A Graph Neural Network gas concentration prediction model based on Spatio-Temporal data

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Abstract. For the problem of low prediction accuracy caused by traditional neural network gas concentration prediction models which did not consider temporal and spatial characteristics of gas data, this paper proposed a Spatial-Temporal graph neural network gas prediction model based on Spatial-Temporal data. Its essence was the integration of graph convolutional network and WaveNet network. In spatial dimension, graph convolutional network was used to aggregate the information of neighbor nodes, and adaptively adjusts the spatial association strength of each node according to the attention mechanism to captured the spatial characteristics of gas data. In temporal dimension, WaveNet network model was introduced, Dilated Causal Convolution was used to extract the temporal characteristics of gas data on temporal dimensions. According to the distance between gas sensors in the mine, the gas data spatial structure was constructed by Thresholded Gaussian kernel function. Experiment with the measured gas temporal and spatial data, using Mean Absolute Error (MAE) as an indicator of predictive accuracy. The experimental results show that the prediction model mentioned in this paper is significantly improved compared with the prediction accuracy of other predictive models.

1. Introduction
Gas outburst is one of the main disasters in coal resource mining projects. Accurate prediction of gas concentration changes in mining areas is the key to preventing gas outburst disasters [1]. The internal mechanism of gas outburst is very complicated, and its mechanism model is still unclear. At present, neural network, chaos theory, grey theory and other methods are mainly used to predict gas concentration, and gas outburst disasters can be judged by predicting gas emission from mining areas.

The traditional neural network prediction model uses a large amount of measured historical data and adopts a temporal series prediction method to realize the prediction of gas concentration. For example, Academician Peng established a set of comprehensive prediction methods for gas outburst dangerous areas based on the Support Vector Machine and Probabilistic Neural Network based on genetic algorithms [2]. Fu combined the Isometric Feature Mapping algorithm with the Weighed Least Square Support Vector Machine algorithm to establish a gas outburst dual coupling algorithm prediction model [3]. Although the above models have improved the accuracy of gas concentration prediction to a certain extent, none of these models consider the interaction of different gas sensors, that is, the spatial characteristics of gas monitoring data. According to the kinetic theory of gases, the distribution of gases is not only related in the temporal dimension, but also has a close relationship with the spatial dimension.
Therefore, if only the temporal dimension of gas data is considered and the spatial attribute is ignored, it will inevitably affect the prediction accuracy.

Spatial-Temporal data is temporal series data with a positional relationship. Spatial-Temporal data widely exists in various fields of real life, such as traffic forecasting, weather forecasting, air quality forecasting, etc. Since the spatial distribution of the gas data sensor collected in the actual mining area is not a regular spatial structure, the gas data collected is non-Euclidean structure data. Graph neural networks can effectively model data in non-Euclidean structures and capture the internal correlation of data. Temporal and spatial are the two most important and universal characteristics of an individual. The Spatial-Temporal graph neural network adds a temporal dimension to the graph neural network, that is, the data of each node in the graph structure is a temporal series that changes with time. Therefore, the Spatial-Temporal graph neural network can simultaneously capture the temporal and spatial correlation of Spatial-Temporal data.

The research of Spatial-Temporal graph neural network mainly focuses on how to add temporal dimension to the graph. Research is mainly concentrated in two directions. A method based on Recurrent Neural Network: For example, Liu combined the Spatial-Temporal graph convolutional network and Long Short Term Memory to establish a ST-GCN-LSTM (Spatial Temporal Graph Convolutional Network Long Short Term Memory) model [4]; the other is a method based on Convolutional Neural Networks. For example, Bing uses graph convolution combined with Temporal convolutional network [5]. Some studies have tried to jump out of the above ideas. For example, Yu used Transformer as a new way to replace the original CNN and RNN to deal with the temporal dimension [6].

