Dynamic Filters in Graph Convolutional Neural Networks*

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Abstract

Over the last few years, we have seen increasing data generated from non-Euclidean domains, which are usually represented as graphs with complex relationships, and Graph Neural Networks (GNN) have gained a high interest because of their potential in processing graph-structured data. In particular, there is a strong interest in exploring the possibilities in performing convolution on graphs using an extension of the GNN architecture, generally referred to as Graph Convolutional Neural Networks (GCNN). Convolution on graphs has been achieved mainly in two forms: spectral and spatial convolutions. Due to the higher flexibility in exploring and exploiting the graph structure of data, recently, there is an increasing interest in investigating the possibilities that the spatial approach can offer. The idea of finding a way to adapt the network behaviour to the inputs they process to maximize the total performances has aroused much interest in the neural networks literature over the years. This paper presents a novel method to adapt the behaviour of a GCNN to the input proposing two ways to perform spatial convolution on graphs using input-based filters which are dynamically generated. Our model also investigates the problem of discovering and refining relations among nodes. The experimental assessment confirms the capabilities of the proposed approach, which achieves satisfying results using simple architectures with a low number of filters.

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1 Introduction

In the last few decades, Convolutional Neural Networks (CNNs) have gained much interest due to their potential and versatility in addressing a large scale of machine learning problems [LeCun et al. (1998), LeCun et al. (2015)], such as image processing [Krizhevsky et al. (2012)] and pattern recognition [Kim (2014)] while achieving great success. The potential of CNNs lies in extracting and processing local information performing convolution on input data using sets of trainable filters with a fixed size. However, the design of the convolution operation in the CNNs allows processing only regular data while, in the real world, there is a considerable amount of data that naturally lie on non-Euclidean domains, needing different techniques to be processed.

These data are often represented by graph-based structures. Graph structures imply several difficulties in using standard data processing techniques, such as the impossibility of using classic CNNs due to the variable number of neighbours for each node (differently from regular data where the filter properties fix the number of neighbours for each node). This aspect has led to new processing techniques such as Graph Neural Networks (GNNs), which gained high interest during the last years.

First attempts [Sperduti and Starita (1997); Gori et al. (2005); Scarselli et al. (2008)] of neural network based on input graphs, generally referred to as Recurrent Graph Neural Networks (RecGNNs), was based on message passing architectures, where an iterative propagation allows to learn the representation of the node of the neighbour’s information. The learned data representations are then used as features for classification or regression tasks. However, as the size of the graphs to be processed increased, these approaches were more and more computationally expensive, and this represented a new challenge to overcome.

Due to the great success of CNNs, GNNs inherits convolution operation producing the Graph Convolutional Neural Networks (GCNNs), which have found their expression in two different approaches. The former are spectral methods (see, for example, [Li et al. (2018); Levie et al. (2018)]), that perform convolution based on graphs signal processing techniques. The latter are spatial methods (see, for example, [Atwood and Towsley (2016); Hechtlinger et al. (2017)]), that instead perform convolution using spatial information of data, similarly to what classical CNNs do. GCNNs share the same idea of message passing with RecGNNs but in a non-iterative manner.

Among the different works proposed in the literature, in [Zhang et al. (2019)] the authors proposed a novel method, the Graph Structure Convolutional Network (GSCN), which performs a spatial convolution learning underlying input graph structure information, improving in this way the overall performances of the network. However, classical Convolutional Networks are based on learned filters having constant values for each input fed to the network. In other words, the filter values are independent of the input values. Instead, adapting the Artificial Neural Network (ANN) behaviour in function of the input is an open research area in the scientific community. For instance, in [Donnarumma et al. (2012)], the authors discuss the biological plausibility of adapting the behaviour...
of neural networks to external inputs. In the GNN field, Simonovsky et al. in Simonovsky and Komodakis (2017) propose the Edge-Conditioned Convolution (ECC) network, which performs spatial convolutions over graph neighbourhoods exploiting edge labels and generating suitable input filters from them. It is worth noticing that ECC leverages structural information (particularly edge labels) to generate sets of convolutional filters without learning information related to the graph structure itself.

