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17th INTERNATIONAL OPERATIONS & MAINTENANCE CONFERENCE IN THE ARAB COUNTRIES OMAINTEC 2019 - 19 November Dubai, United Arab Emirates

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#### Introduction

- Rapid urbanization: 4.7B people to 6.7B by 2050 [United Nations]
- Air and water pollution, unsustainable energy consumption, toxic waste disposal, inadequate urban planning, decreased public health and safety, social vulnerability
- In most large cities of the world, mobility of passengers and freights is not yet sustainable
- Traffic congestion, increase of transport needs, ineffective accessibility, reduced productivity

#### Introduction

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- Traffic congestion, increase of transport needs, ineffective accessibility, reduced productivity

- Solutions:
  - 1. Champion alternatives
  - 2. Enlarge infrastructure
  - 3. Manage traffic flows
- Increase of available data enables innovative and integrated solutions
- Urban computing: intelligent transportation systems (ITS), smart vehicle sharing systems, home automation, smart grid and energy solutions
- Core component of ITS:
  - traffic forecasting

Goal of Traffic Forecasting:

- Measure, model and predict traffic conditions, in real-time, accurately and reliably, in order to
- Optimize the flow and mitigate traffic congestion, and support traffic light control, time of arrival estimates, planning of new road segments

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Very challenging problem:

- Heterogeneous data (e.g., loop counter and floating car data)
- Complex **spatio-temporal** dependencies
- Typically sparse, incomplete and highdimensional data
- Inclusion of **external factors** (e.g., weather conditions, and road accidents)

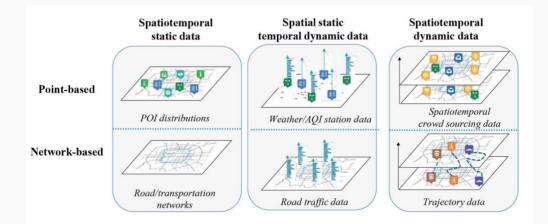
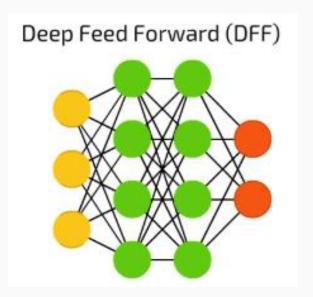


Figure 1: Six types of urban data [9]. Reprinted with permission.

• Traditional approaches can be divided into model-driven and data-driven approaches

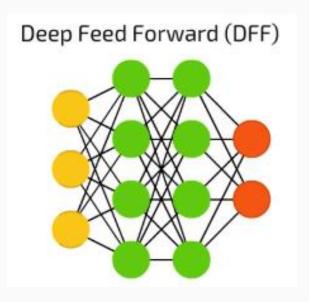
• **Model-driven** methods typically require prior knowledge, detailed modeling, not easily transferable to other cases, significant computational resources • **Traditional data-driven** approaches typically require careful feature engineering, and are not complex enough to model the non-linearity and nonstationarity of the spatio-temporal data

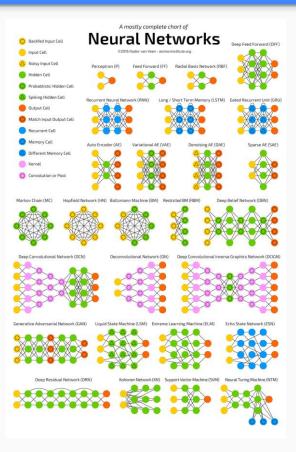
• Deep learning and neural networks



Source: Van Veen, F. & Leijnen, S. (2019). The Neural Network Zoo. Retrieved from https://www.asimovinstitute.org/neural-network-zoo

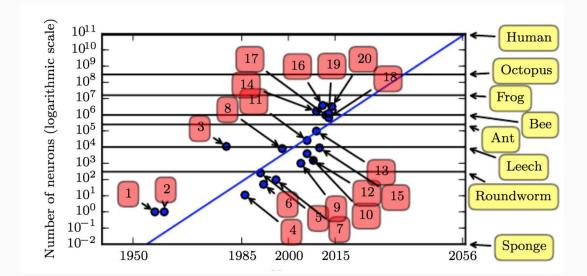
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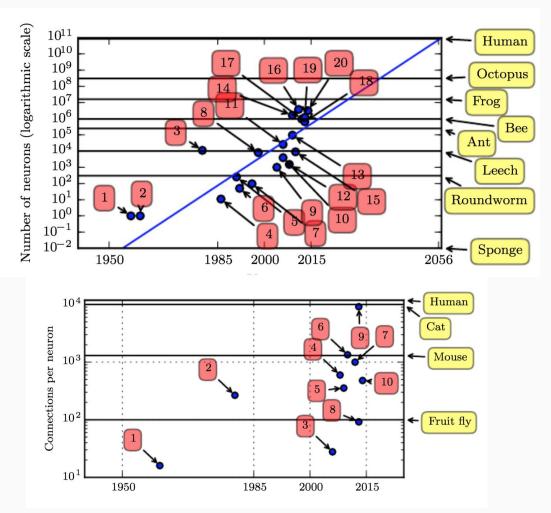
### • # neurons



