datasets that are useful testbeds for analysis and comparison of graph-based machine learning algorithms.

A. Enzymes:

ENZYMES is a data set of protein tertiary structures obtained from Borgwardt et al. [21] consisting of 600 enzymes from the BRENDA enzyme database [15]. In this case the task is to correctly assign each enzyme to one of the six op-level classes.

B. MUTAG:

MUTAG [24] is a data set of 188 mutagenic aromatic and heteroaromatic nitro compounds labeled according to whether they have a mutagenic effect on the Gram-negative bacterium Salmonella typhimurium.

Properties of these protein graph datasets are summarized in Table 1 below.

Table 4.1: *Summary of protein datasets to be used in this thesis.*

	ENZYMES	**MUTAG**
# Graphs	600	188
Mean |V|	32.63	17.93
Mean |E|	62.14	19.79
# Classes	6	2
# Vertex labels	3	7
# Edge labels	-	11

4.2 Implementation

Implementing an evolutionary search algorithm requires plentiful CPU and GPU resource time. Even for small classification tasks, training graph CNNs is a GPU-intensive and time intensive task. Also, given the small size of these protein datasets, the reporting method followed is a standard 10-fold cross validation based aggregated accuracy score. The implementation details of the evolutionary algorithm are explained in this section.

A. Basic Implementation:

The basic implementation of evolutionary algorithm is simple. The experiment is started with set number of model architectures *N* and set number of total cycles *C*. *N* is kept constant for both MUTAG and Enzymes dataset to *10* models. *C* is *40* for MUTAG and is *250* for Enzymes. Other hyperparameters are also initialized to set values. For the first cycle, *N* new models of weak classifiers (weak architectures) are created similar to Real et al. [17]. In this case the weak classifiers are made up of two layers: random fully-connected layer and output classes based fully-connected layer. After creation, in the first cycle, the weak classifiers are trained.

Model training is done using 10-fold cross-validation. The data is divided into a train: validation split of 90:10. Each model is trained for a set number of iterations and validation accuracy score is calculated after the iterations are finished. This is the validation accuracy for that fold. This is repeated for 10 independent folds and the mean validation accuracy is calculated. This mean validation accuracy is the assigned fitness score for the model.

B. Parallel Implementation:

The basic implementation is time consuming and GPU-intensive. To implement the evolutionary search algorithm in GPU-constrained environment, it was necessary to perform parallelization of the algorithm. All the experiments were performed using only 2 Nvidia Tesla P100 GPUs with 12 GB capacity each. Initial architectures are very simple and do not require full capacity of the GPU. Also, given the small size of the datasets, complex architectures would also make optimal use of the GPU space while running a single fold at a time.

To avoid wastage of GPU space and to speed up the training process, this work implements a parallel version of 10-fold cross validation with specified number of folds running parallelly. This is possible as each fold is independent from any other fold and fold data indices can be precomputed easily. The python 'multiprocessing' library [45] helps in parallelization of the code. With this parallel implementation, the training time speed up achieved is directly proportional to the number of parallel folds running simultaneously.

C. Saving and Loading Best model:

With increase in complexity of the architectures, the models start fitting the data and that is reflected in lower loss values. All these models are trained for certain preset value of iterations and validated on validation set. With complex models, it is observed the loss value attains a low point at some iteration of the fold and then explodes to a very high value. This is called loss explosion. This happens because the learning rate is too high.

But in our case of 10-fold cross validation, loss explosion iteration is different for every fold. For some folds, it may not occur at all. In others, it may occur twice. This problem is illustrated in Figure 4.2.1 which is a tensorboard snippet of 10 folds of a single model architecture.

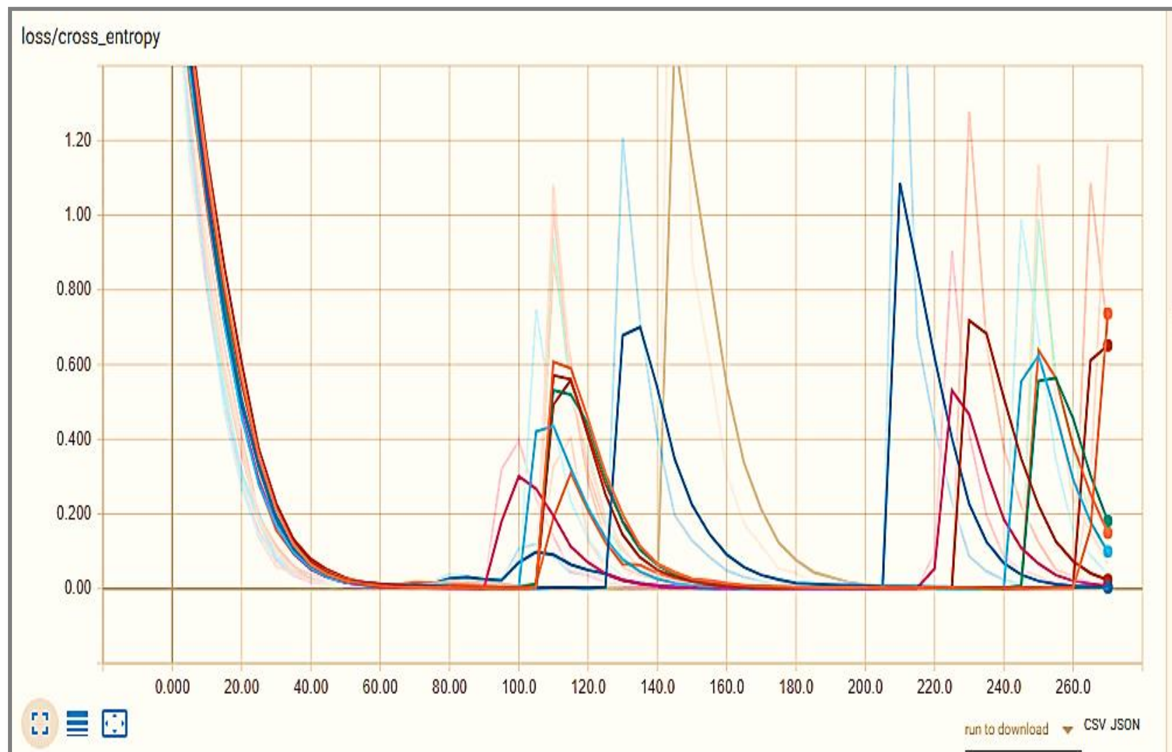


Figure 4.2.1: *Loss explosion within training of a fold of an architecture.*

In such a case, calculating validation score after a preset number of iterations seem counterintuitive as the models, even after fitting the data, may have their training loss explode and result into a poor validation accuracy score for that particular fold. Hence, instead of calculating the score based on the model of a preset iteration, this work incorporates a method of saving the best model based on its training loss value. After the completion of the preset iterations, this best model is loaded, and validation accuracy score is calculated for that particular fold’s model. This method may not always give the best validation score as the model is saved on basis of lower training loss value. Lower training loss value may result in overfitting and degrading the

performance on validation set. But this method reduces hyperparameters by removing the need to set the right number of training iterations.

