Multivariate Time Series Regression with Graph Neural Networks

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Abstract

Machine learning, with its advances in Deep Learning has shown great potential in analysing time series in the past. However, in many scenarios, additional information is available that can potentially improve predictions, by incorporating it into the learning methods. This is crucial for data that arises from e.g., sensor networks that contain information about sensor locations. Then, such spatial information can be exploited by modeling it via graph structures, along with the sequential (time) information. Recent advances in adapting Deep Learning to graphs have shown promising potential in various graph-related tasks. However, these
methods have not been adapted for time series related tasks to a great extent. Specifically, most attempts have essentially consolidated around Spatial-Temporal Graph Neural Networks for time series forecasting with small sequence lengths. Generally, these architectures are not suited for regression or classification tasks that contain large sequences of data. Therefore, in this work, we propose an architecture capable of processing these long sequences in a multivariate time series regression task, using the benefits of Graph Neural Networks to improve predictions. Our model is tested on two seismic datasets that contain earthquake waveforms, where the goal is to predict intensity measurements of ground shaking at a set of stations. Our findings demonstrate promising results of our approach, which are discussed in depth with an additional ablation study.

**Keywords:** Graph Neural Networks, Time Series, Convolutional Neural Networks, Sensors, Regression, Earthquake Ground Motion, Seismic Network

## 1 Introduction

In today’s world, advances in hardware and wireless network technology have opened the path for energy-efficient, multi-functional and low-cost sensors [1]. Spread across a large geographical region, a set of sensors can then form a sensor network used for data collection and analysis [2], in particular considering large-scale time series data. Example domains where such real-world sensor data is analyzed include, e.g., traffic [3], weather [4] and seismology [5], regarding time series anomaly detection, forecasting, segmentation, as well as regression and classification. Exemplary standard techniques to tackle such problems are Gaussian processes [6], ARIMA [7] and XGBoost [8].

Recently, however, there have been considerable advances in Deep Learning methods, in particular with respect to their ability to automatically find structure in the data leading to powerful (implicit) feature construction and well performing models. In particular, the advances of using Convolutional Neural Networks (CNNs) have attracted a lot of interest due to their power to extract meaningful features from the raw time series, e.g., [9, 10]. However, if only the time series data are examined, then some aspects of the sensor data are left unseen, i.e., the spatial relations for datasets that have a grounding in a geographical sense.

Therefore, researchers have developed Deep Learning techniques to perform time series analysis like forecasting [11], anomaly detection [12] and imputation [13], with data arising from networks (i.e., graphs), called Graph Neural Networks (now referred to as GNNs), which we also focus on in this paper. However, these models focus on tasks that are vastly different from regression or classification analysis (e.g., time series forecasting).

In contrast to previous research, in this paper we tackle the problem of time series regression with GNNs, for which we present an architecture to perform multivariate time series regression using GNNs.
Previous attempts for tackling similar time series problems with graph-based methods have been made by [5, 14, 15], yet each have some shortcomings. [5] mention that they designed a Deep Learning approach using a GNN. However, they only append the (latitude, longitude) information to the time series being handled by a CNN. Therefore, while prediction scores improved, no actual GNN layers were used. Second, [14] proposed a graph partitioning algorithm that works together with a CNN. However, they make use of classical graph theory techniques and a GNN method is not applied. Lastly, [15] recently suggested a method that uses CNNs and GNNs for seismic event classification. However, (1) their model focuses on time series classification instead of regression, (2) no spatial or (3) meta information about the stations is added, (4) only three nodes are examined for each observation and (5) global average-pooling is used which removes many (informative) features.

Therefore, to the best of the author's knowledge, this is the first attempt to create a larger scale Deep Learning architecture that can process multivariate time series for such a regression task. By combining the capabilities of a CNN (feature extraction) and a GNN (spatial information), our model can manage the feature sizes that are common in high-frequency time series data arising from multiple sensors.

We test our proposed models on network-based seismic data. The model is inspired by the work presented in [16] and [17], which functions as our baseline. In their work, the maximum ground-shaking at a set of seismic stations is predicted by tackling this as a regression problem. Their model used CNNs to extract useful features from the time series. We start from their work as a departure point, and illustrate how to design the Deep Learning model structure using GNNs for such a task.

Our contributions are summarized as follows:

1. We propose a method to perform multivariate regression on time series originating from graph-structured data. For this, we present an architecture utilising CNNs and GNNs that is also adjustable for other use cases, e.g., time series classification tasks.
2. We evaluate our model thoroughly on two seismological datasets that differ significantly from one another evidencing the generality and potential of the proposed GNN-based architecture. We discuss our results in detail and perform a comparison against the baseline model proposed in [16].
3. Finally, we systematically analyze the capabilities of our model in detail by comprehensive experimentation adjusting several hyperparameters in our proposed workflow.