Source: Deep Learning - Ian Goodfellow et al, MIT PRESS - 2017

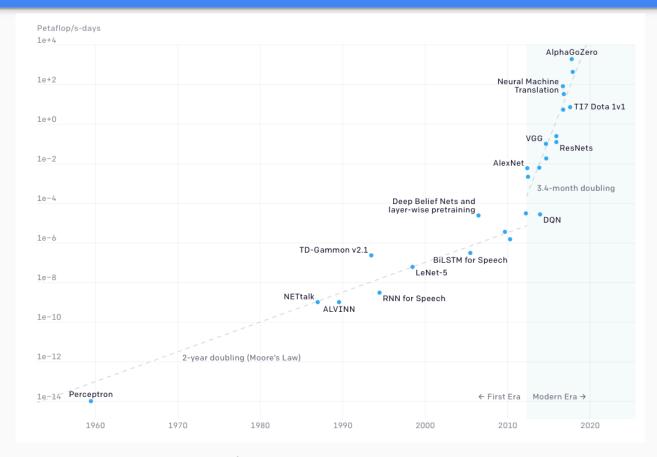
• # neurons

### # connections



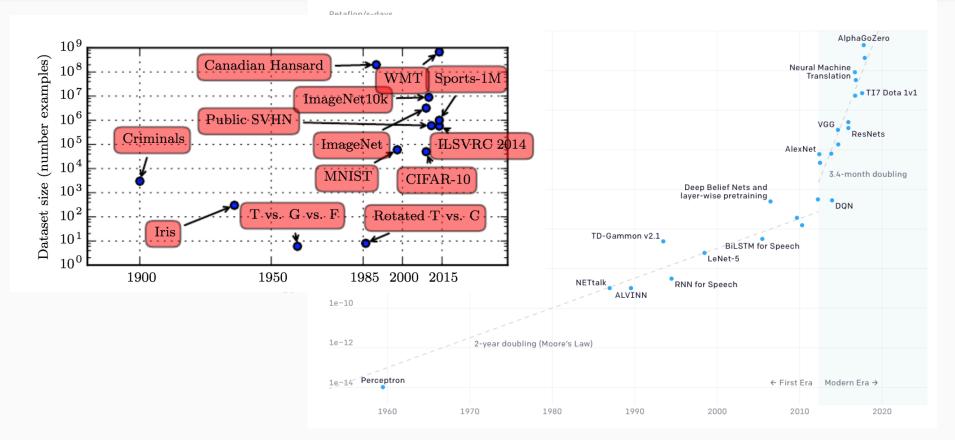
Source: *Deep Learning* - Ian Goodfellow et al, MIT PRESS - 2017

#### Neural networks (datasets and compute)

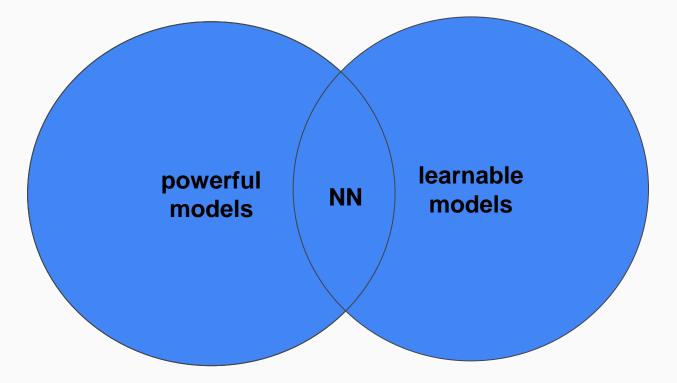


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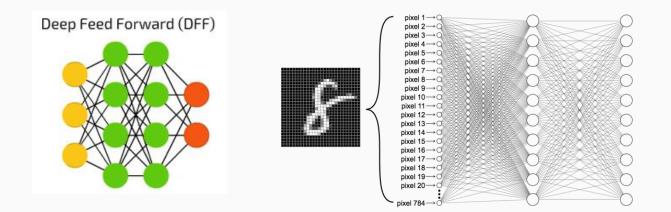


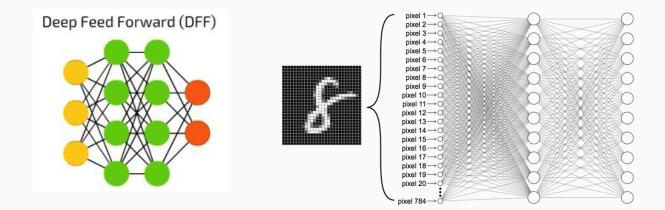
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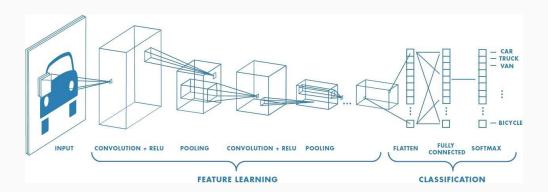