Chapter 5

Results and Analysis

5.1 Results

A. Comparisons with Other methods:

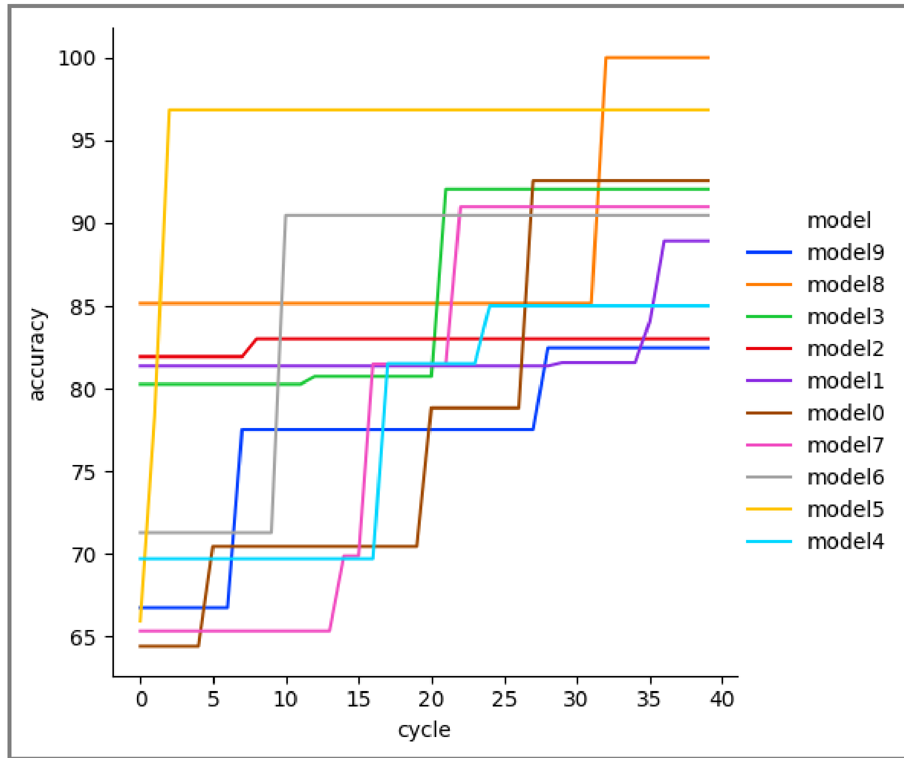
In this work, experiments were done on the protein graph structure datasets of Enzymes and Mutag. The scores obtained after evolution were able to beat the state-of-the-art accuracy score on Mutag dataset and got comparable to state of the art accuracy score on Enzymes dataset. Table 5.1.1 shows the accuracy scores of different methods on these two datasets. It must be noted that this work is based on Dominguez et. al. [14] and Such et. al. [5, 22]. And this work beats the accuracy scores posted by their methods on these two datasets.

Table 5.1.1: 10-fold cross validation accuracy score comparisons between different methods.

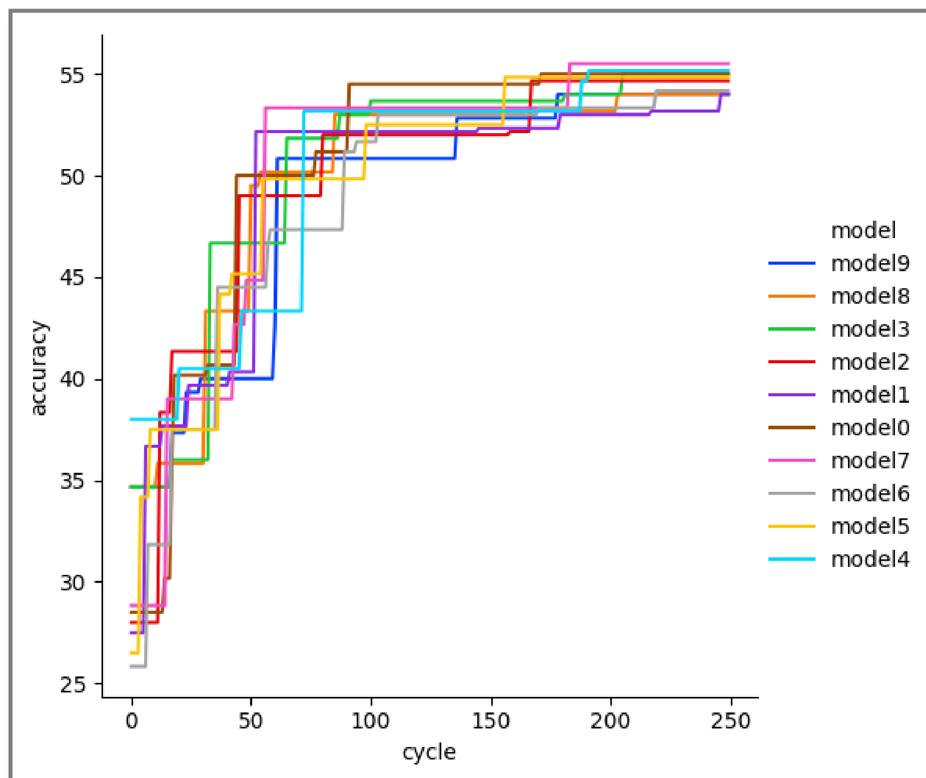
	MUTAG	ENZYMES
PATCHY-SAN [18]	92.63%	-
Deep WL [4]	87.44%	53.43%
Donini et al. [20]	93.00%	-
structure2vec [23]	88.28%	61.10%
WL [25]	83.78%	59.05%
WL-OA [20]	84.5%	59.90%
Morris et al. [16]	87.2%	**61.80%**
ECC [12]	89.44%	53.50%
Manual method	98.42%	53.00%
Test-and-Mutate (baseline)	**100.00%**[1]	48.33%
Test-and-Mutate-with-Probability	**100.00%**[1]	55.50%

Figure 5.1.1 shows the evolution of models over cycles for both, Enzymes and Mutag dataset. The experiments shown in Figure 5.1.1 achieve best results using evolutionary approach for the respective datasets.

