Connecting the dots:

Multivariate Time Series Forecasting with Graph Neural Networks

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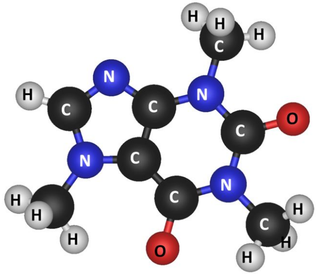
KDD '20, August 23–27, 2020, Virtual Event, USA

ACM ISBN 978-1-4503-7998-4/20/08…$15.00
https://doi.org/10.1145/XXXXXX.XXXXXX

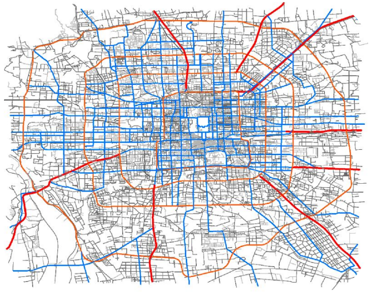
Zonghan Wu, Shirui Pan, Guodong Long, Jing Jiang, Xiaojun Chang, and Chengqi Zhang. 2020. Connecting the Dots: Multivariate Time Series Forecasting with Graph Neural Networks. In *26th ACM SIGKDD Conference on Knowledge Discovery and Data Mining (KDD '20), August 23–27, 2020, Virtual Event, USA*. ACM, New York, NY, USA, 11 pages. https://doi.org/10.1145/XXXXXX.XXXXXX

Intro on Graph Neural Networks (GNNs)

- Neural networks that can directly be applied to graphs
- When data represented as a graph
  - objects = nodes
  - relations = edges
- Motivation:
  - Deal with abstract concepts like relationships and interactions
  - Exploit that the data is representable as a graph
  - Intuitive



https://courses.lumenlearning.com/introchem/chapter/molecules/

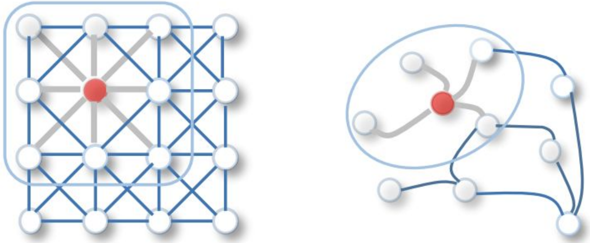


Road2Vec, 2017, K. Liu, S. Gao.

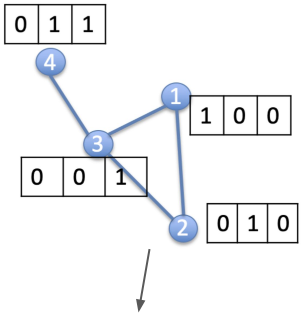
https://towardsdatascience.com/the-power-of-weak-ties-f1049c93f3a3

Graph Convolution

- Find spatial relationships between nodes
- Aggregate features from neighbours
- Generalization of CNNs, with
    - No ordering of neighbors
    - Different # of neighbors
- Adjacency matrix to represent neighbors
- Receptive field increases



A Comprehensive Survey on Graph Neural Networks, 2019, Wu et al

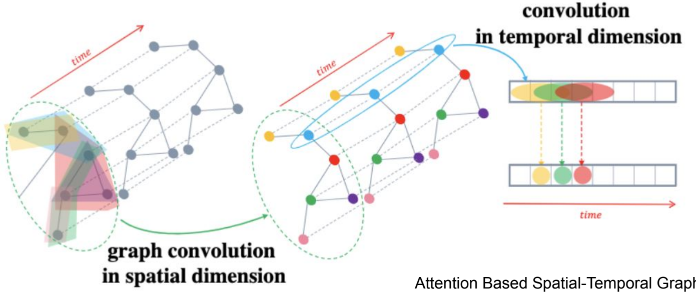


$$\begin{bmatrix} 1 & 1 & 1 & 0 \\ 1 & 1 & 1 & 0 \\ 1 & 1 & 1 & 1 \\ 0 & 0 & 1 & 1 \end{bmatrix} \times \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 1 \end{bmatrix} = \begin{bmatrix} \mathbf{1} & \mathbf{1} & \mathbf{1} \\ 1 & 1 & 1 \\ 1 & 2 & 2 \\ 0 & 1 & 2 \end{bmatrix}$$

