

The Combination of GCN and CNN in Spatial-Temporal Domain

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Background Knowledge

The principle of the Convolution Neural Network (CNN)

Technically, the convolution in deep learning is actually a "cross-correlation" operation, which is different from the convolution in signal processing. The main parameters of the convolution operation are **kernel**, **stride**, **padding** and **output channel**. Among them, the kernel is learnable and the receptive field of the convolution operation; stride is the number of pixels moved per step when the kernel traverses the input; padding adds a circle of 0s around the input feature map; output channel refers to the number of kernels.

The Matrix Form of Convolution in PyTorch CPU implementation

Patch: It is the area the input and traversing kernel perform multiplication, which mean a step stride can generate a patch.

Image is from [14]

The Generation of the matrix form in CPU PyTorch source code

First, All the patches will form the corresponding row of the matrix, which is so call image to rows.

Second, the flattened kernels are also formed as a matrix.

Finally, the convolution is formed as a matrix multiplication between the patching image and unfolding kernels.

Here is the source code in CPU PyTorch for this implementation. For more detailed implementation information please kindly refer to the link.

[https://github.com/pytorch/pytorch/blob/e9902358df14dc4809e4f50b1208](https://github.com/pytorch/pytorch/blob/e9902358df14dc4809e4f50b12088a5200a1862d/aten/src/ATen/native/ConvolutionMM2d.cpp) [8a5200a1862d/aten/src/ATen/native/ConvolutionMM2d.cpp](https://github.com/pytorch/pytorch/blob/e9902358df14dc4809e4f50b12088a5200a1862d/aten/src/ATen/native/ConvolutionMM2d.cpp)

The feature maps of the CNN

Deeper layer can capture global features by stacking convolution layers, which might help the classification.

To visualize the features maps, a cat image with shape (256,256,3) is fed into the CNN model.

Code and results are from [3]

The Encoder-Decoder Architecture in CNN

Here is a conventional architecture of encoder-decoder, which can be used for supervised learning and unsupervised learning. If the output is the same as the input, we call it as Autoencoder:

Code and results are from [4]

Here is one computer vision domain example for autoencoder

```
mport torch.nn as nn
class AutoEncoder(nn.Module):
 def \_init (self):super (AutoEncoder, self). __init_()
   self. encoderConv = nn. Sequential(nn.Conv2d(1, 16, 3, stride=3, padding=1),nn.ReLU(True),
    nn. MaxPool2d(2), \# [16, 5, 5]
    nn. Conv2d(16, 8, 3, stride=1, padding=1), \frac{\pi}{16} [8, 5, 5]
    nn. ReLU(True),
     nn. MaxPool2d(2), \# [8, 2, 2]
   self.decoderConv = nn.Sequential(nn. ConvTranspose2d(8, 16, 3, stride=2), \# [16, 5, 5]
    nn. ReLU(True),
     nn. ConvTranspose2d(16, 8, 5, stride=3, padding=1),nn.ReLU(True),
     nn. ConvTranspose2d(8, 1, 2, stride=2, padding=1), \# [1, 28, 2]
     nn.ReLU(True)
def forward (self, x):
   x1 = self.encodeerConv(x)x = self.decoderConv(x1)return x1, x
```


As we can see, the reconstructed outcomes look the same as the input in most cases, which means that the latent state in the lower dimension space can somehow represent the corresponding image. 7/37

Graph Convolution Neural Network (GCN)

The GCN is similar to CNN since it is obtained from the CNN. For a convolution in deep learning, two main steps should be considered: i) how to identify the neighbors and ii) how to aggregate the neighbors.

For the first point, how the GCN find the neighbors? We use adjacency matrix A to identify neighbors.

For the second point, how the GCN aggregate the neighbors? The GCN use sum method to aggregate the neighbors which is same as CNN.

$$
H^{l+1} = \sigma(AH^lW^l + B)
$$

where A is the adjacent matrix denoting the neighbors, $H^{(l)}$ is the nodes' attribute and $W^{(l)}$ is the kernel and B is the bias. 8/37

GCN V.S CNN

To empress understanding, we compare GCN and CNN: the CNN uses the around pixels as neighbors while the neighbors in GCN should be identified by an adjacency matrix. For the aggregation method, both GCN and CNN sum up neighbors together as the final result.