[1] Skeptical to report 100% accuracy score. But given the automated evolutionary algorithm, issue seems to be with dataset. Hence evaluation and analysis done mostly on other comparatively difficult dataset. Other manual methods also getting close to 100 % accuracy. Also, note, this is maximum accuracy of *N* models, not mean accuracy.



(a)



(b)

Figure 5.1.1: *Model evolution over cycles for* ***(a)*** *Mutag dataset and* ***(b)*** *Enzymes dataset.*

B. Comparisons with Manual method:

The experiments based on evolutionary algorithm clearly top the results to that of the manual experiments. Also, these experiments have significantly less running time than that taken by manual designers to design specific architectures and tune hyperparameters to achieve optimal performance. Both these results are summarized in Table 5.1.2.

Table 5.1.2: Comparison of running times and best accuracy scores between manual and evolutionary approaches.

Method	MUTAG		Enzymes	
	Accuracy	*Time*	*Accuracy*	*Time*
Manual	98.42%	5 days	53.00%	18 days
Evolutionary	***100.00%***	***20 mins***	***55.50%***	***9 days***

C. Model Architectures:

Evolutionary algorithms, unlike manual design methods, provide a pool of model architectures which have undergone various mutations and hyperparameter tunings to achieve close to optimal performance. This section provides certain model architectures found in the pool of models, after the experiment was finished for a dataset.

a. Mutag dataset:

For this dataset, the most surprising result was that none of the top models contained any type graph convolution layers. Most models had fully-connected layers and reduce-max pooling layers. Model architectures yielding top accuracy score are shown in Figure 5.1.2. The contrast between manual and evolutionary network design is aptly displayed in the figure.

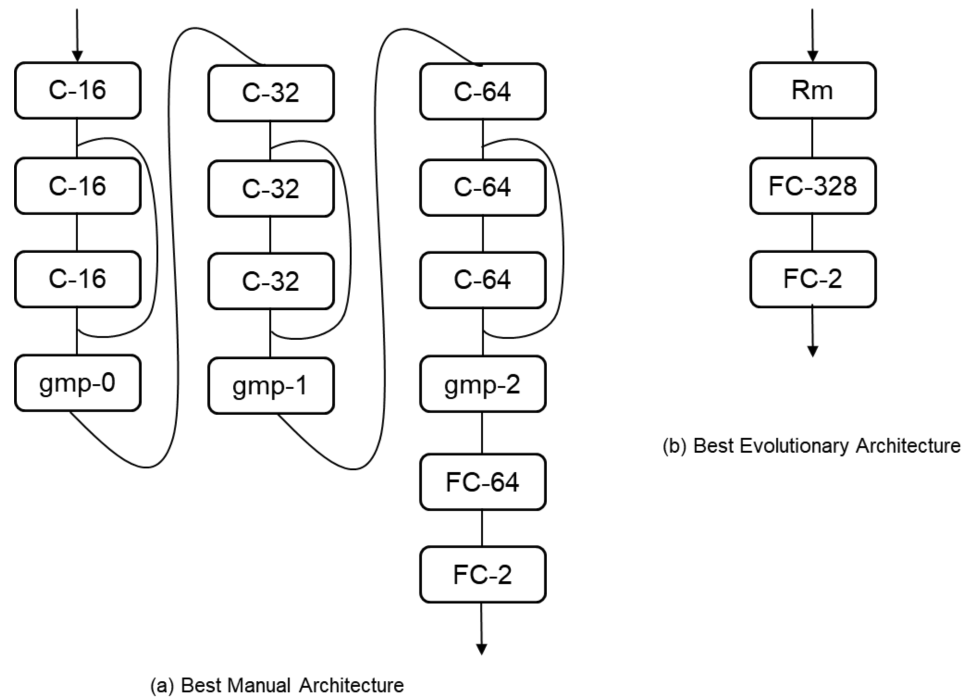


Figure 5.1.2: (a) *Best architecture designed manually.* ***(b)*** *Best architecture generated by evolution.*

b. Enzymes dataset:

For this dataset, the pool of models had less diversity. Top model architectures were tuned for hyperparameters to get comparable accuracy score. This being a more complex dataset with more output classes and more input samples, most architecture elements are found in these architectures. Graph embed pooling, the dense pooling method, is helpful for this dataset and is thus present in one of the top architectures. Model architectures yielding top accuracy score are shown in Figure 5.1.3.