Adjacency matrix (A) Feature matrix (X)

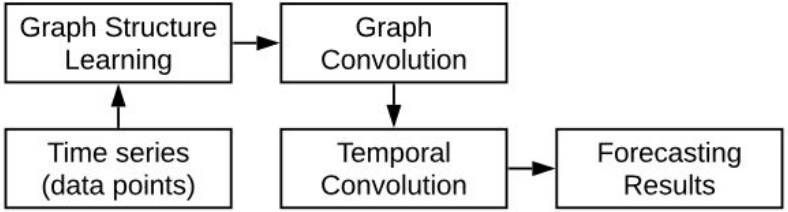
Back to the paper: Motivation, challenges and contributions

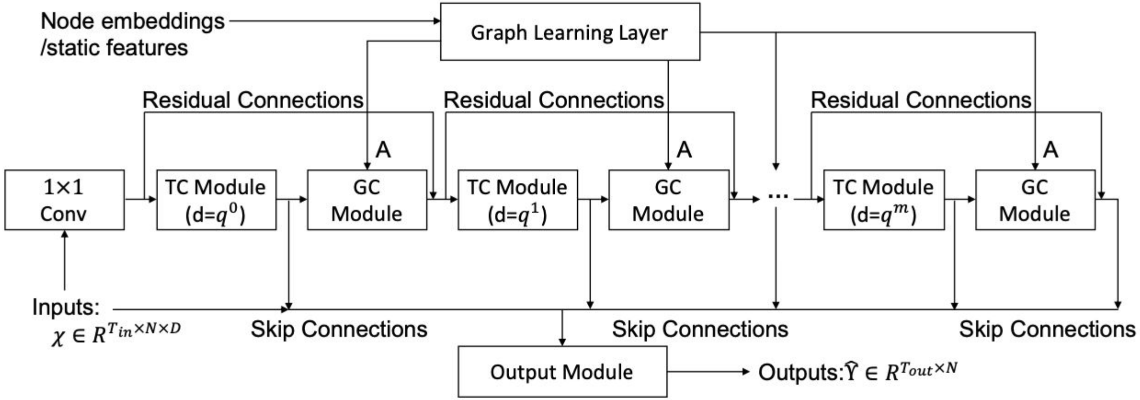
- Existing GNN on multivariate TS data:
  - Model the dependencies between variables as a graph
  - Utilize the spatial relations when predicting future values
  - “Spatial-temporal GNN”
- Challenges:
  - 1) Unknown graph structure
  - 2) Graph learning
- Main contributions of this paper:
  - General GNN for multivariate time series
  - Handle data without explicit graph structure
  - Joint framework for modeling multivariate time series and learning graph structure



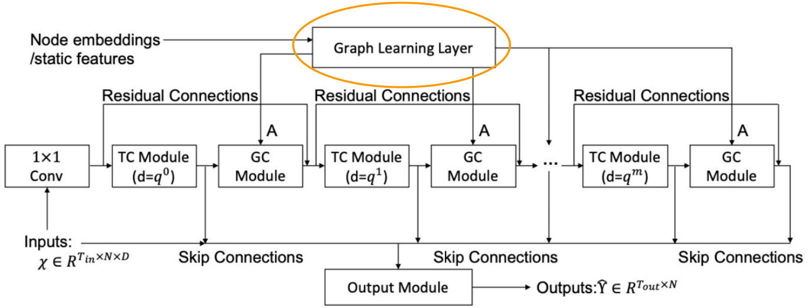
Attention Based Spatial-Temporal Graph Convolutional Networks for Traffic Flow Forecasting, 2019, Guo et al.