In this paper, we exploit the possibility of dynamically changing the behaviour as a function of the input and propose a novel method to perform spatial convolution on graph-structured data using fixed-sized filters while learning graph structural information and adapting the network’s behaviour to each input. To this aim, we propose two different approaches in performing dynamical filtering operations (see Section 3):

1. **Global** dynamic filtering operations, where a unique input-dependent set of filters is used to extract features from a single input graph;

2. **Local** dynamic filtering operations, where for each given input graph, convolution is performed using neighbourhood-dependent sets of filters leading to a more adaptable convolution operation on the input.

This paper is organized as follows. Section 2 briefly reviews the related literature; Section 3 describes the proposed method; the experimental assessment is described in Section 4 while in Section 5 the obtained results are presented and discussed. The concluding Section 6 is left to final remarks.

## 2 Related works

We are proposing an ANN architecture that exploits both the concept of dynamically changing the behaviour of a generic ANN and that of convolution on graph-structured data based on GNNs.

In this section, we will first report the related works on ANNs with a dynamically changing behaviour. Then, we give a general description of the Graph Neural Network. Finally, we summarise related works on GCNNs.

### 2.1 Dynamically changeable behaviours in ANNs

A dynamical change of an ANN’s behaviour is achieved by adapting the network parameters to each input instance, and it allows to perform input-suited processing.

The idea of controlling the behaviours of an ANN through auxiliary inputs has a long history in the literature Jordan (1990); Schmidhuber (1992); Nishimoto et al. (2008); Paine and Tani (2004); Noelle and Cottrell (1995); Siegelmann (2012); Eliasmith (2005); Bishop (1994); Donnarumma et al. (2012). For example, in Paine and Tani (2004) a set of external neural units, called control neurons, are bidirectionally connected to all the neurons belonging to a lower
layer network influencing their functions and favouring the generation of particular motor primitives. In Bishop (1994); Bishop et al. (1995), the authors describe a way to represent general conditional probability densities \( p(t|x) \) by considering a parametric model for the distribution of \( t \), expressed as a neural network whose parameters are determined by the outputs of another neural network with \( x \) as input.

More recently, in Jia et al. (2016) the authors defined the dynamic changes in ANNs’ behaviours in the context of traditional CNNs using the dynamic filter module to execute the convolution operation. Dynamic filter module consists of two parts: a filter-generating network, that generates filters’ parameters from a given input, and a dynamic filtering layer, that applies those generated filters to another input. Moreover, the dynamic filtering layer is instantiated in two different ways: a dynamic convolutional layer, wherever the filtering operation is translation invariant, and a dynamic local filtering layer, wherever the filtering operation is not translation invariant, and it implies the using of specific local filters over all the input’s positions. However, this method is developed in the context of classic CNNs; by contrast, in Simonovsky and Komodakis (2017), the authors attempt to perform a dynamic spatial convolution on graphs. The authors proposed the Edge-Conditioned Convolution (ECC), which uses a filter-generating network to output edge-specific filters for each input sample dynamically.

Inspired by what is described in Jia et al. (2016); Simonovsky and Komodakis (2017), in this work, we perform an adaptive convolution on input graphs using filters dynamically generated by a filter-generating network, thus obtaining a dynamical change in the behaviour of the GCNN. We would like to point out that, differently from the ECC proposed in Simonovsky and Komodakis (2017) where convolutional filters are edge-based, our proposal (see Section 3) considers node-based filters, tweaking in this way the filtering operation on nodes themselves. Moreover, according to Jia et al. (2016), our approach is proposed either as a dynamic convolutional layer or as a dynamic local filtering layer. In the former, a set of filters is globally shared by all the neighbourhoods during the convolution, and it is dependent on all the input nodes; in the latter, sets of filters are locally generated for each neighbourhood during the convolution.

2.2 Graph Neural Networks

The first proposal of a neural network model for graph-structured data was made in Scarselli et al. (2008). This model builds on the idea that graph nodes represent concepts related to each other via edges. Each node \( n \) is represented by a feature vector \( x_n \), and each edge \((i, j)\) is described by a feature vector \( x_{e_{(i,j)}} \). This model leverages information exchange among nodes and their neighbours to update their features iteratively (message passing mechanism). Following the formalisation given in Wu et al. (2020), the hidden state of the node \( v \) is
updated as follows:

$$h_v^{(t)} = \sum_{u \in N(v)} f_w(x_v, x_{e(v,u)}, x_u, h_u^{(t-1)})$$

where $f_w(\cdot)$ is a parametric function, $N(v)$ is the neighbourhood of the node $v$, and $h(0)$ is randomly initialised for each node. Further details can be found in Scarselli et al. (2008). In the literature, iterative graph processing techniques based on neural networks with a message passing architecture are generally referred as RecGNNs.