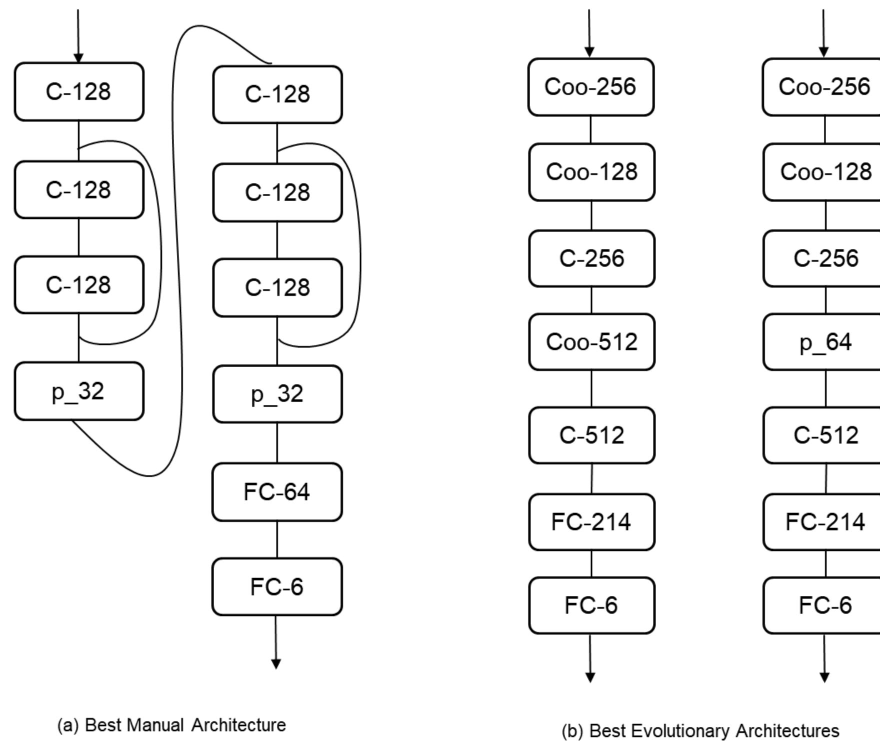


Figure 5.1.3: (a)*Best architecture designed manually.* ***(b)*** *Top architectures generated by evolution.*

5.2 Analysis

A. Mutation Probability Analysis:

Mutation probability was an important parameter boosting the performance of the evolutionary algorithm. It helped the algorithm converge faster to better model architectures with higher validation scores. The variance between validation scores in the pool of models reduces with probability. Also, the variance between different experiments decreases after introduction of mutation probability.

This can be observed in the Figure 5.2.1. It can be seen that high variance between scores is present between the experiments with no mutation probabilities (top row in Figure 5.2.1). Also, experiments with mutation probabilities (bottom row in Figure 5.2.1) achieve higher max and mean scores over time, but they are also running for a greater number of cycles. So, for a fair comparison, we compare it with the

convergence rate. If we observe the max. and mean accuracy value at 100 cycles, it can be easily seen that experiments with mutation probabilities converge to higher mean and max. accuracy values.

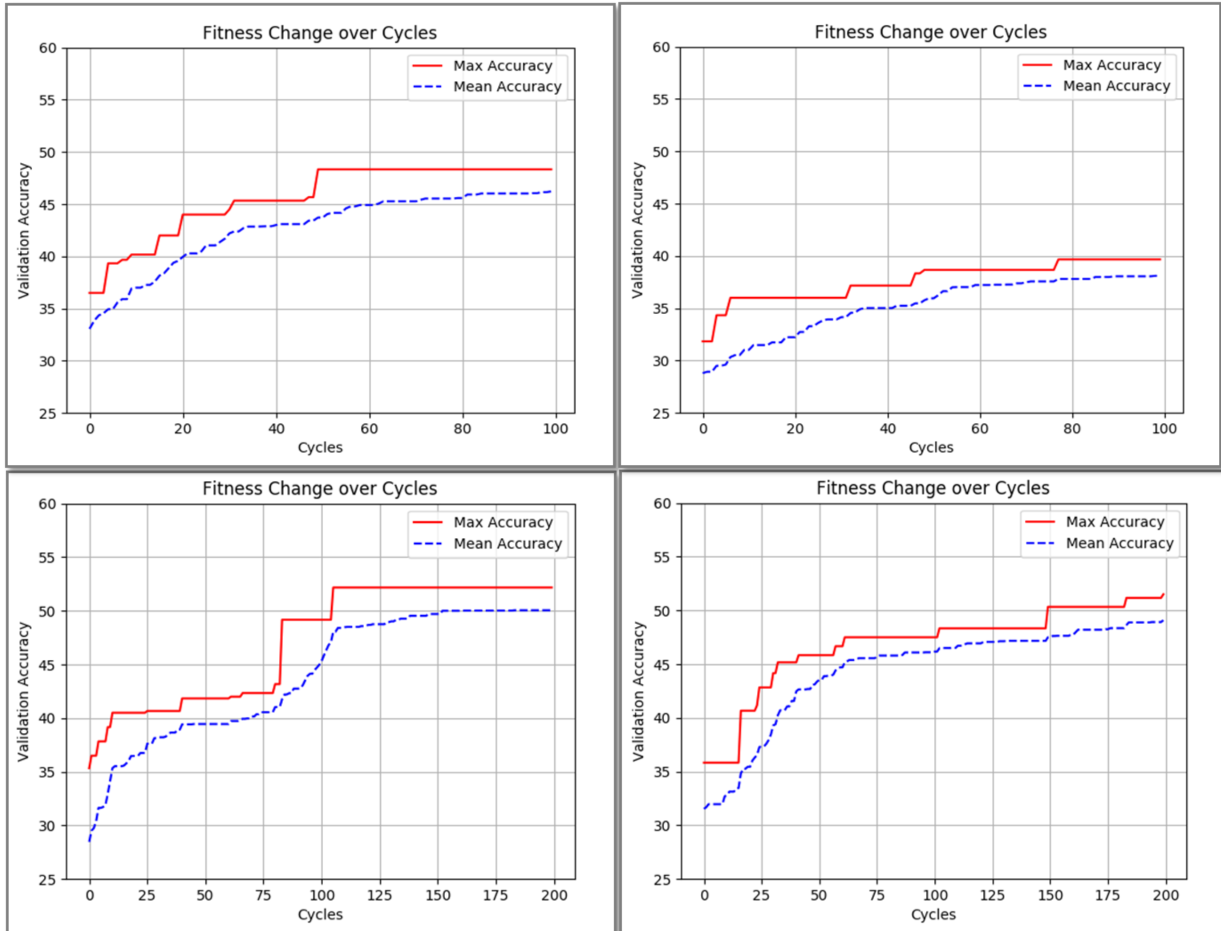
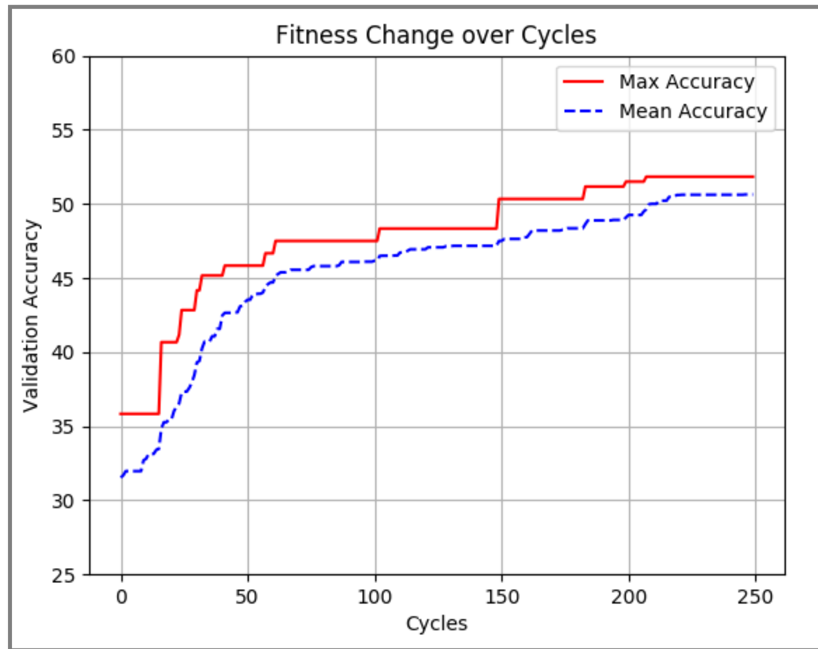