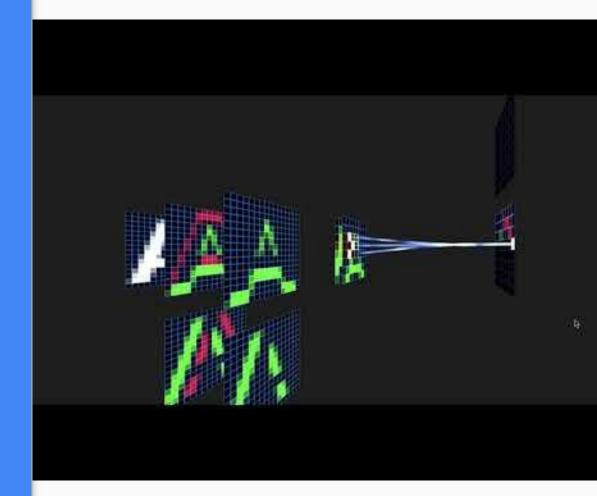
Deep Feed Forward (DFF)





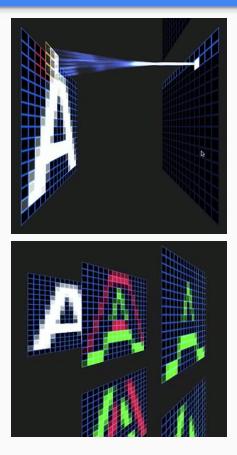


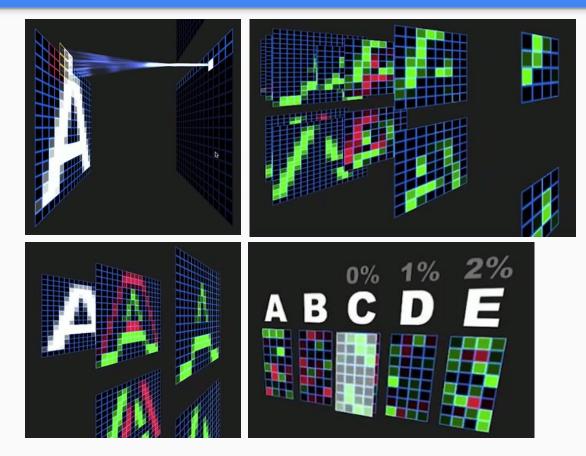




#### https://youtu.be/9KuhzUX1\_Ks

Source: Otavio Good - A visual and intuitive understanding of deep learning



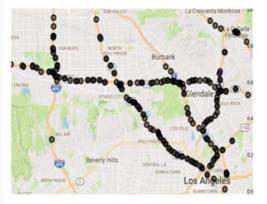




(a) METR-LA



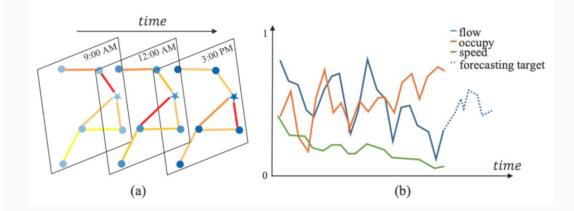
(b) PEMS-BAY

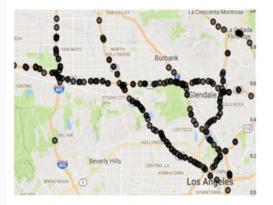


(a) METR-LA



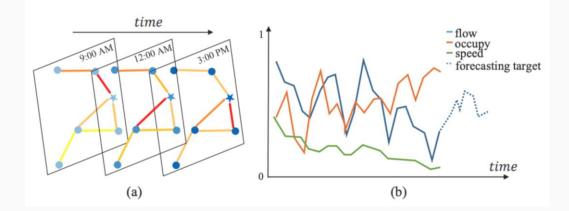


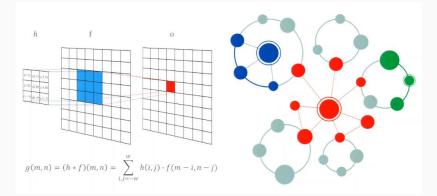




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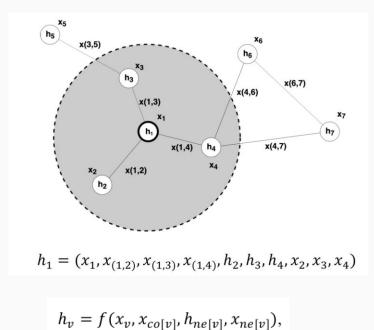
(b) PEMS-BAY

Category	References		
Recurrent Graph Neural Networks	[39], [47]–[50]		
Convolutional Graph Neural Networks	[37], [40], [51]–[53]		
Graph Attention Networks	[54], [55]		
Graph Autoencoders	[56]–[61]		

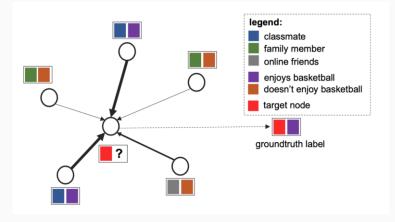
Table 1. Categorization of graph neural network models and representative publications.