To face the computational costs of these methods, several kinds of neural network models were proposed in literature, often with the aim of generalise classical and established neural networks processing to graph data such as Generative Adversarial Network (GAN) Goodfellow et al. (2014), attentional mechanisms Baldanau et al. (2014), or CNNs.

2.3 Graph Convolutional Neural Networks

A particular focus was given in the literature to perform convolution on graph-structured data. GCNNs share the idea of message passing adopted by RecGNNs but implement it in a non-iterative manner: information is exchanged between neighbours using different convolutional layers, each with different filters Wu et al. (2020). However, the non-Euclidean characteristic of graphs (e.g., their irregular structure) makes the convolution and filtering operations not as well-defined as those on images. For this reason, in the past decades, researchers have been working on how to conduct convolution operations on graphs distinguishing two different approaches:

- the **spectral approach**, that relies on the graph spectral theory, involving graph signal processing, such as graph filtering and graph wavelets (see, for example, Henaff et al. (2015); Li et al. (2018); Levie et al. (2018));

- the **spatial approach**, that leverages on structural information to perform convolution, such as aggregations of graph signals within the node neighbourhood (see, for example, Atwood and Towsley (2016); Hechtlinger et al. (2017)).

We point out that although spectral architectures have been explored successfully in several works, such as Henaff et al. (2015); Li et al. (2018); Levie et al. (2018), one of the main problems of GCNNs in the spectral domain is that the graph structure is fixed for all the inputs because of the use of the graph Laplacian in the training stage. Although strategies to use GCNNs with different inputs graph structures were proposed Li et al. (2018), this problem is generally not present in the spatial domain.

Recently, many spatial domain methods have been proposed in the literature. For example, in Niepert et al. (2016) the authors present PATCHY-SAN,
a GCNN model inspired by the classical image-based CNN. In [Atwood and Towsley (2016) and Hechtlinger et al. (2017)] two different methods to generalise the convolutional operator using random walks for neighbourhood locating were reported. In [Wu et al. (2019)] the complexity of a graph neural network was reduced, collapsing the network layers into a single linear transformation. Nevertheless, in the most significant part of the proposed methods the graph structure of the inputs is given a priori, that is, the input structure has to be defined before the network training stage. Interestingly, in [Zhang et al. (2019)] the authors proposed a method to learn or refine the graph structure together with the network parameters. However, this method, as for the classical CNNs, relies on learned filters whose values are fixed and equals for all the inputs.

The method we propose in this paper, following [Zhang et al. (2019)], adopts the approach to learn or refine the graph structure together with the network parameters. However, it also modifies the network’s behaviour using dynamically generated convolutional filters computed by a filter-generating network, as suggested in [Jia et al. (2016)].

To summarise, our proposal consists of performing a spatial convolution on graph-structured data merging two different aspects: to learn or refine information related to the input graph structure and to adapt the GCNNs behaviour to its input. Implementing an input-adaptable filtering operation brings two main advantages, as the experimental results will show: an improvement in the overall performances and a more compact model in terms of trainable parameters.

3 Method description

In this work, we propose a GCNN-based architecture whose convolutional filters change in function of the input features. Differently from similar works as [Simonovsky and Komodakis (2017)], where filters depend on the graph edges, we propose a dynamic behaviour architecture based on the graph nodes’ features. In this section, after a brief introduction of graphs’ notation, a detailed description of our proposal is given.

3.1 Notations

Let \( G = (V, E) \) be an undirected or directed graph where \( V \) is a finite set of \( N \) nodes, and \( E \) is a finite set of edges. We define in boldface \( x^i \in \mathbb{R}^{1 \times J} \) the input feature vector related to the node \( i \in V \), where \( J \) is the number of input channels, and \( y^i \in \mathbb{R}^{1 \times M} \) its output feature vector, where \( M \) is the number of output channels. Let \( X \in \mathbb{R}^{N \times J} \) denote the matrix representation of an input graph as an embedding of the feature vectors of its nodes.