Figure 5.2.1: *Top row (Fig.* ***(a)***, ***(b)****) are experiments with no probability associated with mutations (baseline algorithm). Bottom row (Fig.* ***(c)***, ***(d)****) are experiments with probabilities associated with mutations.*

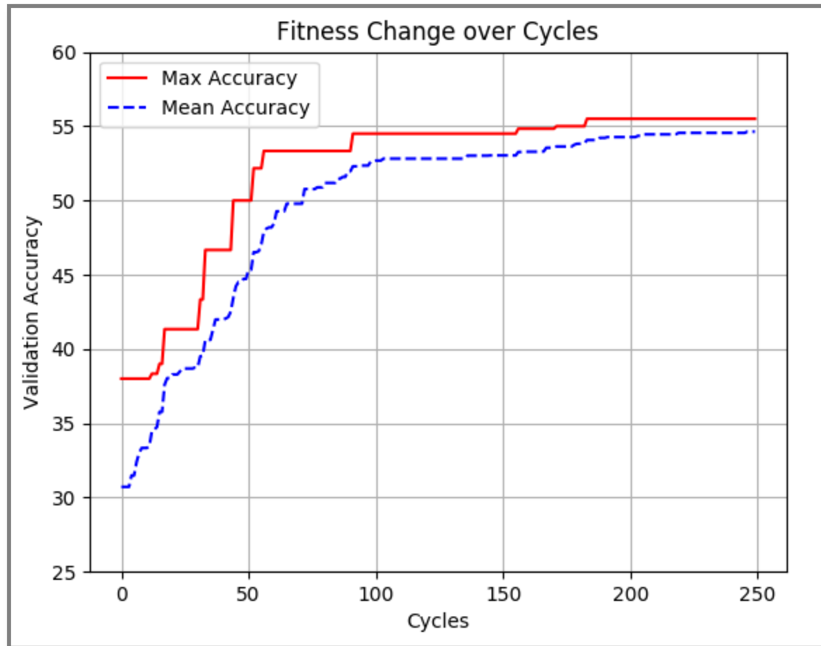
B. Weight Loading Analysis:

Mutation probability was an important parameter for the evolutionary algorithm. To further reduce the converging time, weights of selected layers were loaded from the previous architecture, based on the mutation. This helps the current architecture by having better initial conditions. This can be observed in the Figures 5.2.2 (a) and (b).

The radical time reduction in achieving top score is easily spotted on comparing the two results. Also, weight loading reduces the variance in accuracy scores among the pool of models. Thus, weight loading along with mutation probability, is able to generate quickly a pool of high performing model architectures with very close accuracy scores.



(a)



(b)

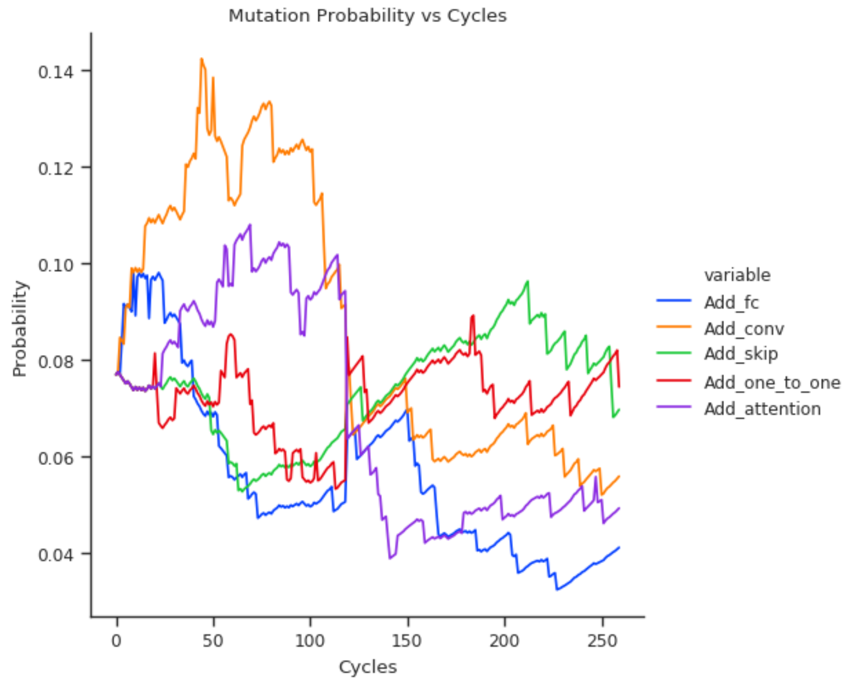
Figure 5.2.2: *This figure emphasizes the importance of weight loading. Fig.* ***(a)*** *is based on experiment which involved no weight loading, Fig* ***(b)*** *is based on experiment with weight loading.*