Like the CNN, the stacking convolution layer can enlarge the receptive field of the model, the GCN can be stacked to capture multi-hop neighbor features

Besides, the Encoder-Decoder Architecture can be also applied into the graph structure data.

Image is from [6] $\qquad \qquad$ Image is from [7] $\qquad \qquad$ 9/37

The principle of the Recurrence Neural Network (RNN)

Recurrent Neural Networks (RNNs) are a class of neural network that are helpful in modeling sequence data. They specialize in processing sequences and are often used in NLP because of their effectiveness in handling text. The most common used RNN models are Long Short-Term Memory (LSTM) and Gate Recurrent Unit (GRU).

A type of fully connective neural network recurrent in the temporal domain

Images are from [8][9]

What about Attention V.S RNN?

- Attention needs to calculate the correlation at each time step, the time complexity of the simple attention is $O(n^2)$.
- The time complexity of RNN is $O(n)$, where n is the length of the sequence.
- Parameters are shared in temporal domain
- The current output is mainly relied on the previous output.

The introduction of the LSTM

Long Short-Term Memory (LSTM) is a type of RNN that is specifically designed to handle sequential data, such as time series, speech, and text. LSTM networks are capable of learning order dependence in sequence prediction problems.

 $S(x) = \frac{1}{1+e^{-x}}$

Input Gate
$$
i_t = \sigma(W_i \cdot [h_{t-1}, x_t] + b_i)
$$

\nForget Gate $f_t = \sigma(W_f \cdot [h_{t-1}, x_t] + b_f)$
\n $\tilde{C}_t = \tanh(W_C \cdot [h_{t-1}, x_t] + b_C)$
\nMemory Cell $C_t = f_t * C_{t-1} + i_t * \tilde{C}_t$
\nOutput Gate $o_t = \sigma(W_o \cdot [h_{t-1}, x_t] + b_o)$
\nOutput $h_t = o_t * \tanh(C_t)$

Usually, σ is chosen as a sigmoid function S(x).

How we handle the video data which are time-series images? **Spatial-temporal domain model**

An intuitive way is that we first apply the CNN to the images. After that, we flatten the CNN result as a vector and then feed into the RNN model. However, this manner can not handle spatial-temporal feature at the same time since it handles spatial and temporal features separately.

Images are from [11][10]

The intuitive way Considering the LSTM, can we integrate the convolution into the LSTM? Rather than just conducting CNN and LSTM separately

The ConvLSTM for video prediction

ConvLSTM is a type of recurrent neural network for spatial-temporal prediction that has convolutional structures in both the input-to-state and state-to-state transitions. It determines the future state of a certain cell by the inputs and past states of its local neighbors.

Note that:

- The input-to-state transition means the input X_t transits to H_t
- The state-to-state transition means the H_{t-1} , C_{t-1} transits to H_t , C_t

the ConvLSTM is similar to the LSTM while the matrix multiplication is replaced as convolution

Input Gate $i_t = \sigma(W_{xi} * \mathcal{X}_t + W_{hi} * \mathcal{H}_{t-1} + W_{ci} \circ \mathcal{C}_{t-1} + b_i)$ Forget Gate $f_t = \sigma(W_{xf} * \mathcal{X}_t + W_{hf} * \mathcal{H}_{t-1} + W_{cf} \circ \mathcal{C}_{t-1} + b_f)$ $\tilde{\mathcal{C}}_t = \tanh(W_{xc} * \mathcal{X}_t + W_{hc} * \mathcal{H}_{t-1} + b_c)$ Memory Cell $\mathcal{C}_t = f_t \circ \mathcal{C}_{t-1} + i_t \circ \tilde{\mathcal{C}}_t$ Output Gate $o_t = \sigma(W_{xo} * \mathcal{X}_t + W_{ho} * \mathcal{H}_{t-1} + W_{co} \circ \mathcal{C}_t + b_o)$ Output $\mathcal{H}_t = o_t \circ \tanh(\mathcal{C}_t)$

where $*$ is the convolution operation for spatial feature. \circ is the elementwise multiplication. As the spatial-temporal feature can be capture in one operator, the ConvLSTM can handle video prediction task.