Overall architecture





Graph Learning Layer



- **In short: Learning the adjacency matrix, A**
- Wants uni-directed edges -> asymmetric **A**
- The subtraction and ReLU in (3) makes **A** asymmetric
- Selects the top-k closest nodes as neighbors
- Rest is set to zero
- Resulting **A** passed to all the Graph Convolution Modules

$$\mathbf{M}_1 = tanh(\alpha \mathbf{E}_1 \mathbf{\Theta}_1) \tag{1}$$

$$\mathbf{M}_2 = tanh(\alpha \mathbf{E}_2 \mathbf{\Theta}_2) \tag{2}$$

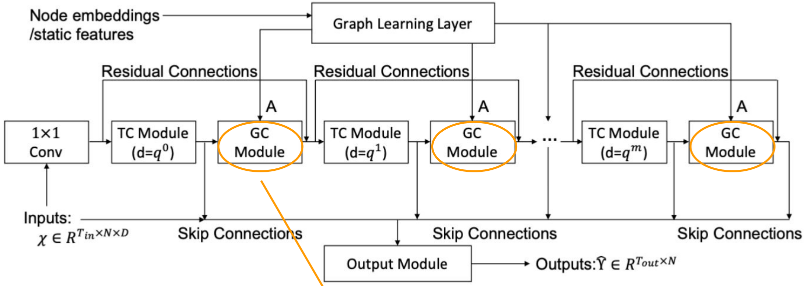
$$\mathbf{A} = ReLU(tanh(\alpha(\mathbf{M}_1 \mathbf{M}_2^T - \mathbf{M}_2 \mathbf{M}_1^T))) \tag{3}$$

$$for\ i = 1, 2, \cdots, N \tag{4}$$

$$\mathbf{idx} = argtopk(\mathbf{A}[i,:]) \tag{5}$$

$$\mathbf{A}[i, -\mathbf{idx}] = 0, \tag{6}$$

Graph Convolution Module



- **In short: Learning spatial dependencies**
- 1) Information propagation: $H^k = \beta H_{in} + (1-\beta)\tilde{A}H^{k-1}$
  - Calculate information from different 'hops'

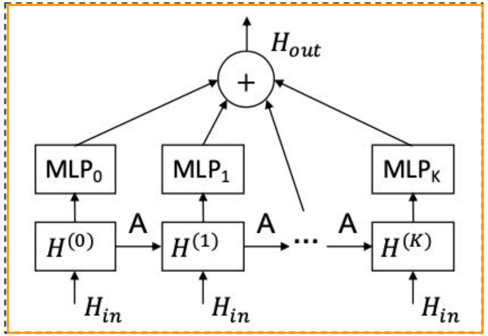
    1) H^0 : each node contains info about itself

    2) H^1 : each node contains info also about its neighbours

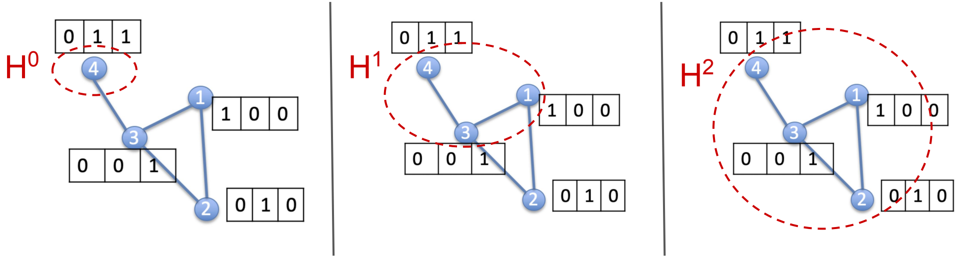
    3) H^2 : each node contains info about neighbours and their neighbours

    ...

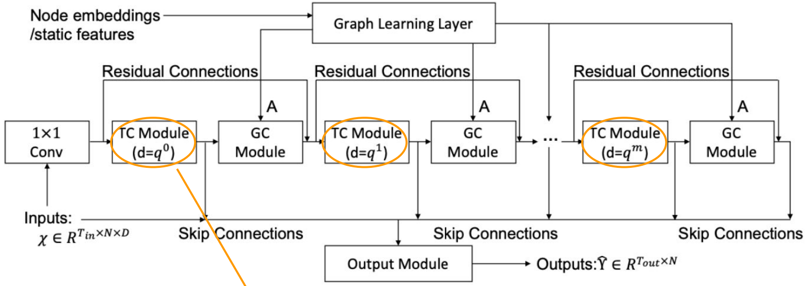
mix-hop propagation layer



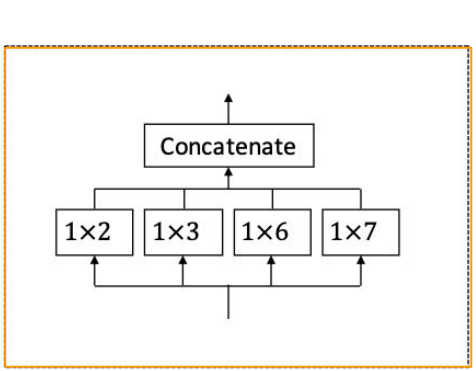
- 2) Information selection: $H_{out} = \sum_{k=0}^{K} H^{(k)} W^{(k)}$
  - Weigh the different hops
  - W is adjusted by MLP



Temporal Convolution Module



- **In short: Capture temporal dependencies**



Want to

1) Capture temporal patterns of various ranges
2) Handle very long sequences

How?