The rest of the paper is structured as follows: We discuss related work in Section 2, which provides the necessary background on Deep Learning, graphs and GNNs. Next, our method and training settings are explained in Section 3. After that, Section 4 introduces the used datasets, presents our results and discusses these in context of a model-based comparison. Finally, Section 5 concludes with a summary and outlines interesting directions for future work.
2 Background and Related Work

In the following, we briefly outline background and related work on graphs and Deep Learning in general, CNNs, GNNs and its utilization in time series, as well as the implementation of Deep Learning for seismic analysis.

2.1 Deep Learning on Complex Data

Traditional machine learning often requires considerable effort from the user to construct meaningful features, which is time-consuming and error-prone [9]. Deep Learning provides a way for automatic feature extraction with the help of multiple layers that can utilise nonlinear processing. In particular, this also relates to complex representations such as time series and graphs. Therefore, Deep Learning offers strong processing and learning on complex data.

Initially, the Multi-layer Perceptron (MLP) was developed in which all network layers are fully linked [18]. While being powerful, due to its high computation time the depth of the network is limited. Therefore, researchers have found ways to create more advanced architectures for specific tasks. One of the most prominent and successful outcomes of this effort is the CNN discussed in the next section.

2.2 Convolutional Neural Networks (CNN)

A CNN is a regularized MLP that is specialized in handling data structures with multiple dimensions (e.g., pictures with color channels). It uses a feed-forward structure with convolutions instead of more general matrix multiplications. CNNs are widely adopted in Natural Language Processing and Computer Vision. A CNN has an advantage over MLPs due to its use of weight sharing, sampling and local receptive fields [19]. In order to create output, the convolutional layers convolve the input using filters and activation functions.

More formally, a convolution operation is defined as:

$$y^{l+1}_i(j) = k^l_i \ast M^l(j) + b^l_i$$

where $y^{l+1}_i(j)$ denotes the input of the $j$-th neuron in the feature map $i$ of layer $l+1$, $k^l_i$ the weights of the $i$-th filter kernel in layer $l$, $M^l$ the $j$-th local region in layer $l$ and $b^l_i$ the bias. An activation function is applied after each convolutional layer to retrieve the nonlinear features. An example of a commonly used activation function is the Rectified Linear Unit (ReLU):

$$\text{ReLU}(x) = \max(0, x)$$

where $x$ is the convolutional layers output. ReLU is a piecewise linear function that will directly output the input if positive, otherwise, it will return zero. Another common activation function is the hyperbolic tangent (TanH) [20]:

$$\text{TanH}(x) = \frac{e^x - e^{-x}}{e^x + e^{-x}} = 1 - \frac{2}{1 + e^{2x}} \in [-1, 1]$$
where $e$ is Euler’s mathematical constant. The advantage of TanH is that negative values can be returned, which is useful if your desired output data distribution contains those.

2.3 Graphs

Before discussing the extension of Deep Learning models to graphs, we first introduce some background and basic notation in this area. Essentially, the field of Deep Learning with graphs focuses on a data structure called a graph, that models the relationship between a set of objects (nodes or vertices $V$) and their connections/interrelationships (given by a set of edges $E$ linking the respective nodes/vertices); see Figure 1b below for an example. Graphs can model various systems across numerous areas such as social networks, physical systems and knowledge graphs. Most commonly, the tasks at hand are: node-classification, link prediction, graph-classification and node clustering [21].

More formally, we define a graph as $G = (V, E)$ where $V$ is the set of nodes and $E$ the set of edges. An edge $e_{ij} = (v_i, v_j)$ connects nodes $v_i$ and $v_j$. A common way to represent and store a graph is with an Adjacency matrix $A \in \mathbb{R}^{N \times N}$ where $N = |V|$, which is a square matrix such $A_{ij} = 1$ if there is an edge from node $v_i$ to node $v_j$, and 0 otherwise. The number of neighbors of a node $v$ is known as the degree of $v$ and is denoted by $D_{ii} = \sum_j A_{ij}$, where $D$ is then the diagonal degree matrix. Edges can be undirected and directed. Undirected edges contain no notion of source and destination, e.g., the absolute distance between two nodes is always equal no matter from which node the measurement starts. Directed edges do contain direction, e.g., whether somebody follows someone else on a social network or not.

However, nodes, edges and entire graphs can have features as well, such that a feature vector $a = (a_1, a_2, \ldots, a_n)$ of individual features $a_i \in \Omega_A$ out of a feature domain $\Omega_A$ is assigned to the nodes (and/or edges). Such features can be applied in Deep Learning using GNNs as we will see below. Fundamentally, node features can be used to predict the label of an entire graph as well, which would be a global graph feature. GNN problems therefore mostly consist of node-level, edge-level and graph-level tasks.

2.4 Deep Learning on Graphs

Essentially, while the CNN has been an amazing breakthrough, there was still a need to bridge the gap between Deep Learning and graphs. Specifically, the standard CNN convolutions are not applicable to graph-structured data due to its non-euclidean nature. In particular, one cannot convolve a $n \times n$ grid over a graph the same way as with an image, for example, as is visible in Figure 1. In Figure 1a, both the red and blue boxes convolve over the same $n$ numbers. In Figure 1b, the red box convolves three nodes, except the blue box convolves over two nodes. Therefore, extensive effort was put into finding ways to define convolutions over graphs.
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Fig. 1: (a) Matrix-based convolution on an image / time series or a (b) graph where a convolution is a lot harder to define.