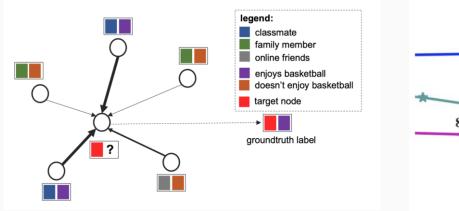
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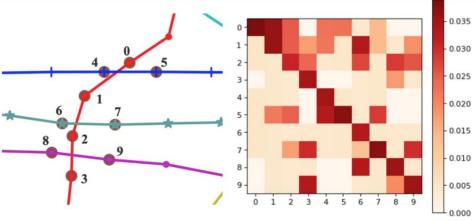
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 $\boldsymbol{o}_v = g(\boldsymbol{h}_v, \boldsymbol{x}_v),$ 

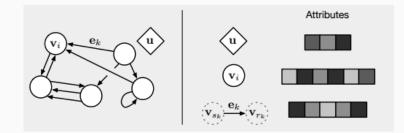




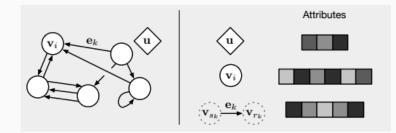


(c) Attention matrix obtained from the spatial attention mechanism.

# Graph Network (GN) Blocks

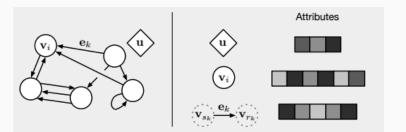


# Graph Network (GN) Blocks



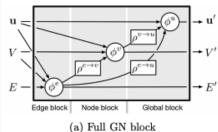
$$\begin{split} e_{k}{}' &= \varphi^{e}(e_{k},h_{rk},h_{sk},u), \qquad e_{i}{}^{*'} &= \rho^{e \to h}(E_{i}{}'), \\ h_{i}{}' &= \varphi^{h}(e_{i}{}^{*'},h_{i},u), \qquad e^{*'} &= \rho^{e \to u}(E'), \\ u' &= \varphi^{u}(e^{*'},h^{*'},u), \qquad h^{*'} &= \rho^{h \to u}(H'), \end{split}$$

## Graph Network (GN) Blocks



$$\begin{aligned} e_{k}{}' &= \varphi^{e}(e_{k}, h_{rk}, h_{sk}, u), \qquad e_{i}{}^{*'} &= \rho^{e \to h}(E_{i}{}'), \\ h_{i}{}' &= \varphi^{h}(e_{i}{}^{*'}, h_{i}, u), \qquad e^{*'} &= \rho^{e \to u}(E'), \end{aligned}$$

 $u' = \varphi^u(e^{*'}, h^{*'}, u), \qquad h^{*'} = \rho^{h \to u}(H'),$ 



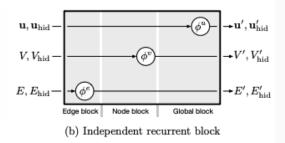
Node block

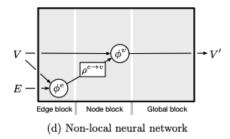
(c) Message-passing neural network

+ u

 $\rightarrow V'$ 

Global block





J. Rico, J. Barateiro, A. Oliveira - Graph Neural Networks for Traffic Forecasting (OMAINTEC 2019)

Edge block

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E

### GNN for Traffic Forecasting

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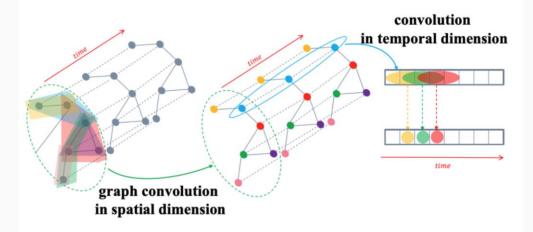
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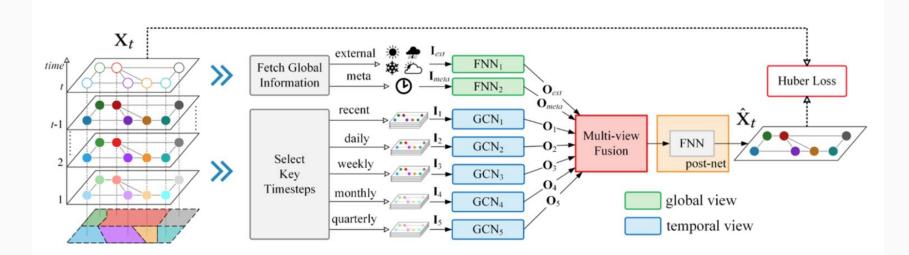
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### GNN for Traffic Forecasting