The Motivation of the Combination

Introduction of the spatial-temporal task for Near-surface Temperature

The Near-surface Temperature prediction (NTP) is one of the application task of weather forecast in spatialtemporal domain. The model can be formulated as follows:

$$
\tilde {\cal X}_{t+1}, \ldots \tilde {\cal X}_{t+\beta} = \mathop{\rm arg\,max} p({\cal X}_{t+1}, \ldots {\cal X}_{t+\beta} \vert {\cal X}_t, \ldots {\cal X}_{t-\alpha+1}),
$$

PS: The unit of the temperature is Kelvin. The formula of the transform is K=^oC+273.15

All images which do not mention are from [13]

Observation in real-world application

Pearson Coefficient

$$
\rho\left(\mathbf{x},\mathbf{y}\right)=\frac{\sum_{i=1}^{n}\left(\mathbf{x}_{i}-\bar{\mathbf{x}}\right)\left(\mathbf{y}_{i}-\bar{\mathbf{y}}\right)}{\sqrt{\sum_{i=1}^{n}\left(\mathbf{x}_{i}-\bar{\mathbf{x}}\right)^{2}}\sqrt{\sum_{i=1}^{n}\left(\mathbf{y}_{i}-\bar{\mathbf{y}}\right)^{2}}},
$$

Difference distances identify by different colors

we can make three key observations:

- (i) the grid pairs with a close distance have a high correlation, which reflects the short-range spatial correlations; suitable for CNN
- (ii) the grid pairs with a long-distance may still have a strong correlation, which indicates the existence of long-range spatial correlations; suitable for GCN
- (iii) the grid pairs with the same distance may have varying correlations, which shows that the spatial correlations are quite complex. suitable for spatial attention, a technique to reweight pixels based on their importance.

The observations imply that both long- and short-range spatial correlations would be beneficial for near-surface temperature prediction and grids with the same distances may have different contributions.

Fig. 1. An illustrative example of long- and short-range spatial correlations for near-surface temperature.

Methodology

The Main Idea of the **L**ong- and **S**hort range **Conv**olution LS-Conv

The LS-Conv is design to capture long- and short- range spatial correlation in a convolution operator by unifying GCN and CNN.

Here is the conventional convolution procedure

the LS-Conv replaces scalar multiplication with graph convolution

We choose a data-driven method to generate the learnable adjacency matrix. After that, we flatten the input image into a matrix for long-range spatial correlation capturing. After the graph convolution, we fold the result back to an image and select the corresponding row to integrate the short-range spatial correlation. 18/37

The Overview of the LS-Conv

Here is the whole overview of the LS-Conv. Given an input X, The Node-based Spatial Attention is first applied to evaluate the importance of each grid of the X aiming to distinguish important nodes for long-range spatial correlations construction. Meanwhile, the learnable node embedding is initiated, which denotes the channel information of the corresponding grid. After the NSA, the LAGC module learns an adaptive adjacent matrix to model the long-range spatial correlations by using graph convolution kernel from LS-Conv kernel. Finally, in the LSI, these GCN outputs are aggregated in a CNN manner, where each GCN result is similar to the element-wise product result between kernel and input in conventional CNN. Consequently, these results will be summed together and placed at the corresponding position of the output Y.

The Mechanism of Node-based Spatial Attention (NSA)

Spatial attention is a form of attention mechanism that focuses on specific regions of an image. It is used in computer vision tasks to improve the performance of CNNs by allowing them to focus on important regions of an image. As the input image can be viewed as nodes of the adaptive adjacency matrix, so we also call this module Node-based spatial attention (NSA).

PS: Conv1@1 means the Conv2d operation with 1*1 kernel size

Long-range adaptive graph constructor (LAGC)

we review the convention GCN, which is shown as follows:

$$
(\mathbf{X} *_{G} \Theta) = \left(\mathbf{I}_{N} + \mathbf{D}^{-\frac{1}{2}} \mathbf{A} \mathbf{D}^{-\frac{1}{2}}\right) \mathbf{X} \Theta + \mathbf{b},
$$

where D is the degree matrix, $D[i, i] = \sum_{j=1}^{N} A[i, j]$ and $D[i, j] = 0$. The term $D^{-1/2}AD^{-1/2}$ is called adjacency matrix normalization. I_N is the identity matrix also called the self-loop factor which means that the GCN consider both neighbors and itself.