In order to obtain neighbourhoods with a sufficient number of nodes to which apply a filter of dimension \( K \), we select the \( k \)-nearest neighbours of each node using some node distance definition, for example, the classical shortest path distance [Buckley and Harary (1990)]. Neighbourhoods are uniquely defined for
each node. We will generally refer to the neighbourhood of a given node \( n \) as \( N(n) \).

### 3.2 Proposed approach

This work aims to perform convolution on graphs using dynamically generated filters conditioned on a given input. As we have described above, otherwise from ECC in Simonovsky and Komodakis (2017), where convolution is performed using dynamical *edge-based* filters, our intent consists in using *node-based* filters dynamically generated from nodes’ feature vectors.

Considering an input graph \( X \), using a filter-generating network \( h(\cdot) \) with parameters \( \theta \) we can generate a set of node-specific filters \( F = h_\theta(X) \) to achieve a dynamic convolution on input graphs. Supposing to compute the \( m \)-th output channel of the node \( n \), following the formulation proposed in Zhang et al. (2019) our proposal can be formalised as follows:

\[
y_n^m = f\left( \sum_{j=1}^{J} \sum_{l=1}^{K} A_{nl} F_{jlm} x_s^{(n,l)}(\cdot) \right)
\]

where \( s(n,l) \) returns the index of the \( l \)-th neighbour of \( N(n) \), \( A_{nl} \) represents a correlation degree between each node \( n \) and its \( l \)-th neighbour, according to the definition given in Zhang et al. (2019), \( F_{jlm} \) are the filters generated by the filter-generating network \( h_\theta(\cdot) \). Thus, two different types of parameters, \( A \) and \( \theta \), have to be learned during the training stage.

We remark that, following what is described in Jia et al. (2016), the proposed approach will be implemented in two different ways:

1. **Dynamic Convolutional Graph Neural Network** (D-ConvGNN): the filter-generating network, defined as \( h_\theta : \mathbb{R}^{N \times J} \rightarrow \mathbb{R}^{J \times K \times M} \), takes as input the the input graph and generates a unique set of filters shared among all the neighbourhoods;

2. **Dynamic Local Convolutional Graph Neural Network** (DL-ConvGNN): the filter-generating network, defined as \( h_\theta = \mathbb{R}^{K \times J} \rightarrow \mathbb{R}^{J \times K \times M} \), for a given node \( n \), takes as input the embedded feature vectors of its neighbourhood \( N(n) \) and generates a local set of filters.

Both of the implementations are depicted in Figure 1. We will refer to the convolutional layer involving the dynamic filtering layer as **D-ConvGNN**, and to the one involving the dynamic local filtering layer as **DL-ConvGNN**.

The resulting \( A_{nl} \) matrix expresses the strength of the learned relationship between the node \( n \) and its \( l \)-th neighbour after the training stage so that it can be viewed as *a posteriori knowledge*. As it was reported in Zhang et al. (2019), all entries in \( A \) were initialised with a constant \( c \).

Moreover, according to what is made in Zhang et al. (2019), a sparse constraint, defined as an \( L_1 \) norm on the \( A \) matrix, is considered to let the layer...
emphasise only important relations among the neighbourhoods. The sparse constraint is added to a general loss function of the entire network following a Lagrangian form:

$$\mathcal{L}(\hat{Y}, Y) = \mathcal{L}_b(\hat{Y}, Y) + \gamma \sum_i P \|A^i\|$$

where $\hat{Y}$ are the predicted labels, $Y$ represents the ground truth, $\mathcal{L}_b$ is a basic loss function (such as Cross-Entropy Loss for classification tasks or MSE for regression tasks), $P$ is the number of D-ConvGNN/DL-ConvGNN layers, $A^i$ is the a posteriori knowledge learned by the $i$-th layer and $\gamma$ is the Lagrange multiplier balancing the effect of basic loss and the sparse constraint.

The use of a dynamic approach in performing the filtering operation, as the experimental results will show, involves the use of a fewer number of convolutional filters leading to a simpler architecture having, in some cases, a fewer number of trainable parameters. Moreover, in this approach, the dynamic behaviour is enhanced differently from ECC by the contribution of the underlying structural graph information learned by the $A$ matrix.