2.5 Graph Neural Networks

GNNs are Deep Learning based methods that are adapted for the graph domain. Historically, there are two main classes of methods that GNNs used: (1) Spectral methods and (2) Spatial methods. Spectral methods use the eigenvectors and eigenvalues of a matrix with eigendecomposition, and perform convolutions with the Graph Fourier Transformation and inverse Graph Fourier transform. These transformations of the signal $x$ are defined as $F(x) = U^T x$ and $F^{-1}(x) = U x$ where $U$ represents the matrix of eigenvectors of the normalized graph Laplacian $L = I - D^{-1/2} A D^{-1/2}$, $D$ is the degree matrix of the Adjacency matrix $A$ and $I$ refers to the identity matrix of length $|V|$ [22].

Spatial methods use message passing techniques which look at the local neighborhood of nodes and perform calculations on their top-k neighbors. With a node aggregation/update function $f$, an updated node representation $Z$ could then be defined as $Z = f(G)X$ where $G$ refers to the Adjacency or Laplacian matrix, and $X$ to the node features of the nodes in $G$ [23]. However, a serious issue with spatial methods is determining the convolution procedure with differently sized node neighborhoods [22].

To conclude, there are two typical operations when designing GNNs: Spatial methods focus more on the connectivity of the graph, while Spectral methods focus on the eigenvalues and eigenvectors of a graph [23]. As we will see later, both techniques were recently brought together by work of e.g., [24].

In general, the history of creating Deep Learning models for graphs is surprisingly long. For example, Recursive Neural Networks were already adapted to work on directed acyclic graphs in the 1990s [25]. However, one recent paper that revamped the interest in using Deep Learning on graphs was written by Bruna et al [26]. They propose two ways that use hierarchical clustering and the spectrum of the graph Laplacian to perform convolutions on low-dimensional graphs. This highlights the origin of the aforementioned spectral methods, which mostly come from Spectral Graph Theory [27]. Afterwards, the Chebnet [28] was introduced that improved the convolution procedure with fast localized convolution filters. They overcome the problem of non-localized filters in the spectral domain, and the problem of matching local neighborhoods in the
spatial domain by introducing a special filter parametrization. This approach is then simplified by Kipf and Welling [24] into the now so-called Graph Convolutional Networks (GCNs), which are also used in this paper. They define their propagation rule (convolution in a graph) as follows:

$$H^{(l+1)} = \sigma \left( \tilde{D}^{-\frac{1}{2}} \tilde{A} \tilde{D}^{-\frac{1}{2}} H^{(l)} W(l) \right)$$  \hspace{1cm} (4)$$

where \(H^{(l)} \in \mathbb{R}^{N \times D}\) is the matrix of activations of the \(l\)th layer, \(\sigma\) denotes the selected activation function, \(\tilde{D} = \sum_j \tilde{A}_{ij}\) refers to the degree matrix; matrix \(\tilde{A} = A + I_N\) is the Adjacency matrix of the undirected graph \(G\) with the added self-connections \(I_N\) to include a node’s own node features, \(H^{(0)} = X\) where \(X\) are the node features and \(W^{(l)}\) the trainable weight matrix for a specific layer. This equation produces a node-specific output of size \(N \times F\) features in which \(F\) is the number of desired output features for each node \(N\). Based on this, we will now discuss extensions for time series analysis.

2.6 Graph Neural Networks for Time Series Analysis

Considering the connection between GNNs and classical time series analysis, most effort is visible in forecasting time series [11, 29]. These approaches adapt existing neural network architectures to use operators from the graph domain. Examples are Gated Recurrent GNNs that utilise the spectral convolutions from [28]. Also, Diffusion-Convolutional Networks are introduced that take into account the in and out-degree of nodes to capture the spatial dependencies of nodes better, which is beneficial in e.g., traffic prediction use cases [30]. Later on, Spatio-Temporal Graph Convolutional Neural Networks are introduced that interchange the convolution procedure between temporal and spatial dimensions [31]. In addition, GNNs have been used to perform anomaly detection in time series data. [12] propose an attention-based GNN that used the results of a forecast to classify deviating predictions as anomalies. In addition, [13] propose GRIL (Graph Recurrent Imputation Layer), a Spatial-Temporal GNN that reconstruct missing data by learning spatial-temporal representations.