Model	Ref.	Scope	Predicts	Data source	Datasets	Open dataset?	Code available?
ST-GCN	[92]	Fw, Ur	S	L	BJER4, PeMS	X, √	✓
DCRNN	[83]	Fw	s	L	METR-LA, PeMS	1	✓
MRes-RGNN	[87]	Fw	S	L	METR-LA, PeMS	1	x
TGC-LSTM	[7]	Fw, Ur	s	L, FCD	LOOP, INRIX	√, X	x
ASTGCN	[8]	Fw	F, S	L	PeMSD4, PeMSD8	1	✓
STDGI	[86]	Fw	s	L	METR-LA	1	✓
MVGCN	[90]	Ur	F	FCD	TaxiNYC, TaxiBJ, BikeDC, BikeNYC	1	x
DST-GCNN	[82]	Fw, Ur	S, V	L, FCD	METR-LA, TaxiBJ	1	x
GSRNN	[91]	Ur	F	FCD	BikeNYC, TaxiBJ	1	x
Graph Wavenet	[84]	Fw	s	L	METR-LA, PeMS	1	✓
3D-TGCN	[6]	Fw	s	L	PeMS	1	x
ST-UNet	[93]	Fw	s	L	METR-LA, PeMS	1	x
GaAN	[55]	Fw	s	L	METR-LA	1	x
Motif-GCRNN	[88]	Ur	s	FCD	TaxiChengdu	x	x
STGi-ResNet	[85]	Ur	F	FCD	Didi Chengdu	1	X
T-GCN	[94]	Fw, Ur	S	FCD	SZ-taxi, Los-loop	<b>X</b> , √	X
FlowConvGRU	[97]	Ur	F	FCD	TaxiNYC, TaxiCD	1	x

## **GNN for Traffic Forecasting**



Multi-view Graph Convolutional Networks (MVGCN) [90]

# Conclusions, Challenges and Opportunities

- Deep learning and in particular, Graph Neural Networks, have achieved state of the art results in prediction tasks, including traffic prediction
- Several challenges and opportunities lie ahead, in the next decades

- Opportunities:
  - More and better data
  - More computational resources
- Challenges:
  - Uncertainty estimates
  - Interpretability
  - Integration with downstream applications
  - Data ageing and concept drift
  - Travel time prediction
  - Better evaluation metrics
  - Systematic inclusion of exogenous factors