The advantages of the proposed approach can be summarised as follows:

- It inherits the standard convolution operation from classical CNNs. The convolution is performed on each node with its nearest neighbours applying sets of fixed-sized filters.
- It learns underlying input structural information. While processing a node with its neighbourhood, the structural information learned emphasises node relationships, increasing the overall performances.
- Its behaviours changes according to the input. Filters used for the convolution are dynamically generated using an external module based on the input graphs.
- Convolution operations are locally and globally adaptive. Dynamic filters can be input dependent and shareable over all the inputs’ neighbourhoods, or neighbourhood-dependent, allowing the convolution to be locally dynamic.
- Dynamic behavioural of the convolutional filters leads to design simpler architectures. Promising results can be achieved using a fewer number of convolutional filters than a non-dynamic approach.

4 Experimental assessment

We conducted the experimental assessment of our method, running two series of experiments. At first, we conducted preliminary experiments on the well-known benchmark dataset MNIST modelling grid-structured data as graphs to test
Figure 1: A graphical description of the D-ConvGNN (a) and DL-ConvGNN (b) layers in processing a node - marked in red - using filters of dimension $K = 5$. Using the D-ConvGNN method (a), a unique set of filters dependent on all the nodes’ feature vectors of the input graph is dynamically generated and shared among all of its neighbourhoods. On the contrary, filter sets are dynamically generated in each neighbourhood using the DL-ConvGNN method (b), and they are dependent only on the nodes’ feature vectors of the neighbourhoods themselves (neighbourhood dependent filters are marked by the same colour of the node that is being processed). Finally, jointly with the nodes’ entries of the $A$ matrix (marked by the same colour), in both cases, input signals of the neighbourhoods are weighted summed to compute the nodes’ outputs.

our proposal’s feasibility. In this first series of experiments, we compared the performances of our approach with the ones achieved by non-dynamic GCNN methods. We point out that in this series of experiments, we are not interested in obtaining better results than other approaches presented in the literature, but we want to validate the feasibility of our method experimentally. In the second series of experiments, we have applied our approach in some of the experimental scenarios reported in Zhang et al. (2019) in order to make a comparison with a non-dynamic convolution neural network on general graph-structured data. In
particular, we chose DPP4, 20NEWS and Reuters-21578 datasets.

We aim to overcome the results reported in the literature while keeping the number of convolutional filters low and using filter-generating networks with simple architectures (such as shallow neural networks) for both the D-ConvGNN and the DL-ConvGNN. Table 1 there is a summary of the datasets selected in our experiments. It is essential to underline that all the experiments were carried out using the identical experimental setups reported in the reference papers to make a fair comparison.

| Dataset         | Learning Task        | #graphs | |V| | #classes |
|-----------------|----------------------|---------|-----|-----|----------|
| MNIST           | Graph Classification | 70000   | 717 | 10  |
| DPP4            | Graph Regression     | 8193    | 2153| -   |
| 20NEWS          | Graph Classification | 17236   | 10000| 20  |
| Reuters-21578   | Graph Classification | 8931    | 1500 | 90  |

Table 1: Datasets selected for the experiments

4.1 MNIST

We used the widely known MNIST handwritten digits dataset for running the first series of experiments. In order to make a comparison with a spatial GCNN method, we focused on the experiments described in Hechtlinger et al. (2017). In particular, we focused on making a comparison using an experimental setup on the MNIST dataset proposed in Hechtlinger et al. (2017) where, after the exclusion of constant pixels, images are modelled as graphs computing pixels’ relationships using their correlation matrix: a directed edge links two pixels (nodes) if their correlation in absolute value exceeds a fixed threshold value.

Again, in Hechtlinger et al. (2017), the authors have considered $K = 6$ neighbours per node to perform the filtering operations. This task can be defined as a 10-classes classification problem; each sample is described by a graph whose set of vertices has cardinality $|V| = 717$; each node is described by 1 feature; this dataset was reported already split in training (60000 samples) and test (10000 samples) sets.