C. Mutation analysis:

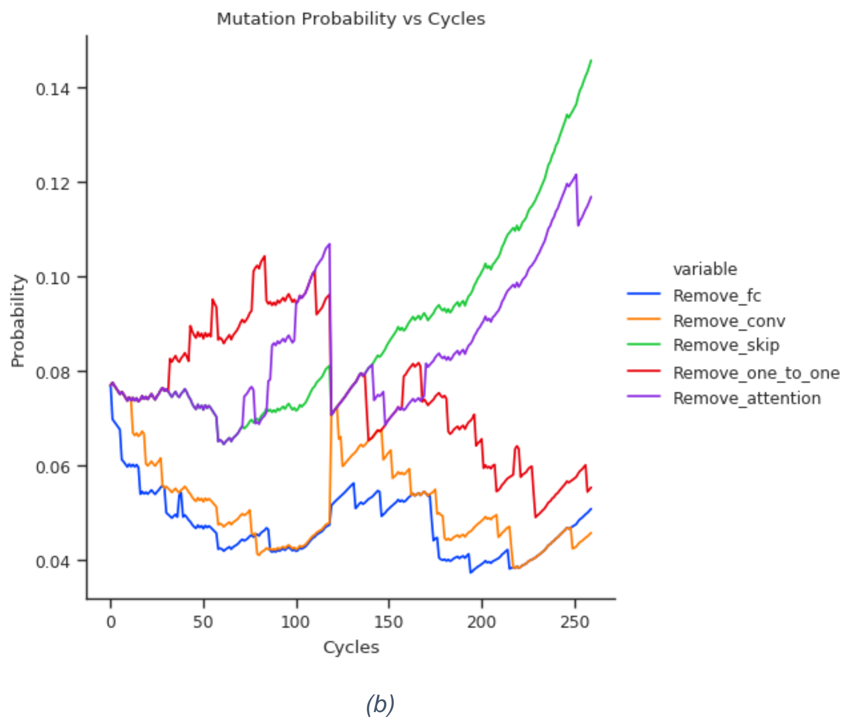
Different mutations play an important role in converging to pool of better model architectures. The importance of a mutation changes over time. Adding a fully connected layer may be helpful at the start, but over time adding a fully-connected layer may prove counter-productive to the manual designer. The same can be said with other feature extraction mutations. Figure 5.2.3 shows the change in mutation probability over cycles for every mutation in the Enzymes experiment with top results. It can be observed that 'add' mutations are prominent at the start and 'remove' mutations are prominent at the end.

Pooling gains importance only when the model is complex and has been saturated after learning low level features. Pooling helps in reducing the graph structure and increases the receptive field helping the model learn higher order features. Learning rate and regularization factors are tuned almost all through the

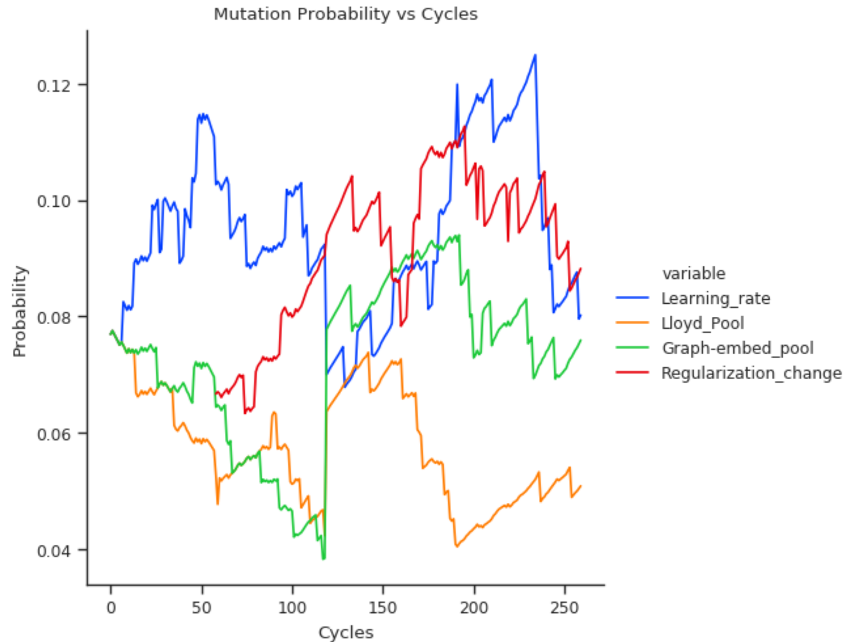
training cycles. This shows that this evolutionary process is attaining to a better model in a way similar to that of a manual designer.



(a)



(b)



(c)

Figure 5.2.3: *Evolution of different mutations' probability over cycles.* ***(a)*** *shows the 'add' mutations and their probability change over cycles.* ***(b)*** *shows the 'remove' mutations and their probability change over cycles.* ***(c)*** *shows the pooling and parameter mutations and their change over cycles. All these figures show the importance of a mutation within the cycle period.*

D. Hyperparameter reduction:

Evolutionary algorithms are more efficient in terms of hyperparameters. The main hyperparameters to set for the evolutionary algorithm are:

i. Total Cycles

ii. Number of models

iii. Iterations per fold of training

iv. Probability reward

v. Probability cycle

Other parameters like learning rate and regularization parameters can optionally be initialized. While manually designing a model architecture, the hyperparameters needed to be considered are:

i. Learning rate parameters (starter learning rate, learning rate step, learning rate decay)
ii. Regularization parameters (L1 and L2 regularizations)
iii. Depth of the architecture (Total number of layers in an architecture)
iv. Type of layers in the architecture. (convolutional, fully-connected etc.)
v. Iterations per fold of training
vi. Layer units for every layer (Size of individual output units in each layer)
vii. Batch size parameters
viii. Pooling parameters (pool ratio, pool size, type of pooling)

It can easily be seen that the evolutionary algorithm drastically reduces the number of hyperparameters. This gives two-fold benefits. The evolutionary algorithm tunes all the hyperparameter it introduces. The manual effort of choosing as well as tuning the hyperparameter is decreased. This gives designers more time to improve the underlying theory behind their algorithms whilst being less anxious about optimizing the model architectures.

Chapter 6

Conclusions and Discussions

6.1 Conclusions

This thesis work shows the feasibility of evolutionary algorithms for graph CNN architecture search. This thesis work researches on various evolutionary algorithms and provides a suitable and simple evolutionary algorithm to design graph CNN architectures. The algorithms described for evolving graph CNN architectures can be applied to different datasets and can generate dataset-specific graph CNN architectures. It achieves comparable to state-of-the-art accuracy on classification of protein graph structures using graph CNN model provided by Petroski Such et al. [22] and Dominguez et al. [14].