However, when modeling time series data using GNNs, most of the proposed models combine GNNs with RNNs and LSTMs that are designed for modelling data with a focus on the dependency of time [32]. More critically, they are focusing on modeling the long-term dependencies in a set of data. For example, a typical time series use case would be modeling the long and short-term dependencies in traffic data sampled every \(n\) minutes, such as performed by [11, 29, 33]. In these papers, the data imputed into the models are often in the range of 6-12 observations to predict the next few observations. However, when the task is to classify or perform regression to predict some metric, there is a lack of long-term dependency in the data. Especially in the case of high-frequency data, or when the entire phenomena that is analysed takes place in a time-frame of 0-50 seconds, whereas typical forecasting-related datasets contain days, weeks or months of data where the sampling rate is lower.
2.7 Deep Learning for Seismic Analysis

Over the past decades, huge volumes of continuous seismic data have been collected [34, 35]. This data can be modeled as complex networks, i.e., graphs forming seismograph networks consisting of observations from multiple stations. With the availability of large datasets and advances in machine learning, the seismological community has also seen a rise in the use of machine and Deep Learning. Exemplary use cases are magnitude estimation [36] and earthquake detection [37]. Specifically for waveform analysis, the CNN has been applied several times. For example, [38] developed a CNN for single-station localization, magnitude and depth estimation. In addition, CNNs were developed for P- and S-wave arrival times picking [e.g., 37, 39]. Others used multi-station waveforms which were analysed for the estimation of the location of earthquakes [5] or earthquake early warning [40].

The work of [5, 14, 15] comes most close to the goals of our work. Each of these papers tried to use time series related data in combination with graphs to improve predictions. [5] used classical CNNs that attached the (latitude, longitude) locations of the sensors to the waveforms to improve predictions, which differs from our goal to use GNN layers. In other words, metadata was used to enhance their CNN model, except no graph layers were applied. [14] propose a technique that combines CNNs with graph partitioning to group time series together based on spatial information. This procedure increases the quality of the within-group features, and improves predictions, but no GNNs were utilised. Lastly, [15] present a method that uses CNNs and GNNs for seismic event classification. However, no spatial information is provided to the model (Adjacency matrices only containing 1’s are created), no meta-information about the nodes is added, only three stations are examined simultaneously, their method focuses on time series classification and the features of the GNN are average pooled (which loses too much valuable feature information).

Here, we propose a technique that will use the full power of GNNs to perform time series analysis. To the best of our knowledge, no GNN-based method was used to perform such a time series regression task before.

3 Method

In this section, we propose the model architecture for the Multivariate Time Series Regression GNN. The full architecture is shown in Figure 3, which we will introduce via an abstract overview first, before we discuss it in detail.

3.1 Basic Model Architecture

Figure 2 presents an abstracted overview of the building blocks of our proposed architecture, which can therefore also be instantiated for other tasks, such as time series classification. In summary, our proposed architecture of a GNN for time series regression contains the following main contributions compared to previous work, as we will detail below:
1. To obtain node features, we apply a 1D CNN for feature extraction on the individual nodes using a wide kernel [9, 41] on the input data as in [16].
2. A GNN (utilizing GCN layers from [24]) of \( n \) layers is implemented for processing these feature vectors calculated by the CNN as node features. While in other GNN papers the node features each measure a unique aspect about a node (e.g., the age and friend count in a social network), we demonstrate that GCNs can also learn from features that are sequential in time.
3. Finally, we flatten the entire GCN feature output to retain enough information for later on dense layers for a desired task, whereas the standard procedure is average or max-pooling [28, 42, 43].

### 3.2 Model Implementation

This section introduces the version of our abstracted implementation applied to a regression task on seismic data. Our proposed model uses 10 seconds of 3-channel seismic waveform data as input in the first block (see Figure 3 and Section 4.1 for a full overview of the model and the dataset). After that, CNN, GNN and post-processing layers are applied.

#### 3.2.1 CNN for Feature Extraction

In the second block of our model, two 1D CNN layers act as feature extractors by using wide kernel sizes, small strides, increasing filters, regularization of \( \lambda = 10^{-4} \) and a ReLU activation function, which has proven to be useful for 1D time series data [16, 41]. The function of these CNN layers is to learn the temporal patterns of each station. Afterwards, the last two dimensions of the second CNN are flattened to make the dimensions fitted for the GNN layers, which typically need an input of \((N, F)\) where \(N\) refers to the number of nodes in the graph, and \(F\) to a one-dimensional vector of node features \([x_1, x_2 \ldots x_n]\). To this partially flattened feature vector, the node features (latitude, longitude) of each node are added as node meta data.
3.2.2 GNN Processing

Next, it follows the GNN layers where the GCN was used from [24]. While in [16] the third CNN layer gathers the cross-station information, here the GCN takes this role, since the GCNs use the features from the CNN as node features for each node. More concretely, each node \( N \) in the GCN receives one of the CNN feature vectors of dimension \((N, F)\) as node features where \( F \) is the length of the feature vector. The two GCN layers use these features of the nodes by reducing them to \((N, 64)\) by both containing 64 filters. The GCN layers, therefore, act as dimensionality reducers. Considering the hyperparameters of the GCN, experimentation revealed that starting with a ReLU activation function followed by a TanH works best, in combination with a dropout in between the two layers. In addition, bias was set to false (as suggested by [24]) and the same kernel regularizer was used as in the CNN layers.

3.2.3 Postprocessing

A standard procedure in the GNN literature is using global graph pooling operators such as max or average-pooling [28, 42, 43]. These pooling techniques reduce the dimensions of a GNN layer to one feature for each node in the graph. However, as a result this procedure removes many meaningful features that are calculated by the CNN in the previous layers. Therefore, the output of the final GCN layer is flattened to retain as many features as possible for later inference.