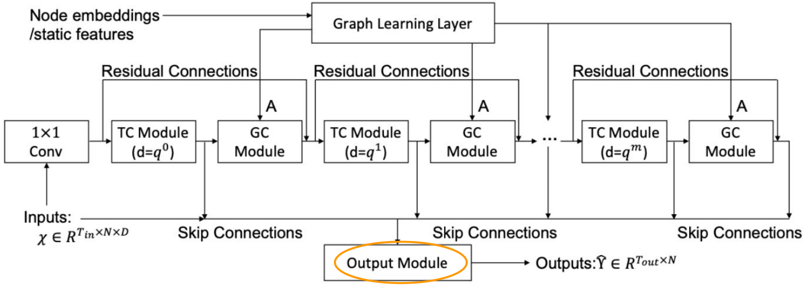
1) Inception:

Concatenate 1D convolutions with different filter sizes

2) Dilated convolution:

Increase dilation factor (d) for each TC module

Output Module



- Two 1x1 convolutions
- Transforms output into desired output dimension
- Use MAE
- Train using regular stochastic gradient descent

Experiments

- Validate their model on single-step and multi-step forecasting

Table 2: Baseline comparison under single-step forecasting for multivariate time series methods.

Dataset		Solar-Energy				Traffic				Electricity				Exchange-Rate			
		Horizon				Horizon				Horizon				Horizon			
Methods	Metrics	3	6	12	24	3	6	12	24	3	6	12	24	3	6	12	24
AR	RSE	0.2435	0.3790	0.5911	0.8699	0.5991	0.6218	0.6252	0.63	0.0995	0.1035	0.1050	0.1054	0.0228	0.0279	0.0353	0.0445
	CORR	0.9710	0.9263	0.8107	0.5314	0.7752	0.7568	0.7544	0.7519	0.8845	0.8632	0.8591	0.8595	0.9734	0.9656	0.9526	0.9357
VARMLP	RSE	0.1922	0.2679	0.4244	0.6841	0.5582	0.6579	0.6023	0.6146	0.1393	0.1620	0.1557	0.1274	0.0265	0.0394	0.0407	0.0578
	CORR	0.9829	0.9655	0.9058	0.7149	0.8245	0.7695	0.7929	0.7891	0.8708	0.8389	0.8192	0.8679	0.8609	0.8725	0.8280	0.7675
GP	RSE	0.2259	0.3286	0.5200	0.7973	0.6082	0.6772	0.6406	0.5995	0.1500	0.1907	0.1621	0.1273	0.0239	0.0272	0.0394	0.0580
	CORR	0.9751	0.9448	0.8518	0.5971	0.7831	0.7406	0.7671	0.7909	0.8670	0.8334	0.8394	0.8818	0.8713	0.8193	0.8484	0.8278
RNN-GRU	RSE	0.1932	0.2628	0.4163	0.4852	0.5358	0.5522	0.5562	0.5633	0.1102	0.1144	0.1183	0.1295	0.0192	0.0264	0.0408	0.0626
	CORR	0.9823	0.9675	0.9150	0.8823	0.8511	0.8405	0.8345	0.8300	0.8597	0.8623	0.8472	0.8651	0.9786	**0.9712**	0.9531	0.9223
LSTNet-skip	RSE	0.1843	0.2559	0.3254	0.4643	0.4777	0.4893	0.4950	0.4973	0.0864	0.0931	0.1007	0.1007	0.0226	0.0280	0.0356	0.0449
	CORR	0.9843	0.9690	0.9467	0.8870	0.8721	0.8690	0.8614	0.8588	0.9283	0.9135	0.9077	0.9119	0.9735	0.9658	0.9511	0.9354
TPA-LSTM	RSE	0.1803	**0.2347**	0.3234	0.4389	0.4487	0.4658	0.4641	0.4765	0.0823	0.0916	0.0964	0.1006	**0.0174**	**0.0241**	**0.0341**	**0.0444**
	CORR	0.9850	**0.9742**	0.9487	0.9081	0.8812	0.8717	0.8717	0.8629	0.9439	0.9337	0.9250	0.9133	**0.9790**	0.9709	0.9564	0.9381
MTGNN	RSE	**0.1778**	0.2348	**0.3109**	**0.4270**	**0.4162**	0.4754	**0.4461**	**0.4535**	**0.0745**	0.0878	**0.0916**	**0.0953**	0.0194	0.0259	0.0349	0.0456
	CORR	**0.9852**	0.9726	**0.9509**	0.9031	**0.8963**	0.8667	**0.8794**	**0.8810**	**0.9474**	0.9316	**0.9278**	**0.9234**	0.9786	0.9708	0.9551	0.9372
MTGNN+sampling	RSE	0.1875	0.2521	0.3347	0.4386	0.4170	**0.4435**	0.4469	0.4537	0.0762	**0.0862**	0.0938	0.0976	0.0212	0.0271	0.0350	0.0454
	CORR	0.9834	0.9687	0.9440	0.8990	0.8960	**0.8815**	0.8793	0.8758	0.9467	**0.9354**	0.9261	0.9219	0.9788	0.9704	**0.9574**	**0.9382**