Based on the fact that actual gas concentration data is temporal series data with spatial attributes, this paper proposes a Spatial-Temporal graph neural network gas concentration prediction model AGCN-WaveNet (Attention Graph Convolutional Networks WaveNet, AGCN-WaveNet) based on Spatial-Temporal data. This model can not only consider the influence of the previous gas concentration data of a single node on the current gas concentration, but also the influence of the gas concentration of its neighbor nodes on the gas concentration of the node. Because the changes in gas concentration data of adjacent nodes in the mining area are interrelated, considering the spatial attributes of the gas data can greatly improve the prediction accuracy of the model. Finally, based on the real gas concentration spatiotemporal data, this paper verifies the effectiveness of the proposed Spatial-Temporal graph neural network prediction model.

2. Materials and Methods

2.1 Problem Definition

The purpose of gas temporal and spatial concentration prediction is to predict the future gas concentration based on the historical gas concentration data collected by multiple sensors in the mine. Use a graph \( G = (V; E) \) and its adjacency matrix \( A \) to represent the gas data monitoring point network of the working face of the mining area. Where \( V \) is the node of the graph formed by sensors on the mining face, and \( E \) is the edge of the graph formed by the relationship between the sensors. For each time point \( t \), the graph \( G \) has a dynamic feature matrix \( X_t \), and the dimension of \( X_t \) is \( N \times P \), where \( P \) is the number of features of the input data. Therefore, the gas concentration prediction problem can be expressed as learning a function \( F \) to obtain the feature matrix of \( T_1 \) time steps in the future according to the historical feature matrix of \( T_1 \) time steps and graph \( G \). The mathematical description is:

\[
X^{(t-T_1)}; X^{(t-T_1+1)},...,X^{(t)},G \xrightarrow{F(*)} [X^{(t+1)},...,X^{(t+T_1)}]
\]  

(1)

2.2 Gas concentration prediction model based on AGCN-WaveNet

2.2.1 Spatial convolution

Figure 1 shows a working face of Shijiazhuang coal mine, where each sensor in the mine is regarded as a different node in the graph structure. According to the distance between each sensors, a threshold
Gaussian kernel weighting function is used to define the edge weight between vertices [7], and the Gaussian kernel weighting function is defined as:

$$W_{ij} = \begin{cases} \exp\left(-\frac{[dist(i, j)]^2}{2\theta^2}\right) & \text{dist}(i, j) \leq k \\ 0 & \text{otherwise} \end{cases}$$

(2)

where, $k$ and $\theta$ are parameters, and $\text{dist}(i, j)$ is the distance between sensors.

In the spatial dimension, this paper uses graph convolutional network to extract information from gas data. For a given graph structure in space, the graph convolutional network enables each node on the graph to efficiently extract node spatial features by aggregating the feature information of all its neighbor nodes.

Literature [8] proposed a diffusion convolutional layer, which regards the signal transfer on the graph as random diffusion, and simulates the diffusion process of the graph signal with N finite steps. The diffusion convolutional layer can be expressed as:

$$Z = \sum_{n=0}^{N} P^n X W_n$$

(3)

where, $P$ is the random diffusion matrix on the graph, and $P_{ij}$ represents the probability of node $i$ diffusing to node $j$. $P^n$ can be regarded as the probability of spreading from node $i$ to node $j$ through $n$ steps. $D$ is the degree matrix of $A$, and $P$ can be expressed as:

$$P = D^{-1} A$$

(4)

The attention mechanism can filter out the most important information to the target, and then improve the recognition accuracy [9]. The graph structure constructed by distance does not necessarily reflect the complete spatial dependence relationship, and may lead to partial lack of spatial relationship. The partial lack of spatial relationship will cause the graph convolutional network to not fully capture the spatial characteristics of the gas data, which will affect the prediction accuracy. In this paper, the attention mechanism is used to adaptively adjust the strength of the spatial relationship between nodes, so that the model can capture the spatial characteristics of gas data more accurately.

$$A_s = \text{soft max}\left(V \cdot \sigma\left((XW_1)W_2(W_3X)^T + b\right)\right)$$

(5)
where, V and \( W_1, W_2, W_3 \) are the parameters to be trained, \( \sigma \) are the Sigmoid function, X is the input feature matrix, and \( A_t \) is the normalized attention matrix. \( A_t \) and the initialized adjacency matrix are multiplied to realize the dynamic adjustment of the spatial relationship.