A way to simultaneously tune hyperparameters while performing architecture search is presented by the evolutionary algorithm. It easily tops the manually designed architectures for protein graph classification using this model of graph CNNs.

6.2 Discussions

Architecture design is a tedious task, one that requires focus and attention to models. This algorithm has shown that not only can it build better model architectures, but it also can do so in drastically less time. From the architecture search done by the algorithm as observed from plot depicting individual mutation probabilities, it can be seen that the evolution process is similar to that of a manual designer: ‘add’ mutations at the beginning, ‘remove’ mutations at the end, ‘pool’ mutations introduced after building complex architectures and tuning learning rate parameter throughout is similar to the changes that a human designer would follow.

This algorithm gets rid of inherent biases seen in section 5c for architectures generated for Mutag. Special features like layer specific weight loading and saving best model help in faster convergence of the experiment to generate a pool of highly skilled architectures. This work provides an efficient solution to automate the task architecture design of graph CNNs.

6.3 Future works

This evolutionary algorithm provided in this thesis work is an apt choice for architecture search on small datasets in a limited resource environment. This work can be extended further. Some possible extensions are:

- Apply the evolutionary algorithm for CNN architecture search on benchmark image datasets.
- Scale parallel implementation into a full-fledged distributed implementation over multiple GPUs to decrease training time and increase speed up.
- Generate new algorithm that generates architectures by combination of more than one architecture.

Bibliography

[1] M. Suganuma, S. Shirakawa, and T. Nagao, “A Genetic Programming Approach to Designing Convolutional Neural Network Architectures,” in *Proceedings of the Genetic and Evolutionary Computation Conference*, New York, NY, USA, 2017, pp. 497–504.

[2] K. O. Stanley, D. B. D’Ambrosio, and J. Gauci, “A Hypercube-Based Encoding for Evolving Large-Scale Neural Networks,” *Artificial Life*, vol. 15, no. 2, pp. 185–212, Apr. 2009.

[3] K. Stanley, “Compositional pattern producing networks: A novel abstraction of development,” *Genetic Programming and Evolvable Machines*, vol. 8, pp. 131–162, 2007.

[4] P. Yanardag and S. V. N. Vishwanathan, “Deep Graph Kernels,” in *Proceedings of the 21th ACM SIGKDD International Conference on Knowledge Discovery and Data Mining*, New York, NY, USA, 2015, pp. 1365–1374.

[5] F. Petroski Such, “Deep Learning Architectures for Novel Problems,” *Theses*, Feb. 2017.

[6] F. P. Such, V. Madhavan, E. Conti, J. Lehman, K. O. Stanley, and J. Clune, “Deep neuroevolution: genetic algorithms are a competitive alternative for training deep neural networks for reinforcement learning,” *arXiv preprint arXiv:1712.06567*, 2017.

[7] K. He, X. Zhang, S. Ren, and J. Sun, “Deep Residual Learning for Image Recognition,” in *2016 IEEE Conference on Computer Vision and Pattern Recognition (CVPR)*, 2016, pp. 770–778.

[8] K. He, X. Zhang, S. Ren, and J. Sun, “Delving Deep into Rectifiers: Surpassing Human-Level Performance on ImageNet Classification,” in *Proceedings of the 2015 IEEE International Conference on Computer Vision (ICCV)*, Washington, DC, USA, 2015, pp. 1026–1034.

[9] G. Huang, Z. Liu, L. van der Maaten, and K. Q. Weinberger, “Densely connected convolutional networks,” in *Proceedings of the IEEE Conference on Computer Vision and Pattern Recognition*, 2017.

[10] G. F. Miller, P. M. Todd, and S. U. Hegde, “Designing Neural Networks using Genetic Algorithms.,” in *ICGA*, 1989, vol. 89, pp. 379–384.

[11] H. Dai, B. Dai, and L. Song, “Discriminative Embeddings of Latent Variable Models for Structured Data,” in *International Conference on Machine Learning*, 2016, pp. 2702–2711.

[12] M. Simonovsky and N. Komodakis, “Dynamic Edge-Conditioned Filters in Convolutional Neural Networks on Graphs,” in *2017 IEEE Conference on Computer Vision and Pattern Recognition (CVPR 2017)*, 2017.

[13] K. O. Stanley and R. Miikkulainen, “Evolving Neural Networks Through Augmenting Topologies,” *Evol. Comput.*, vol. 10, no. 2, pp. 99–127, Jun. 2002.

[14] M. Dominguez, R. Dhamdhere, A. Petkar, S. Jain, S. Sah, and R. Ptucha, “General-Purpose Point Cloud Feature Extractor,” in *Winter Applications of Computer Vision 2018*, 2018.

[15] N I. Schomburg *et al.*, “BRENDA, the enzyme database: updates and major new developments,” *Nucleic Acids Research*, vol. 32, no. suppl_1, pp. D431–D433, Jan. 2004.

[16] C. Morris, K. Kersting, and P. Mutzel, “Glocalized Weisfeiler-Lehman Graph Kernels: Global-Local Feature Maps of Graphs,” in *2017 IEEE International Conference on Data Mining (ICDM)*, 2017, pp. 327–336.

[17] E. Real *et al.*, “Large-Scale Evolution of Image Classifiers,” in *International Conference on Machine Learning*, 2017, pp. 2902–2911.

[18] M. Niepert, M. Ahmed, and K. Kutzkov, “Learning convolutional neural networks for graphs,” in *International conference on machine learning*, 2016, pp. 2014–2023.

[19] K. He, G. Gkioxari, P. Dollár, and R. Girshick, “Mask r-cnn,” in *Computer Vision (ICCV), 2017 IEEE International Conference on*, 2017, pp. 2980–2988.

[20] M. Donini, N. Navarin, I. Lauriola, F. Aiolli, and F. Costa, “Fast Hyperparameter Selection for Graph Kernels via Subsampling and Multiple Kernel Learning.”