As performed by [16], a normalization value (the largest amplitude seen across all stations that measured the specific earthquake within the input time window) is added to the flatten layer, followed by a dense layer with 128 units. As will be explained in Section 4 in more detail, 5 dense layers of size \((N)\) with linear activation functions (values between -6 and +1 have to be predicted) are applied next. These 5 dense layers represent the regressions target variables called PGV, PGA, SA(0.3 s), SA(1 s) and SA(3 s) for each of the nodes.

3.3 Software and computer

Python was used combined with Tensorflow\(^1\) and Keras\(^2\) to develop the proposed models. The GCN layer is derived from Spektral\(^3\). Calculations are done with support of Numpy \(^4\) and table formatting with Pandas \(^5\). Furthermore, to reduce the overall training time, the models are trained on a dedicated server with two Intel Xeon CPUs (3.2GHz), 256GB RAM and a Nvidia Quadro RTX3956000 (24GB) GPU. After training, the models are fairly small (around 6MB) and are deployable, e.g., on standard PC hardware as well as edge computing platforms.

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\(^1\)https://www.tensorflow.org/
\(^2\)https://keras.io/
\(^3\)https://graphneural.network/
\(^4\)https://numpy.org/
\(^5\)https://pandas.pydata.org/
3.3.1 Model Training

For training, five runs of five-fold cross validation were performed (for stable results) by splitting the data in a random split with seed = 1, taking the best epoch of each fold. The average mean squared errors of all runs were taken as the result. The memory of Tensorflow and Keras was reset in every iteration of the k-fold cross validation.

![Diagram of the proposed architecture](image)

**Fig. 3**: Overview of the proposed architecture. The crucial steps are the flattening of the CNN output that retains the dimension of the number of nodes, in order to suit it for the dimensions the GCN layers need as node feature input. In addition, the output of the final GCN layer is not average or max-pooled, but flattened to retain as much information as possible.
The model used a batch size of 30 and 100 training epochs with early stopping - patience of 10. For the optimization, the adaptive stochastic optimization algorithm RMSprop (Root Mean Square Propagation) was used with mostly standard values (learning rate of 0.0001 with 0.9 rho, no epsilon and a decay of 0). RMSprop works by dividing the learning rate by an exponentially decaying average of squared gradients \[20\]. As a result, when the gradient steps are excessively large, RMSProp automatically reduces the size of the gradient steps toward (local) minima (large steps could result into overshooting).

4 Results

To assess the performance of our proposed GCN model, data from the CI and CW seismic datasets that include hundreds of earthquake signals from \[44\] were used. We start by introducing these datasets in detail. After that, we detail the experimentation. Specifically, we provide the MSE scores of each model and visualize the differences between them.

4.1 Dataset

We perform regression on two datasets recorded by the Italian national seismic network \[45, 46\], described fully in \[16, 17\]. Seismic data is an ideal candidate to test our method, since the seismic measurements contain (1) an enormous amount of data, and (2) sensors that are geographically grounded. Each sensor in the dataset continuously records the amplitudes of the seismic waves resulting from earthquake occurrences along three components of ground motion (i.e., 3 dimensions): up-down, north-south, and east-west. The data recorded by the sensors (i.e., seismometer or accelerometers) located at the stations are crucial for seismologists to understand the nature of the recorded earthquakes (e.g., magnitude, location, focal mechanism, ...).

Because information can be transmitted faster than the seismic waves travel (P-waves travel usually at average velocities of $\sim 5 - 6 \text{ km/s}$ and S-waves roughly at half the velocity of the P-waves in the shallow Earth's crust), seismologists have developed algorithms to predict e.g., the maximum intensity measurements (IMs) of ground shaking at a set of locations, caused by an earthquake, using only the very first stations (i.e., those closest to the epicenter) that have recorded the earthquake already. In the seismological literature this objective is known as “earthquake early warning” (EEW). In general, EEW systems estimate earthquake parameters (magnitude, location, etc.) quickly and provide a warning about the incoming ground motion that will occur at selected locations. This is achieved by using the initial parts of the seismic stations recordings and adopting specialized techniques.

In our algorithm, the recordings from the closest stations are used by the model to give warnings through direct approximations of the IMs at the stations farther away. The IMs used here include peak ground acceleration (PGA), peak ground velocity (PGV) and spectral acceleration (SA) at 0.3, 1 and 3 second periods and represent the labelled data of our model. That is, by using
the earthquake recordings from the stations nearby the epicenter, recorded within 10 s from the origin time of the earthquake, we make predictions of the maximum ground shaking at the stations farther away. These stations have not yet recorded the earthquake-related ground motion at all or its maximum. We, however, provide the recordings of all the stations in the network to the model, both of those that recorded the earthquake ground motions and those that have not. The pattern of the recorded waveforms from all the stations provides a “footprint” of the earthquake location, although the latter is not estimated in our scheme. An example of an earthquake (red solid star) drawn from our CI dataset is shown in Figure 4. The vertical red line in Figure 4a illustrates that, at the end of the 10-second window, only the FEMA station has recorded a large part of the earthquake and the other stations farther to the northwest (cf. Figure 4b) have not yet recorded the first P waves. Our hypothesis is that this task is highly suited for GNNs.