### 2.2.2 Temporal Convolution

In the temporal dimension, this paper uses the WaveNet model to capture the temporal characteristics of gas Spatial-Temporal data [9]. The WaveNet model was originally used for natural language processing problems. The latest research shows that the WaveNet model also has good performance for handling temporal problems.

The basic unit of WaveNet is causal convolution, for a given input \( X=(x_1, x_2, ..., x_T) \) and convolution kernel \( F_1=(f_1, f_2, ..., f_K) \), the causal convolution of \( x \) and \( f \) at step \( t \) is

\[
(X * F_1)(t) = \sum_{s=0}^{K-1} f(s)x(t-s)
\]

(6)

The disadvantage of causal convolution is that when a larger receptive field is needed, the receptive field can only be improved by continuously increasing the number of network layers and increasing the convolution kernel, which greatly increases the number of network layers and the complexity of the model. This article uses dilated causal convolution to improve the defect. The essence is to make the convolution kernel skip the input value with a certain expansion factor through a given expansion factor, so that the model can obtain a larger receptive field when the number of layers is small.

For a given input \( X=(x_1, x_2, ..., x_T) \) convolution kernel \( F_2=(f_1, f_2, ..., f_K) \) and dilation factor, the causal convolution of \( x \) and \( f \) at step \( t \) is

\[
(X * F_2)(t) = \sum_{s=0}^{K-1} f(s)x(t-s \times d)
\]

(7)

where, \( d \) is dilation factor.

### 2.2.3 AGCN-WaveNet Model Framework

Figure 2 shows the framework of the gas prediction model based on AGCN-WaveNet. The prediction model is composed of a graph convolutional layer and a gated dilated convolutional layer to form a Spatial-Temporal layer. The gated dilated convolutional layer is composed of two dilated causal convolutional layers. By using multiple Spatial-Temporal layers, the AGCN-WaveNet prediction model can handle spatial correlations at different temporal levels.
The input data extracts the Spatial-Temporal features through the Spatial-Temporal layer and connects the residuals with the original input to reduce the loss of information during the cycle. Different expansion factors are used in the K spatiotemporal layers, the short-term temporal dependence is captured at the bottom layer, and the long-term temporal dependence is captured when K is relatively large. The output of the model can be obtained by connecting the results of the K spatiotemporal layers and then passing through the two linear layers.

3. Results & Discussion

The experimental data adopts the measured data of gas concentration in a mining area in Shijiazhuang. The data set division method is: extract the time period from 2017-10-30 to 2017-11-17, a total of 19 days as the training set, 2017-11-18 02:12:00 to 2017-11-18 12:12:00, a total of ten hours of data as the test set, 2017-11-18 12:12:00 to 2017-11-18 18:12:00, a total of ten hours of data as the verification set. The above-mentioned time points were sampled from the sensors in different areas of the mine shown in Figure 1. Data is collected every 2 minutes.

In the experiment, the length of the input gas data temporal series is set to 15 and the output length is set to 5. That is, the gas concentration data of 10 minutes is predicted by the gas concentration data of the previous 30 minutes. AGCN-WaveNet adopts the expansion factor of each layer of 10 Spatial-Temporal layers as (1, 2, 1, 2, ...). The diffusion step size in the graph convolutional layer is set to 2, and dropout=0.3 is set in the graph convolutional layer to prevent the model from overfitting. The optimizer selects the Adam optimizer to optimize the model, the initial learning rate is 0.001, and the number of training rounds is set to 30.