Many graph-based task can easyly find neighbors. However, in meteorological task, it is hard for us to identify the neighbors. So we propose a data-driven method to learn the neighbors:

$$
\mathbf{D}^{-\frac{1}{2}} \mathbf{A} \mathbf{D}^{-\frac{1}{2}} = \text{SoftMax}\left(\text{ReLU}\left(\mathbf{E}_{\mathcal{G}} \mathbf{E}_{\mathcal{G}}^{T}\right)\right),
$$

$$
\mathbf{Z} = \left(\mathbf{I}_{N} + \mathbf{D}^{-\frac{1}{2}} \mathbf{A} \mathbf{D}^{-\frac{1}{2}}\right) \mathbf{X} \boldsymbol{\Theta} + \mathbf{b},
$$

 E_g is the learnable node embedding corresponding to the grid in the input X. The multiplication of E_g and E_g^T can be viewed as measuring the similarity of other node embedding vector. The ReLU activation function aims to guarantee the positive value in the learnable adjacent matrix and the SoftMax activation function is designed for the normalization. In this way, we design a data-driven adjacency matrix generation method to capture the meteorological long-range spatial correlation. 21/37

Long- and short-range integrator (LSI)

We first conduct the graph constraint for the input X, which has shape $(c, n \times m)$. Then, a graph convolution is performed with the help of the LS-Conv kernel aiming to capture long-range spatial correlation. After the graph convolution, the result is reshaped into a new shape (n, m, f). Finally, we select the corresponding result based on the location of the LS-Conv kernel, which is same as CNN.

$$
\mathbf{L} = \left(\mathbf{I}_{N} + \mathbf{D}^{-\frac{1}{2}} \mathbf{A} \mathbf{D}^{-\frac{1}{2}}\right) \mathbf{X}, \text{ CNN manner in aggregation}
$$
\n
$$
(\mathbf{X} \star \Theta) (i, j, :)= \sum_{p=1}^{k} \sum_{q=1}^{k} \left[\mathbf{L} \Theta_{p,q,:,:}\right]_{(n,m,f)} (i - p, j - q, :),
$$

graph convolution

- Light green outcomes is generated by the light green LS-Conv kernel, so we pick up the first row in the first column as the final result.
- For the orange outcomes, which is generated by the second LS-Conv kernel. So we pick up the first row in the second column.
- Finally, we conduct sum aggregation in a CNN manner to capture short-range spatial correlation.

Long- and short-range Convolution (LS-Conv)

 $\mathbf{X}=[\text{NSA}(\mathcal{X})]_{(nm,c)},$ Identify the important nodes for long-range spatial correlations ${\bf D}^{-\frac{1}{2}}{\bf A}{\bf D}^{-\frac{1}{2}}=\text{SoftMax}\big(\text{ReLU}({\bf E}_\mathcal{G} {\bf E}_\mathcal{G}^T)\big),\,$ Adjacency matrix is constructed by a data-driven method $\mathbf{L}=\left(\mathbf{I}_{N}+\mathbf{D}^{-\frac{1}{2}}\mathbf{A}\mathbf{D}^{-\frac{1}{2}}\right)\mathbf{X},~~$ Graph constrain is applied to the input $\mathbf{A}(\mathbf{X}\star\Theta)(i,j,:) = \sum\limits_{i=1}^k\sum\limits_{j=1}^k\left[\mathbf{L}\Theta_{p,q,:,:}\right]_{(n,m,f)}(i-p,j-q,:),\;$ Aggregate the GCN result in a CNN manner $n=1$ $q=1$

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ConvLSTM equipped with LS-Conv (LS-NTP)

Upon the LS-Conv, we embed this new operator into the ConvLSTM (we replace the convolution operator with the LS-Conv operator.)

Input Gate
$$
i_t = \sigma (W_{xi} \star \mathcal{X}_t + W_{hi} \star \mathcal{H}_{t-1} + W_{ci} \circ C_{t-1} + b_i)
$$
,
\nForget Gate $f_t = \sigma (W_{xf} \star \mathcal{X}_t + W_{hf} \star \mathcal{H}_{t-1} + W_{cf} \circ C_{t-1} + b_f)$,
\n $\tilde{C}_t = \tanh (W_{xc} \star \mathcal{X}_t + W_{hc} \star \mathcal{H}_{t-1} + b_c)$,
\nMemory Cell $C_t = f_t \circ C_{t-1} + i_t \circ \tilde{C}_t$,
\nOutput Gate $o_t = \sigma (W_{xo} \star \mathcal{X}_t + W_{ho} \star \mathcal{H}_{t-1} + W_{co} \circ C_t + b_o)$,
\nOutput $\mathcal{H}_t = o_t \circ \tanh(C_t)$,

where $X_t \in R^{n \times m \times c}$ is the input tensor at time-step t, \star is the LS-Conv operator, and the \circ is the element-wise multiplication.