The CI Dataset (see Table 1) consists of 915 earthquakes recorded on a set of 39 stations (CI network) in central Italy. The earthquake epicenters and station locations are within the area that consists of latitude $[42^\circ, 42.75^\circ]$ and longitude $[12.3^\circ, 14^\circ]$, with earthquakes happening from the 1st of January until the 29th of November 2016. It contains many spatially concentrated earthquakes and a dense network of stations. Earthquakes have a depth between $1.6 \text{ km} \leq z \leq 28.9 \text{ km}$ and magnitudes in the range $2.9 < M \leq 6.5$. 

Fig. 4: Example of part of the data for one earthquake in the dataset. (a) Rescaled earthquake waveform amplitudes of the earthquake shown in (b) as a solid red star. The blue time series in (a) represents the FEMA station labeled in (b), and the vertical red line shows the end of the 10 s input waveform. Approximate P- and S-wave fronts are shown as circles in green and orange colors, respectively. The stations are shown as solid blue dots.
The CW Dataset consists of 266 earthquakes recorded on a set of 39 other stations (CW network) in central-western Italy. The earthquake epicenters and station locations are within the area bounded by latitudes [41.13°, 46.13°] and longitudes [8.5°, 13.1°], with earthquakes spanning the time period between 1-1-13 and 20-11-17. All the earthquakes are in the depth between 3.3 km and 64.7 km, with magnitudes in the range $2.9 < M \leq 5.1$. Therefore, the CW dataset clearly covers a larger area than the CI dataset and, as Figure 5 illustrates, the earthquakes of the CW dataset are scattered across a large part of central and northern Italy whereas the CI dataset has earthquakes concentrated in one small area.

| Dataset Name | Network 1 | Network 2 |
|--------------|-----------|-----------|
| N Earthquakes | 915       | 266       |
| Stations     | 39        | 39        |
| Magnitudes   | $2.9 \leq M \leq 6.5$ | $2.9 \leq M \leq 5.1$ |
| Periods      | 1-1-16 / 29-11-16 | 1-1-13 / 20-11-17 |
| Depths       | $1.6\text{km} \leq z \leq 28.9\text{km}$ | $3.3\text{km} \leq z \leq 64.7\text{km}$ |
| Epicentral Distances | $0.5\text{km} \leq \Delta \leq 189\text{km}$ | $10\text{km} \leq \Delta \leq 498\text{km}$ |

| Network Nodes | 39 | 39 |
| Network Edges | 722 | 493 |
| $k$           | 0.3 | 0.6 |
| Avg. Degree   | 37.03 | 25.28 |
| Min KM Distance | 159 | 217 |
| Avg. Degree Centrality | 0.97 | 0.67 |

### 4.2 Network Creation

Both sensor networks were created by making use of the geographical locations of the seismic sensors. The Adjacency matrix $A_{i,j}$ was calculated by taking all the pairwise geodesic (the shortest path between two points on a sphere) distances in km between each station (latitude, longitude), and taking the $1 - (\text{min, max})$ scaled distance as the edge weight, since edges with a low distance should have a higher weight. Afterwards, the resulting Adjacency matrix can be filtered on the threshold $k$ to adjust the sparsity in the graph, e.g., the higher the parameter $k$ is set, the fewer edges will retain in the graph.

Then, we transform the Adjacency matrix $A$ into the Laplacian matrix $L = I - D^{-1/2}AD^{-1/2}$ where $D$ refers to the Degree matrix containing the neighbors of each node and $I$ refers to the identity matrix of length $n$ nodes in a graph. A typical Laplacian would only consist of $L = D - A$, however, if nodes have a wide range of varying connectivity, vanishing gradient problems can occur [24]. Therefore, the degree matrix is symmetrically normalized. Lastly, the addition of the identity matrix helps with the GNN to also involve each node’s own node features [24].
The resulting graphs are visible in Figure 5 where the nodes resulting from the seismic stations of the CI and CW datasets are shown in panels a) and b), respectively. Looking at the geographical maps and the coordinates (latitude and longitude) on the axis of the plots, it is clear that the CW network covers a larger land area. In addition, the thickness of the edges in the figure is determined by the distance between two stations. The less distance between two stations, the higher the edge weight. A higher weight will help the GNN with determining which stations will most likely inhibit similar behavior in their sensor readings, improving the prediction of the IMs.

Fig. 5: Overview of the source-receiver geometries of the CI (a) and CW (b) seismic datasets. The blue solid dots correspond to the seismic stations (nodes) and the orange dots refer to the earthquake epicenters. Notice the larger geographical area and the sparseness of the epicenters of the CW dataset when compared to CI. The thickness of the lines connecting the stations (i.e., the edges) are inversely proportional to the distance of the connecting nodes as from the values of the Adjacency matrix.