Table 1 shows the average absolute error (MAE) of the gas concentration prediction results of each sensor by the AGCN-WaveNet network. The calculation formula of the average absolute error is:

$$\text{MAE} = \frac{1}{m} \sum_{i=1}^{m} \left| y_i - y_i^1 \right|$$

(8)

Where, $m$ is the total number of predicted samples, $y$ is the true value, and $y^1$ is the predicted value.

| Sensor  | 2min  | 4min  | 6min  | 8min  | 10min |
|---------|-------|-------|-------|-------|-------|
| Sensor1 | 0.0040| 0.0066| 0.0088| 0.0110| 0.0136|
| Sensor2 | 0.0130| 0.0231| 0.0306| 0.0369| 0.0424|
| Sensor3 | 0.0088| 0.0160| 0.021  | 0.0226| 0.0253|
| Sensor4 | 0.0055| 0.0091| 0.0131| 0.0141| 0.0162|

The relative error of the prediction model for the gas data of 4 sensors in the mine is shown in Table 2:

| relative error | number of samples | average relative error |
|----------------|-------------------|-----------------------|
| <5%            | 805               |                       |
| >=5% and <15%  | 365               | 4.85%                 |
| >=15%          | 30                |                       |

It can be seen from Table 2 that in a total of 1200 prediction samples at the 4 sensors, 67% of the samples have predicted relative errors between 0 and 5%, 97.5% of the samples have predicted relative errors within 15%, and the total average relative error It is 4.85%. Except for a very small number of sample points where the error appears in the larger error range, the vast majority of the sample points are concentrated in the smaller error range.
This experiment uses the gas prediction data of the Sensor 3 as an example, and compares the gas prediction model based on the Spatial-Temporal graph network with the traditional temporal-based comparison of gas prediction models. The prediction effect of AGCN-WaveNet network and WaveNet network on the gas concentration data of Sensor 3 is shown in Figure 3. As can be seen from the figure, compared with the WaveNet network without graph convolution, the gas concentration prediction model based on AGCN-WaveNet better fits the gas concentration change curve in the mine, especially for the longer prediction steps. The situation showed a better fitting effect.

Figure 3 Comparison of prediction effect between AGCN-WaveNet and WaveNet at sensor 3
Table 3 shows the comparison of the prediction accuracy of the gas concentration prediction model based on the Spatial-Temporal graph network, the Autoregressive Moving Average Model (ARMA), and the WaveNet gas concentration prediction model mentioned in this article.

Table 3 Comparison of gas data prediction results at sensor 3

|       | 2min  | 4min  | 6min  | 8min  | 10min |
|-------|-------|-------|-------|-------|-------|
| ARMA  | 0.0117| 0.0209| 0.0287| 0.0359| 0.0409|
| WaveNet | 0.0106| 0.0192| 0.0258| 0.0315| 0.0364|
| AGCN-WaveNet | 0.0088| 0.0160| 0.0210| 0.0226| 0.0253|

It can be seen from Table 3 that the prediction error of the ARMA prediction model is the largest, followed by the WaveNet prediction model, and the prediction error of the AGCN-WaveNet prediction model is the smallest. As the number of prediction steps increases, the advantages of AGCN-WaveNet become more and more significant. When the fifth step is predicted, the prediction accuracy of AGCN-WaveNet is significantly higher than other prediction models. In addition, the prediction accuracy of WaveNet with graph convolution will be further improved compared to WaveNet without graph convolution. The experimental results show that the Spatial-Temporal graph convolution network constructed in this paper can simultaneously capture the temporal and spatial characteristics of gas data, thereby improving the prediction accuracy of the prediction model.

4. Conclusions
1) Aiming at the Spatial-Temporal characteristics of mine gas concentration data, this paper proposes a Spatial-Temporal prediction model of gas concentration. Compared with other commonly used forecasting models, forecasting models can provide longer and more accurate forecasts. It provides new methods and new ideas for preventing gas disasters.

2) Because the gas movement mechanism of the working face is very complicated, the method of defining the correlation only by distance is not comprehensive, and the adaptive adjustment of the correlation of adjacent sensors through the attention mechanism can more effectively express the spatial correlation of the gas data.

3) Changes in factors such as temperature, wind direction, and microseisms in the mine will also affect the changes in gas concentration. This paper does not consider the influence of these factors. This is also the limitation and expansion direction of the AGCN-WaveNet model.

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