Table 3: Baseline comparison under multi-step forecasting for spatial-temporal graph neural networks.

	Horizon 3			Horizon 6			Horizon 12		
	MAE	RMSE	MAPE	MAE	RMSE	MAPE	MAE	RMSE	MAPE
METR-LA									
DCRNN	2.77	5.38	7.30%	3.15	6.45	8.80%	3.60	7.60	10.50%
STGCN	2.88	5.74	7.62%	3.47	7.24	9.57%	4.59	9.40	12.70%
Graph WaveNet	2.69	5.15	6.90%	3.07	6.22	8.37%	3.53	7.37	10.01%
ST-MetaNet	2.69	5.17	6.91%	3.10	6.28	8.57%	3.59	7.52	10.63%
MRA-BGCN	**2.67**	**5.12**	6.80%	3.06	6.17	8.30%	3.49	7.30	10.00%
GMAN	2.77	5.48	7.25%	3.07	6.34	8.35%	**3.40**	**7.21**	**9.72%**
MTGNN	2.69	5.18	6.86%	**3.05**	**6.17**	**8.19%**	3.49	7.23	9.87%
MTGNN+sampling	2.76	5.34	**5.18%**	3.11	6.32	8.47%	3.54	7.38	10.05%
PEMS-BAY									
DCRNN	1.38	2.95	2.90%	1.74	3.97	3.90%	2.07	4.74	4.90%
STGCN	1.36	2.96	2.90%	1.81	4.27	4.17%	2.49	5.69	5.79%
Graph WaveNet	1.30	2.74	**2.73%**	1.63	3.70	3.67%	1.95	4.52	4.63%
ST-MetaNet	1.36	2.90	2.82%	1.76	4.02	4.00%	2.20	5.06	5.45%
MRA-BGCN	**1.29**	**2.72**	2.90%	**1.61**	**3.67**	3.80%	1.91	4.46	4.60%
GMAN	1.34	2.82	2.81%	1.62	3.72	**3.63%**	**1.86**	**4.32**	**4.31%**
MTGNN	1.32	2.79	2.77%	1.65	3.74	3.69%	1.94	4.49	4.53%
MTGNN+sampling	1.34	2.83	2.83%	1.67	3.79	3.78%	1.95	4.49	4.62%

Conclusions

- Framework for multivariate time series forecasting using GNNs
- Graph Learning Layer to **learn** the graph structure
- Spatial dependencies modeled by a Graph Convolution Module
  - Information propagation
  - Information selection
- Temporal dependencies modeled by a Temporal Convolution Module
  - dilated inception layers
- What’s special:
  - No predefined graph structure required
    - learns the adjacency matrix by a graph learning layer
  - General framework, not customized for a single time series domain
  - Reaches SOTA and on-pair SOTA results despite this