4.3 Experimentation: Baseline Models

To make the comparison fair, a slightly modified version of [16] was used as a baseline where the same node features of the GCN model (latitude, longitude) were added due to their influence on the GCN performance. These node features were added in the same manner as performed in [17], where they have shown a considerable impact on the performance. In addition, same as [17], the dropout in [16] has been moved from after the concatenation layer to after the third CNN layer, otherwise a large part of the meta-data could be removed right after it was added.
4.4 Experimentation: IM prediction

The results of the IM prediction are visible in Table 2 and Figure 6. All the algorithms perform better on the CI network than on the CW network. Such behavior is expected due to the following reasons. To start, the CW dataset contains fewer earthquakes (266 against 915) than the CI dataset and, in contrast with the CI, their spatial distribution is sparse. In addition, the CW network covers a vastly larger area, with larger distances between the stations, a larger depth range of the hypocenters and a larger variability in the geological settings.

Table 2: MSE results of each algorithm on the regressed metrics PGV, PGA, SA(0.3 s), SA(1 s), SA(3 s) and the overall mean. The best performing combinations are highlighted in bold.

| Network Type | PGV | PGA | SA(0.3 s) | SA(1 s) | SA(3 s) | Mean |
|--------------|-----|-----|----------|--------|--------|------|
| CI CNN       | 0.212 | 0.228 | 0.227 | 0.231 | 0.272 | 0.234 |
| GCN          | 0.164 | 0.175 | 0.175 | 0.183 | 0.222 | 0.184 |
|              | (-22.64%) | (-23.25%) | (-22.91%) | (-20.78%) | (-18.38%) | (-21.37%) |
| CW CNN       | 0.385 | 0.417 | 0.432 | 0.416 | 0.400 | 0.410 |
| GCN          | 0.331 | 0.357 | 0.383 | 0.362 | 0.320 | 0.351 |
|              | (-14.03%) | (-14.39%) | (-11.34%) | (-12.98%) | (-20.00%) | (-14.39%) |

When examining the individual performance of the models, our GCN model outperforms the original CNN from [16] by a large margin on each of the five metrics of ground motion. Especially in the PGV, PGA and SA(0.3 s) metrics of the CI networks this performance gain is visible. However, a different pattern is visible in the CW network, where the most remarkable difference is visible in SA(3 s). Therefore, a more general view is provided by the mean scores of both networks over each metric. The GCN model outperforms the original CNN with 21.37% in the CI network, and 14.39% in the CW network, resulting in an average performance gain of 17.88%.

Considering the results of the models on each individual earthquake and each IM metric, Figure 7 shows the observed versus the predicted IM values for both the CNN and the GCN models on the same scatter plots. The blue lines (and dots) reveal the performance of the CNN and the green lines (and dots) the GCN. The lines were calculated with an ordinary least squares to better visualize the difference in prediction bias between the two models. It demonstrates that better performance of the GCN model comes also in slight reduction of the bias for large IM values, which is also of great value for the seismological applications (see more in the original CNN paper [16]).

Lastly, the characteristics of all discussed models are visible in Table 3. The models do not deviate concerning Ms/step per epoch. More noticeable are the differences in the number of parameters and model size. The GCN model reduces the parameter size by 6.67%, and decreases the model size by 10.91%.
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4.5 Experimentation: Ablation Study

4.5.1 Tuning hyperparameter $k$.

The graph creation algorithm mentioned in Section 3 used the hyperparameter $k$ to cutoff connections between stations that are too far away. Table 4 presents the results of tuning this parameter on both networks and at what distance the cutoff will be, also highlighting the optimal setting of 0.6 and 0.3 for both networks. While in the CI network the results for $k \in \{0.3, 0.2, 0.1\}$ are almost equal, there is a slight preference for $k = 0.3$ from a computational perspective since less edges results in less convolutions that have to be performed.

It is interesting to see the opposite behavior for both networks concerning the effect of increasing or decreasing $k$. In the CI network, increasing $k$ results in a decrease in performance of our model, whereas the CW network reveals the opposite behavior. An explanation can be found in the different characteristics (see Section 4.1) of both networks, where a low cutoff number results in an optimal number of edges in the CI network, but would result in too many edges in the CW network. Especially in the CW networks, having nearly all edges in the network could confuse the GCN layers, since the stations spread

Table 3: Model characteristics with the parameters in millions and model size in Mb’s.

| Network | Algorithm | Parameters | Ms/step | Model Size |
|---------|-----------|------------|---------|------------|
| CI      | CNN       | 1.35       | 80      | 11         |
|         | GCN       | 1.26 (-6.67%) | 79      | 9.8 (-10.91%) |
| CW      | CNN       | 1.35       | 75      | 11         |
|         | GCN       | 1.26 (-6.67%) | 74      | 9.8 (-10.91%) |
out over larger land area and behave differently earlier than stations in the CI network. Therefore, leaving some weak connections to far away stations intact could decrease the quality of the features. These results highlight how crucial this preprocessing step is when designing graphs, also since some values of $k$ display weaker performance than the baseline models on the CW network.