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#### References

- United Nations, Department of Economic and Social Affairs, Population Division., "World urbanization prospects. the 2018 revision," ST/ESA/SER. A/421, 2019.
- [2] D. Schrank, B. Eisele, and T. Lomax, "2019 Urban Mobility Report," Texas A&M Transportation Institute, 2019.
- [3] I. Lana, J. Del Ser, M. Velez, and E. I. Vlahogianni, "Road Traffic Forecasting: Recent Advances and New Challenges," *IEEE Intell. Transp. Syst. Mag.*, vol. 10, no. 2, pp. 93–109, 2018.
- [4] Y. Zheng, L. Capra, O. Wolfson, and H. Yang, "Urban Computing: Concepts, Methodologies, and Applications," ACM Trans. Intell. Syst. Technol., vol. 5, no. 3, pp. 38:1–38:55, Sep. 2014.
- [5] E. I. Vlahogianni, M. G. Karlaftis, and J. C. Golias, "Short-term traffic forecasting: Where we are and where we're going," *Transp. Res. Part C: Emerg. Technol.*, vol. 43, pp. 3–19, 2014.
- [6] B. Yu, M. Li, J. Zhang, and Z. Zhu, "3D Graph Convolutional Networks with Temporal Graphs: A Spatial Information Free Framework For Traffic Forecasting," arXiv [cs.LG], 03-Mar-2019.
- [7] Z. Cui, K. Henrickson, R. Ke, and Y. Wang, "Traffic Graph Convolutional Recurrent Neural Network: A Deep Learning Framework for Network-Scale Traffic Learning and Forecasting," arXiv [cs.LG], 20-Feb-2018.
- [8] S. Guo, Y. Lin, N. Feng, C. Song, and H. Wan, "Attention Based Spatial-Temporal Graph Convolutional Networks for Traffic Flow Forecasting," in *Proceedings of the AAAI Conference on Artificial Intelligence*, 2019, vol. 33, pp. 922–929.
- [9] Y. Zheng, Urban Computing. MIT Press, 2019.
- [10] Smith Brian L. and Demetsky Michael J., "Traffic Flow Forecasting: Comparison of Modeling Approaches," J. Transp. Eng., vol. 123, no. 4, pp. 261–266, Jul. 1997.
- [11] K. A. Small, E. T. Verhoef, and R. Lindsey, The economics of urban transportation. Routledge, 2007.
- [12] G. A. Davis and N. L. Nihan, "Nonparametric regression and short-term freeway traffic forecasting," J. Transp. Eng., vol. 117, no. 2, pp. 178–188, 1991.
- [13] D. Chowdhury, L. Santen, and A. Schadschneider, "Statistical physics of vehicular traffic and some related systems," *Phys. Rep.*, vol. 329, no. 4, pp. 199–329, May 2000.
- [14] M. Saidallah, A. El Fergougui, and A. E. Elalaoui, "A Comparative Study of Urban Road Traffic Simulators," MATEC Web of Conferences, vol. 81, p. 05002, 2016.
- [15] S. Lee and D. B. Fambro, "Application of Subset Autoregressive Integrated Moving Average Model for Short-Term Freeway Traffic Volume Forecasting," *Transp. Res. Rec.*, vol. 1678, no. 1, pp. 179–188, Jan. 1999.
- [16] Williams Billy M. and Hoel Lester A., "Modeling and Forecasting Vehicular Traffic Flow as a Seasonal ARIMA Process: Theoretical Basis and Empirical Results," J. Transp. Eng., vol. 129, no. 6, pp. 664–672, Nov. 2003.
- [17] L. Zhang, Q. Liu, W. Yang, N. Wei, and D. Dong, "An Improved K-nearest Neighbor Model for Short-term Traffic Flow Prediction," *Procedia - Social and Behavioral Sciences*, vol. 96, pp. 653–662, Nov. 2013.
- [18] H. Su, L. Zhang, and S. Yu, "Short-term Traffic Flow Prediction Based on Incremental Support Vector Regression," in *Third International Conference on Natural Computation (ICNC 2007)*, 2007, vol. 1, pp. 640–645.
- [19] Y. Qi and S. Ishak, "A Hidden Markov Model for short term prediction of traffic conditions on freeways," Transp. Res. Part C: Emerg. Technol., vol. 43, pp. 95–111, Jun. 2014.
- [20] Y. Kamarianakis and P. Prastacos, "Forecasting Traffic Flow Conditions in an Urban Network: Comparison of Multivariate and Univariate Approaches," *Transp. Res. Rec.*, vol. 1857, no. 1, pp. 74–84, Jan. 2003.
- [21] W. Min and L. Wynter, "Real-time road traffic prediction with spatio-temporal correlations," Transp. Res. Part C: Emerg. Technol., vol. 19, no. 4, pp. 606–616, Aug. 2011.
- [22] J. Kwon and K. Murphy, "Modeling freeway traffic with coupled HMMs," Technical report, Univ. California, Berkeley, 2000.
- [23] J. Xu, D. Deng, U. Demiryurek, C. Shahabi, and M. van der Schaar, "Mining the Situation: Spatiotemporal Traffic Prediction With Big Data," *IEEE Journal of Selected Topics in Signal Processing*, vol. 9, no. 4, pp. 702–715, 2015.
- [24] Y. LeCun, Y. Bengio, and G. Hinton, "Deep learning," Nature, vol. 521, no. 7553, pp. 436-444, May 2015.
- [25] A. Krizhevsky, I. Sutskever, and G. E. Hinton, "ImageNet Classification with Deep Convolutional Neural Networks," in Advances in Neural Information Processing Systems 25, F. Pereira, C. J. C. Burges, L. Bottou, and K. O. Weinberger, Eds. Curran Associates, Inc., 2012, pp. 1097–1105.
- [26] R. Collobert, J. Weston, L. Bottou, M. Karlen, K. Kavukcuoglu, and P. Kuksa, "Natural Language Processing (Almost) from Scratch," J. Mach. Learn. Res., vol. 12, no. Aug, pp. 2493–2537, 2011.
- [27] J. Ma, R. P. Sheridan, A. Liaw, G. E. Dahl, and V. Svetnik, "Deep Neural Nets as a Method for Quantitative Structure-Activity Relationships," *Journal of Chemical Information and Modeling*, vol. 55, no. 2, pp. 263–274, 2015.
- [28] H. Wang, N. Wang, and D.-Y. Yeung, "Collaborative Deep Learning for Recommender Systems," in *Proceedings of the 21th ACM SIGKDD International Conference on Knowledge Discovery and Data Mining*, Sydney, NSW, Australia, 2015, pp. 1235–1244.
- [29] V. Mnih et al., "Human-level control through deep reinforcement learning," Nature, vol. 518, no. 7540. pp. 529– 533, 2015.
- [30] W. Huang, G. Song, H. Hong, and K. Xie, "Deep Architecture for Traffic Flow Prediction: Deep Belief Networks With Multitask Learning," *IEEE Trans. Intell. Transp. Syst.*, vol. 15, no. 5, pp. 2191–2201, Oct. 2014.