[21] K. M. Borgwardt, C. S. Ong, S. Schönauer, S. V. N. Vishwanathan, A. J. Smola, and H.-P. Kriegel, “Protein Function Prediction via Graph Kernels,” *Bioinformatics*, vol. 21, no. 1, pp. 47–56, Jan. 2005.

[22] F. P. Such *et al.*, “Robust Spatial Filtering with Graph Convolutional Neural Networks,” *IEEE Journal of Selected Topics in Signal Processing*, vol. 11, no. 6, pp. 884–896, Sep. 2017.

[23] L. F. R. Ribeiro, P. H. P. Saverese, and D. R. Figueiredo, “Struc2Vec: Learning Node Representations from Structural Identity,” in *Proceedings of the 23rd ACM SIGKDD International Conference on Knowledge Discovery and Data Mining*, New York, NY, USA, 2017, pp. 385–394.

[24] A. K. Debnath, R. L. Lopez de Compadre, G. Debnath, A. J. Shusterman, and C. Hansch, “Structure-activity relationship of mutagenic aromatic and heteroaromatic nitro compounds. correlation with molecular orbital energies and hydrophobicity,” *Journal of medicinal chemistry*, vol. 34, no. 2, pp. 786–797, 1991.

[25] N. Shervashidze, P. Schweitzer, E. J. van Leeuwen, K. Mehlhorn, and K. M. Borgwardt, “Weisfeiler-Lehman Graph Kernels,” *Journal of Machine Learning Research*, vol. 12, no. Sep, pp. 2539–2561, 2011.

[26] “Princeton ModelNet.” [Online]. Available: http://modelnet.cs.princeton.edu/. [Accessed: 11-Oct-2018].

[27] “ShapeNet.” [Online]. Available: https://www.shapenet.org/. [Accessed: 11-Oct-2018].

[28] R. Anirudh and J. J. Thiagarajan, “Bootstrapping Graph Convolutional Neural Networks for Autism Spectrum Disorder Classification,” *arXiv:1704.07487 [cs, stat]*, Apr. 2017.

[29] N. Verma, E. Boyer, and J. Verbeek, “FeaStNet: Feature-Steered Graph Convolutions for 3D Shape Analysis,” in *CVPR 2018-IEEE Conference on Computer Vision & Pattern Recognition*, 2018.

[30] B. Baker, O. Gupta, N. Naik, and R. Raskar, “Designing neural network architectures using reinforcement learning,” *arXiv preprint arXiv:1611.02167*, 2016.

[31] B. Zoph and Q. V. Le, “Neural Architecture Search with Reinforcement Learning,” 2017.

[32] “CIFAR-10 and CIFAR-100 datasets.” [Online]. Available: https://www.cs.toronto.edu/~kriz/cifar.html. [Accessed: 11-Oct-2018].

[33] “Detection and Tracking of Pallets using a Laser Rangefinder and Machine Learning Techniques | Request PDF,” *ResearchGate*. [Online]. Available: https://www.researchgate.net/publication/324165524_Detection_and_Tracking_of_Pallets_using_a_Laser_Rangefinder_and_Machine_Learning_Techniques. [Accessed: 11-Oct-2018].

[34] M. Defferrard, X. Bresson, and P. Vandergheynst, “Convolutional Neural Networks on Graphs with Fast Localized Spectral Filtering,” in *Advances in Neural Information Processing Systems*, 2016.

[35] M. Henaff, J. Bruna, and Y. LeCun, “Deep Convolutional Networks on Graph-Structured Data,” *arXiv:1506.05163 [cs]*, Jun. 2015.

[36] A. Sandryhaila and J. M. F. Moura, “Discrete Signal Processing on Graphs,” *IEEE Transactions on Signal Processing*, vol. 61, no. 7, pp. 1644–1656, Apr. 2013.

[37] T. N. Kipf and M. Welling, “Semi-Supervised Classification with Graph Convolutional Networks,” in *International Conference on Learning Representations (ICLR)*, 2017.

[38] J. Bruna, W. Zaremba, A. Szlam, and Y. LeCun, “Spectral Networks and Locally Connected Networks on Graphs,” *arXiv:1312.6203 [cs]*, Dec. 2013.

[39] D. Duvenaud *et al.*, “Convolutional Networks on Graphs for Learning Molecular Fingerprints,” in *Proceedings of the 28th International Conference on Neural Information Processing Systems - Volume 2*, Cambridge, MA, USA, 2015, pp. 2224–2232.

[40] J. Atwood and D. Towsley, “Diffusion-convolutional neural networks,” in *Advances in Neural Information Processing Systems*, 2016, pp. 1993–2001.

[41] K. Simonyan and A. Zisserman, “Very Deep Convolutional Networks for Large-Scale Image Recognition,” *arXiv:1409.1556 [cs]*, Sep. 2014.

[42] A. Krizhevsky, I. Sutskever, and G. E. Hinton, “ImageNet Classification with Deep Convolutional Neural Networks,” in *Advances in Neural Information Processing Systems 25*, F. Pereira, C. J. C. Burges, L. Bottou, and K. Q. Weinberger, Eds. Curran Associates, Inc., 2012, pp. 1097–1105.

[43] C. Fernando *et al.*, “Convolution by evolution: Differentiable pattern producing networks,” in *Proceedings of the Genetic and Evolutionary Computation Conference 2016*, 2016, pp. 109–116.

[44] “Cartesian Genetic Programming - CGP-Library.” [Online]. Available: http://www.cgplibrary.co.uk/files2/CartesianGeneticProgramming-txt.html. [Accessed: 11-Oct-2018].

[45] “16.6. multiprocessing — Process-based ‘threading’ interface — Python 2.7.15 documentation.” [Online]. Available: https://docs.python.org/2/library/multiprocessing.html. [Accessed: 11-Oct-2018].

[46] D. G. Lowe, “Distinctive Image Features from Scale-Invariant Keypoints,” *Int. J. Computer Vision*, vol. 60, no. 2, pp. 91–110, Nov. 2004.

[47] N. Dalal and B. Triggs, “Histograms of oriented gradients for human detection,” in *2005 IEEE Computer Society Conference on Computer Vision and Pattern Recognition (CVPR’05)*, 2005, vol. 1, pp. 886–893 vol. 1.

[48] M. Lin, Q. Chen, and S. Yan, “Network In Network,” *arXiv:1312.4400 [cs]*, Dec. 2013.