### 4.5.2 Variation in different window lengths

Since our GCN model outperforms the original CNN by a certain margin, it is interesting to investigate how short the window length of the earthquake signal can be made until the performance equalizes. Therefore, all the window lengths between 10 seconds and 4 seconds and their corresponding MSE scores (the input size cannot be reduced further with this specific architecture) are displayed in Figure 8 for both models in both datasets.

The input window length can be more than halved before the same performance is reached as the original model reaches on the full input. This reduction also means a reduction of the model parameter size of 1.26 million to around 699 thousand (-44.52%). Especially in this experiment of the ablation study the power of the GCN layers becomes clear. Since GCN layers are designed
Table 4: Ablation results of the minimum distance cutoff hyperparameter $k$ for both networks.

| Network | $k$ | Cutoff (km) | Edges | Avg. Degree | Avg. Degree Centrality | MSE |
|---------|-----|-------------|-------|-------------|------------------------|-----|
| CI      | 0.6 | 92          | 497   | 25.49       | 0.67                   | 0.20|
|         | 0.5 | 115         | 609   | 31.23       | 0.82                   | 0.20|
|         | 0.4 | 138         | 687   | 35.23       | 0.92                   | 0.19|
|         | **0.3** | **159** | **722** | **37.03** | **0.97**              | **0.18**|
|         | 0.2 | 177         | 729   | 37.38       | 0.98                   | 0.18|
|         | 0.1 | 204         | 733   | 37.59       | 0.99                   | 0.18|
| CW      | 0.7 | 162         | 342   | 17.54       | 0.46                   | 0.46|
|         | **0.6** | **217** | **493** | **25.28** | **0.67**              | **0.33**|
|         | 0.5 | 271         | 601   | 30.82       | 0.81                   | 0.37|
|         | 0.4 | 325         | 660   | 33.85       | 0.89                   | 0.36|
|         | 0.3 | 377         | 705   | 36.15       | 0.95                   | 0.44|
|         | 0.2 | 429         | 731   | 37.49       | 0.99                   | 0.47|
|         | 0.1 | 485         | 739   | 37.90       | 0.99                   | 0.52|

Fig. 8: MSE at different window lengths for each model in both networks.
5 Conclusions

In this work, the use of time series regression with Graph Convolutional Networks (GCNs) was displayed. Our method proposed a unique way to leverage features from a CNN as node features in a GCN, and also the deviating principle of flattening the output of the last GCN layer instead of global pooling to retain as much information as possible. The proposed model is tested on two seismic datasets with different characteristics, demonstrating the generalizability of the model. Our model outperforms the CNN-based model [16] by 17.88% on average. Our experiments demonstrate the impressive power of GCNs with processing spatial information, since each of the two models was provided the same input.

The better performance of our model on the CI network compared to the CW network can be explained by the characteristics of the CW dataset. The CW dataset contains less data, covers a larger geographical area and contains earthquakes that are more spread out over the network and along depth.

More crucially, especially when taking into account the use case of early warning systems, our model can match the performance of the original CNN by using less than half of the input window length of both datasets. Such a reduction helps with faster early warnings, along with model parameter reduction, since the parameters were reduced by almost 45%.

One important message which we want to emphasize is that the architecture of the original CNN model by [16] could also be improved from an only CNN perspective (e.g., adding pooling or batch normalization layers, and adding more CNN layers). However, to make the comparison more fair, and to more directly observe the actual effect of the GCN layers on the prediction results, we decided to alter the model architecture as little as possible. Therefore, better architectures could also be designed from that perspective, except that was not the premise of this work.

For future research, other methods of creating the initial Adjacency matrix could be investigated, because the results of the cutoff parameter experiments in the ablation study reveal the substantial effect the graph creation steps have on the performance. Examples include; to keep the top-k edges for each node or using exponential decaying functions as in [27]. In addition, we plan to test our model on other kinds of datasets. For example, both networks now consisted of 39 nodes. It would be interesting how our architecture would scale to datasets featuring 200 or more nodes. In addition, to test the transfer learning capabilities of our model, perhaps adding the spatial information to a pre-trained model on one dataset could make it more adaptable for other tasks with different data characteristics.

Lastly, our architecture was built to be easily adaptable for other tasks. Therefore, we encourage readers to take Figure 2 as a departure point for other analysis tasks. Similarly, we believe that the architecture can be used in other domains featuring time series data recorded by geographically sparse, and non-euclidean geometries.
Declarations

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Availability of data and material
Data are available at [48] (CI dataset) and [49] (CW dataset).

Authors’ contributions
SB and MA conceived of the idea and study, as well as the interpretation of the data, which was performed in a synergistic way together with DJ and AM. SB, MA and JH drafted the manuscript. All authors edited the manuscript. SB implemented the methods and algorithms supported by JH, and ran the experiments, in close collaboration with DJ and AM. DJ and AM provided the baseline model and the data. All authors read, reviewed and approved the final manuscript.

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