- [31] X. Ma, Z. Tao, Y. Wang, H. Yu, and Y. Wang, "Long short-term memory neural network for traffic speed prediction using remote microwave sensor data," *Transp. Res. Part C: Emerg. Technol.*, vol. 54, pp. 187–197, May 2015.
- [32] R. Yu, Y. Li, C. Shahabi, U. Demiryurek, and Y. Liu, "Deep Learning: A Generic Approach for Extreme Condition Traffic Forecasting," in *Proceedings of the 2017 SIAM International Conference on Data Mining*, Society for Industrial and Applied Mathematics, 2017, pp. 777–785.
- [33] Z. Cui, R. Ke, and Y. Wang, "Deep Bidirectional and Unidirectional LSTM Recurrent Neural Network for Network-wide Traffic Speed Prediction," arXiv [cs.LG], 07-Jan-2018.
- [34] X. Ma, Z. Dai, Z. He, J. Ma, Y. Wang, and Y. Wang, "Learning Traffic as Images: A Deep Convolutional Neural Network for Large-Scale Transportation Network Speed Prediction," Sensors, vol. 17, no. 4, Apr. 2017.
- [35] J. Zhang, Y. Zheng, and D. Qi, "Deep spatio-temporal residual networks for citywide crowd flows prediction," in *Thirty-First AAAI Conference on Artificial Intelligence*, 2017.
- [36] H. Yu, Z. Wu, S. Wang, Y. Wang, and X. Ma, "Spatiotemporal Recurrent Convolutional Networks for Traffic Prediction in Transportation Networks," *Sensors*, vol. 17, no. 7, Jun. 2017.
- [37] T. N. Kipf and M. Welling, "Semi-Supervised Classification with Graph Convolutional Networks," arXiv [cs.LG], 09-Sep-2016.
- [38] Q. Liu, M. Allamanis, M. Brockschmidt, and A. Gaunt, "Constrained Graph Variational Autoencoders for Molecule Design," in *Advances in Neural Information Processing Systems 31*, S. Bengio, H. Wallach, H. Larochelle, K. Grauman, N. Cesa-Bianchi, and R. Garnett, Eds. Curran Associates, Inc., 2018, pp. 7795–7804.
- [39] F. Scarselli, M. Gori, A. C. Tsoi, M. Hagenbuchner, and G. Monfardini, "The graph neural network model," *IEEE Trans. Neural Netw.*, vol. 20, no. 1, pp. 61–80, Jan. 2009.
- [40] M. Defferrard, X. Bresson, and P. Vandergheynst, "Convolutional Neural Networks on Graphs with Fast Localized Spectral Filtering," in Advances in Neural Information Processing Systems 29, D. D. Lee, M. Sugiyama, U. V. Luxburg, I. Guyon, and R. Garnett, Eds. Curran Associates, Inc., 2016, pp. 3844–3852.
- [41] P. W. Battaglia et al., "Relational inductive biases, deep learning, and graph networks," arXiv [cs.LG], 04-Jun-2018.
- [42] M. M. Bronstein, J. Bruna, Y. LeCun, A. Szlam, and P. Vandergheynst, "Geometric Deep Learning: Going beyond Euclidean data," *IEEE Signal Process. Mag.*, vol. 34, no. 4, pp. 18–42, Jul. 2017.
- [43] W. L. Hamilton, R. Ying, and J. Leskovec, "Representation Learning on Graphs: Methods and Applications," arXiv [cs.SI], 17-Sep-2017.
- [44] Z. Zhang, P. Cui, and W. Zhu, "Deep Learning on Graphs: A Survey," arXiv [cs.LG], 11-Dec-2018.
- [45] Z. Wu, S. Pan, F. Chen, G. Long, C. Zhang, and P. S. Yu, "A Comprehensive Survey on Graph Neural Networks," arXiv [cs.LG], 03-Jan-2019.
- [46] J. Zhou et al., "Graph Neural Networks: A Review of Methods and Applications," arXiv [cs.LG], 20-Dec-2018.
- [47] Y. Li, D. Tarlow, M. Brockschmidt, and R. Zemel, "Gated Graph Sequence Neural Networks," arXiv [cs.LG], 17-Nov-2015.
- [48] L. Ruiz, F. Gama, and A. Ribeiro, "Gated Graph Convolutional Recurrent Neural Networks," arXiv [cs.LG], 05-Mar-2019.

[49] H. Dai, Z. Kozareva, B. Dai, A. Smola, and L. Song, "Learning Steady-States of Iterative Algorithms over Graphs," in *Proceedings of the 35th International Conference on Machine Learning*, 2018, vol. 80, pp. 1106– 1114.