4.2 Merck Molecular Activity Challenge

The Merck molecular activity is a Kaggle challenge whose main task consists in predicting the biological activities of 15 molecular activity datasets. Each molecule is defined by numerical descriptors generated by its chemical structure. Following different works such as Zhang et al. (2019), Hechtlinger et al. (2017), Henaff et al. (2015), we have experimented our approach on DPP4 dataset which contains 6148 training and 2045 test molecules, defining this task as a regression problem on graph-structured data. As described in Zhang et al. (2019), we have omitted features that are active in less than 20 molecules, resulting in 2153 features per sample. Moreover, following Hechtlinger et al. (2017), we can

1https://www.kaggle.com/c/MerckActivity
refer to the information concerning the correlation structure between features to extract an adjacency matrix to be associated to the DPP4 structure: we consider two descriptors as linked by a directed edge if their correlation in absolute value exceeds a fixed threshold value, exactly as it was described for tests on the MNIST dataset.

According to the standard set by the Kaggle challenge, predictions on the test set are evaluated using the correlation coefficient $R^2$ defined as:

$$R^2 = \text{Corr}(\hat{Y}, Y)^2$$

where $\hat{Y}$ is the predicted activity level, $Y$ is the ground truth, and $\text{Corr}(\cdot)$ is the correlation coefficient. We can define this task as a regression problem; each sample is described by a graph whose set of vertices has cardinality $|V| = 2153$; each node is described by one feature; this dataset was reported already split in training (6148 samples) and test (2045 samples) sets.

4.3 Text categorisation

At last we tested our approach also on a classification task based on two datasets mentioned by Zhang et al. (2019): 20NEWS Joachims (1996) and Reuters-21578 Lewis (1997).

4.3.1 20NEWS dataset

The 20NEWS dataset consists of 20 classes and 17236 samples. Following the preprocessing described in Defferrard et al. (2016), we consider only the 10000 most frequently used words and adopt the bag-of-words model Zhang et al. (2010) to represent each document.

Finally, we adopt the cosine similarity metric between words, described as 100-D vectors generated by word2vec Mikolov et al. (2013), to compute connections among nodes. We can define this task as a 20-classes classification problem; each sample is described by a graph whose set of vertices has cardinality $|V| = 10000$; each node is described by one feature; this dataset is made available already split in training (10167 samples after the preprocessing) and test sets (7069 samples after the preprocessing).

4.3.2 Reuters-21578 dataset

The Reuters-21578 dataset consists of 10788 text documents multi-labelled with 90 different classes. To recreate the same experimental setup described in Zhang et al. (2019), we firstly deleted the multi-label documents, transforming the problem into a single-label one, and then we applied the same preprocessing we made on the 20NEWS dataset, but considering the most 1500 frequently used words to use the bag-of-words model.

We can consider this task as a 90-classes classification problem; each sample is described by a graph whose set of vertices has cardinality $|V| = 1500$; each node is described by one feature; this dataset is available already split in training
set (6399 samples after the preprocessing) and test set (2532 samples after the preprocessing).

5 Results

For each experiment we have adopted a grid search approach for hyperparameters tuning. The ranges of values are reported in the experiments’ related tables 4, 2 and 6.

Except for the first test on the MNIST dataset, in order to check the fairness in the reproduction of the identical experimental setups, we have executed a preliminary analysis in which we have tried to replicate the performance reported by the referenced papers Hechtlinger et al. (2017); Zhang et al. (2019) using their models.

Model performance estimation was performed using an holdout method since each dataset reports a predefined train/test split. Moreover, during the training stage, 30% of the training set was extracted following a stratified sampling to select a validation set.

We chose shallow neural networks with one hidden layer as filter-generating network (FGN) architectures, whose number of nodes was tuned using grid search in each experiment. We denote with \(C_t\) a convolutional layer with \(t\) filters, and with \(FC_t\) a fully connected layer with \(t\) hidden units.

5.1 MNIST

In Table 2 we report the grid search ranges for determining the hyperparameters in the case of the MNIST dataset. In these tests, we used a learning rate scheduler to decrease the learning rate by 30% every 15 epochs. The threshold applied on the features’ correlation values to construct the adjacency matrices was considered a hyperparameter.

| Hyperparameter          | Range               |
|-------------------------|---------------------|
| \(K\)                   | 6                   |
| \(\gamma\)              | \(\{10^{-7}, 10^{-5}\}\) |
| Optimizer               | Adam                |
| Loss                    | Cross-Entropy Loss  |
| Learning Rate           | \(10^{-1}\)         |
| Output Channels         | \{1, 3, 5, 7, 9, 10\} |
| \(c\)                   | \(\{10^{-5}, 10^{-2}\}\) |
| Threshold               | \{0.1, 0.2, ..., 0.9\} |
| FGN Architectures       | \{FC50, FC100, FC150, FC200\} |

Table 2: Grid search settings used for the experiments on MNIST dataset.