> The main difference from ConvLSTM is we replace the convolution operator with the LS-Conv operator.

The framework of the final prediction model

After defining the spatial-temporal model, we use encoder-decoder architecture for the final prediction.

Fig. 5. The framework of encoder-decoder upon LS-NTP.

Experiments

Main Comparison

Table 3

The overall comparisons results for the near-surface temperature prediction.

PS:

- SSIM is an index for measuring the similarity between two images.
- PSNR uses to measure image quality for image distortion.

The comparison on each predictive time-step

We also compare the LS-NTP with other methods in the four mentioned indexes on each predictive timestep.

Fig. 8. Performance against different forecast lead time steps on ERA5.

Ablation Study

To measures the effectiveness of the proposed components, we conduct ablation study

- w/o NSA, which does not consider spatial attention in LS-Conv operator;
- w/o LAGC, which does not consider adaptive graph in LS-Conv operator;
- w NSA & LAGC, which ablates both the NSA and LAGC modules;
- w/o LSI, which means we do not apply CNN after the adaptive graph convolution;
- DAGG-ConvLSTM, which leverages the DAGG [15] to perform the adaptive graph convolution.

Table 4

The ablation study results for near-surface temperature prediction.

The ablation study results are shown in Table. As we can see that the performance suffer different degree decreases by ablating different components.

Analysis & Result

Q1: How does a long distance affect the performance?

We set a distance to filter out the entries in the adjacency matrix as zeros, whose distances to the corresponding grid are larger than a threshold d. Here d varies from 0 km to 6000 km (the largest distance of the selected zone).

- When $d = 0$, the setting means no long-range spatial correlations are considered;
- When $d = 6000$ the setting is equivalent to the original LS-NTP.

ong- and short-range spatial correlations for near-surface temperature

Q2: How does the LS-Conv kernel affect the short-range spatial correlations?

```
we vary the LS-Conv kernel from 1 \times 1 to 7 \times 7
```
- the kernel of LS-Conv is 1×1 means we omit the short-range spatial correlations
- the kernel of LS-Conv is 3×3 means we consider short-range in 3×3 area and consider long-range spatial correlation outside this area.

Table 5

Analysis of LS-NTP kernel size K@K.

K@K	ERA5 (per $1 h$)				$NCEP$ (per 6 h)			
	MAEJ					RMSEL SSIM TPSNR TMAEL RMSEL SSIM TPSNR		
1@1	0.939	1.233	0.878	46.308	1.799	2.386	0.910	40.380
3@3	0.897	1.176	0.883	46.639	1.740	2.318	0.915	40.646
5@5	1.034	1.357	0.869	45.585	1.792	2.397	0.908	40.377
7@7	1.118	1.455	0.845	44.937	1.860	2.465	0.908	40.123

 A 3 \times 3 kernel size reaches the best performance, which means considering non short-range spatial correlation or too large short-range spatial correlation helps little of the performance improvement.

Q3: Can a larger convolution kernel capture the long-range spatial correlations?

To answer this question, we enlarge the kernel size of the baseline models from 3×3 to 9×9 in baseline model which kernel uses for the spatial correlation capturing.

simply enlarge the convolution kernel size might introduce noisy information leading to a performance decreasing.

Q4: Can we visualize the long-range spatial correlations?

As we have used a data-driven method to learn the long-range spatial correlations, we select the column of the adjacency matrix which means the long-range spatial correlation learned by the model. We visual two cases in two datasets.

(a) The visualization of a specific column of (b) The visualization of a specific column of the learned adaptive graph matrix the learned adaptive graph matrix on the map

Fig. 11. The validation of long-range spatial correlation on the ERA5 dataset.

(a) The visualization of a specific column of (b) The visualization of a specific column of the learned adaptive graph matrix the learned adaptive graph matrix on the map

Fig. 12. The validation of long-range spatial correlation on the NCEP dataset.

the adaptive learning long-range spatial correlations are very obvious and reasonable 34/37

Q6: Can we visualize the predictive error performance

Fig. 15. The MAE metric of the results on the ERA5 dataset.

Fig. 16. The MAE metric of the results on the NCEP dataset.

Thank you for listening

Q&A

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