As we can see from the results in Table 3 our approach achieves an accuracy that can be considered comparable with the one reached by Hechtlinger et al.
Moreover, our dynamic approach leads to achieving good performances with a simpler architecture: the graph CNN model achieves its best error rate using two convolutional layers with 20 filters; both the D-ConvGNN and DL-ConvGNN models achieve comparable results using one convolutional layer with 5 dynamically generated filters. Furthermore, it is also important to point out how the use of DL-ConvGNN can lead to a lower number of trainable parameters against the other approaches.

| Method                     | Architecture | #params | Accuracy (%) |
|----------------------------|--------------|---------|--------------|
| Graph CNN (Hechtlinger et al.) | C20-C20      | 145970  | 98.41        |
| D-ConvGNN (ours)           | C5           | 152397  | 97.85        |
| DL-ConvGNN (ours)          | C5           | 49447   | 97.61        |

Table 3: Results on the MNIST dataset.

5.2 Merck Molecular Activity Challenge

The grid search ranges for determining the hyperparameters for experiments with the DPP4 dataset are reported in Table 4. As for the MNIST case, the threshold value to apply to the features’ correlation values to extract the adjacency matrices was chosen as a hyperparameter.

| Hyperparameter  | Range       |
|-----------------|-------------|
| K               | 16          |
| γ               | 10^{-7}     |
| Optimizer       | Adam        |
| Loss            | MSE         |
| Learning Rate   | 1^{-3}      |
| Output Channels | 1           |
| c               | {10^{-5}, 10^{-4}, ... , 10^{-1}} |
| Threshold       | {0.1, 0.2, ..., 0.9} |
| FGN Architectures | {FC50, FC100, FC150, FC200} |

Table 4: Grid search settings used for experiments on DPP4 dataset.

For the evaluation of performance we use the $R^2$ correlation coefficient as stated in Section 4.2. As reported in Table 5 our approach outperforms the result reached by the GSCN method. It is possible to see that the proposed dynamic approach needs only one convolutional filter against the 10 convolutional filters needed by the non-dynamic approach to reach its best result. We also underline that DL-ConvGNN has a lower number of trainable hyperparameters than the other methods in this experiment.

5.3 Text categorization

Since both 20NEWS and Reuters-21578 datasets were preprocessed by almost the same pipeline, which led to a similar data representation, we used the same
grid search ranges reported in Table 5, for both of the datasets. The preprocessing pipeline used for these tasks followed what was done and shared by Defferrard et al. (2016).

| Hyperparameter       | Range             |
|----------------------|-------------------|
| K                    | 25                |
| γ                    | 0                 |
| Optimizer            | Adam              |
| Loss                 | Cross-Entropy Loss|
| Learning Rate        | $10^{-3}$         |
| Output Channels      | $\{1, 2, ..., 10\}$|
| c                    | $\{10^{-5}, 10^{-4}, ..., 1\}$|
| FGN Architectures    | $\{\text{FC50, FC100, FC150, FC200, FC250}\}$|

Table 6: Grid search ranges used for experiments on Reuters-21578 and 20NEWS datasets.

### 5.3.1 20NEWS dataset

During our preliminary analysis, although we tried to replicate the performances as described in Zhang et al. (2019) using the same experimental setup, we could not achieve the GSCN score reported in Zhang et al. (2019) for the batch of experiments on the 20NEWS dataset, probably because in some differences in the processing pipeline. For this reason, in order to make a comparison with our results, we have considered our best GSCN’s score that is reported in Table 7. As we can notice, our approach outperformed the GSCN’s result using a lower number of filters also in this case.

| Method                              | Architecture | Accuracy |
|-------------------------------------|--------------|----------|
| GSCN (Zhang et al.)                 | C16-FC100    | 68.83    |
| GSCN (Zhang et al., our implementation) | C16-FC100    | 60.36    |
| D-ConvGNN (ours)                    | C5-FC100     | 63.15    |
| DL-ConvGNN (ours)                   | C3-FC100     | 62.85    |

Table 7: Results on the 20NEWS dataset.

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2https://github.com/mdef/cnn_graph
5.3.2 Reuters-21578 dataset

As one can see from Table 8, our approach outperforms the result reached by the GSCN method. These results still confirm that our dynamic approach uses fewer convolutional filters to achieve more satisfactory performance than a non-dynamic approach.

| Method               | Architecture | Precision | Recall | F1-measure |
|----------------------|--------------|-----------|--------|------------|
| GSCN (Zhang et al.)  | C16-FC100    | 77.93     | 71.31  | 73.25      |
| D-ConvGNN (ours)    | C3-FC100     | 92.62     | 93.01  | 92.58      |
| DL-ConvGNN (ours)   | C6-FC100     | 92.45     | 93.05  | 92.56      |

Table 8: Results on the Reuters-21578 dataset.

5.4 Discussion

According to the results shown above, our dynamic approach allows us to consider simpler architecture than non-dynamic ones. This aspect was first observed during the experiments on the MNIST dataset, where very simple architectures have led to results comparable with the ones achieved by complex architectures. A similar observation was made while comparing the tests made in Zhang et al. (2019) where, using the same architectures, we have empirically seen that our approach needs a fewer number of convolutional filters to process information while achieving better results. This aspect leads, in general, to design convolutional architectures that will be more compact than the standard ones, where a considerable number of filters and convolutional layers are usually taken into account to extract meaningful information.

To make a comparison between the D-ConvGNN and DL-ConvGNN models, we have not observed particular differences in performances between these two models. It is relevant to point out that, due to the nature of its filter-generating network, the DL-ConvGNN needs a considerably lower number of trainable parameters with respect to D-ConvGNN: this aspect, for example, was emphasised in Table 5 during the experiments on the DPP4 dataset where, considering one convolutional filter and same architectures for the filter-generating networks in both of the models, D-ConvGNN presents 470619 learnable parameters against the 41569 presented by DL-ConvGNN.

It is important to point out that the use of the A matrix as described in Zhang et al. (2019) and adopted here, limits the use of this convolutional layer only to dataset whose samples are described by a fixed graph topology: we remind that $A_{nl}$ contains the learned structural information about the $n$-th node and its $l$-th neighbour, and this relation is fixed in each sample. This limit does not allow to directly compare with the ECC model where instead, the convolution operation is not constrained to a fixed samples’ topology. In future work, we would like to handle this limit to extend the functionality of this layer to datasets with non-fixed topologies among the samples, such as ENZYMES Schomburg et al. (2004) and MUTAG Debnath et al. (1991).
6 Conclusion

In this work, we have proposed a dynamic method to perform convolution on graph-structured data. Combining the idea of having dynamically changeable behaviours in ANNs and convolutional graph neural networks, this work aimed to present a graph convolutional layer capable of performing convolution using node-specific filters in order to achieve an input-suitable filtering operation. To perform convolution on graphs, we decided to adopt a spatial approach, focusing on the characteristic of the GSCN model presented in [Zhang et al. (2019)] in learning graph structural information during the training stage. Moreover, referring to what has been done by Jia et al. in [Jia et al. (2016)] on CNNs, we have considered altering, in a dynamic fashion, the behaviour of our convolutional layer with the using of an external module, the filter-generating network. In this way, the proposed graph convolutional layer learns and applies input-suited filters, making the filtering operation customizable according to its input graph, and enhancing the overall performances using the learned structural information. Furthermore, we have considered two versions of this dynamic convolutional layer: the D-ConvGNN, which generates dynamic filters conditioned to the signals of the entire input graph, and the DL-ConvGNN, which generates local dynamic filters conditioned to the neighbourhoods’ signals.

To assess the improvements in using a dynamic approach to generate convolutional filters, a series of experiment was made to compare our approach with non-dynamic spatial GCNNs, focusing on the GSCN model. Moreover, it empirically emerged that a dynamic approach requires a low number of convolutional filters to achieve satisfying results, involving a lower number of learnable parameters specially in the case of the DL-ConvGNN.

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