- [50] J. You, R. Ying, X. Ren, W. L. Hamilton, and J. Leskovec, "GraphRNN: Generating Realistic Graphs with Deep Auto-regressive Models," arXiv [cs.LG], 24-Feb-2018.
- [51] J. Bruna, W. Zaremba, A. Szlam, and Y. LeCun, "Spectral Networks and Locally Connected Networks on Graphs," arXiv [cs.LG], 21-Dec-2013.
- [52] O. Levy and Y. Goldberg, "Neural Word Embedding as Implicit Matrix Factorization," in Advances in Neural Information Processing Systems 27, Z. Ghahramani, M. Welling, C. Cortes, N. D. Lawrence, and K. Q. Weinberger. Eds. Curran Associates. Inc., 2014. no. 2177–2185.
- [53] D. K. Duvenaud et al., "Convolutional Networks on Graphs for Learning Molecular Fingerprints," in Advances in Neural Information Processing Systems 28, C. Cortes, N. D. Lawrence, D. D. Lee, M. Sugiyama, and R. Garnett, Eds. Curran Associates, Inc., 2015, pp. 2224–2232.
- [54] P. Veličković, G. Cucurull, A. Casanova, A. Romero, P. Liò, and Y. Bengio, "Graph Attention Networks," arXiv [stat.ML], 30-Oct-2017.
- [55] J. Zhang, X. Shi, J. Xie, H. Ma, I. King, and D.-Y. Yeung, "GaAN: Gated Attention Networks for Learning on Large and Spatiotemporal Graphs," arXiv [cs.LG], 20-Mar-2018.
- [56] D. Wang, P. Cui, and W. Zhu, "Structural Deep Network Embedding," in Proceedings of the 22Nd ACM SIGKDD International Conference on Knowledge Discovery and Data Mining, San Francisco, California, USA, 2016, pp. 1225–1234.
- [57] T. N. Kipf and M. Welling, "Variational Graph Auto-Encoders," arXiv [stat.ML], 21-Nov-2016.
- [58] Y. Li, O. Vinyals, C. Dyer, R. Pascanu, and P. Battaglia, "Learning Deep Generative Models of Graphs," arXiv [cs.LG], 08-Mar-2018.
- [59] M. Simonovsky and N. Komodakis, "GraphVAE: Towards Generation of Small Graphs Using Variational Autoencoders," in Artificial Neural Networks and Machine Learning – ICANN 2018, 2018, pp. 412–422.

#### References

- [60] N. De Cao and T. Kipf, "MolGAN: An implicit generative model for small molecular graphs," arXiv [stat.ML], 30-May-2018.
- [61] S. Pan, R. Hu, S.-F. Fung, G. Long, J. Jiang, and C. Zhang, "Learning Graph Embedding With Adversarial Training Methods," *IEEE Transactions on Cybernetics*. pp. 1–13, 2019.
- [62] A. Sperduti and A. Starita, "Supervised neural networks for the classification of structures," *IEEE Trans. Neural Netw.*, vol. 8, no. 3, pp. 714–735, 1997.
- [63] M. Gori, G. Monfardini, and F. Scarselli, "A new model for learning in graph domains," in *Proceedings. 2005 IEEE International Joint Conference on Neural Networks, 2005.*, 2005, vol. 2, pp. 729–734 vol. 2.
- [64] M. A. Khamsi and W. A. Kirk, An Introduction to Metric Spaces and Fixed Point Theory. John Wiley & Sons, 2011.
- [65] J. Chung, C. Gulcehre, K. Cho, and Y. Bengio, "Empirical Evaluation of Gated Recurrent Neural Networks on Sequence Modeling," arXiv [cs.NE], 11-Dec-2014.
- [66] C. Gallicchio and A. Micheli, "Graph Echo State Networks," in The 2010 International Joint Conference on Neural Networks (IJCNN), 2010, pp. 1–8.
- [67] C. Zhuang and Q. Ma, "Dual graph convolutional networks for graph-based semi-supervised classification," Proceedings of the 2018 World Wide Web Conference, 2018.
- [68] D. Bahdanau, K. Cho, and Y. Bengio, "Neural Machine Translation by Jointly Learning to Align and Translate," arXiv [cs.CL], 01-Sep-2014.
- [69] A. Vaswani et al., "Attention is All you Need," in Advances in Neural Information Processing Systems 30, I. Guyon, U. V. Luxburg, S. Bengio, H. Wallach, R. Fergus, S. Vishwanathan, and R. Garnett, Eds. Curran Associates, Inc., 2017, pp. 5998–6008.
- [70] J. B. Lee, R. A. Rossi, S. Kim, N. K. Ahmed, and E. Koh, "Attention Models in Graphs: A Survey," arXiv [cs.Al], 20-Jul-2018.
- [71] P. Vincent, H. Larochelle, I. Lajoie, Y. Bengio, and P.-A. Manzagol, "Stacked Denoising Autoencoders: Learning Useful Representations in a Deep Network with a Local Denoising Criterion," J. Mach. Learn. Res., vol. 11, no. Dec, pp. 3371–3408, 2010.
- [72] D. P. Kingma and M. Welling, "Auto-Encoding Variational Bayes," arXiv [stat.ML], 20-Dec-2013.
- [73] I. Goodfellow et al., "Generative Adversarial Nets," in Advances in Neural Information Processing Systems 27, Z. Ghahramani, M. Welling, C. Cortes, N. D. Lawrence, and K. Q. Weinberger, Eds. Curran Associates, Inc., 2014, pp. 2672–2680.
- [74] X. Wang, R. Girshick, A. Gupta, and K. He, "Non-local neural networks," in Proceedings of the IEEE Conference on Computer Vision and Pattern Recognition, 2018, pp. 7794–7803.
- [75] J. Gilmer, S. S. Schoenholz, P. F. Riley, O. Vinyals, and G. E. Dahl, "Neural Message Passing for Quantum Chemistry," in *Proceedings of the 34th International Conference on Machine Learning - Volume 70*, 2017, pp. 1263–1272.
- [76] A. Paszke et al., "Automatic differentiation in PyTorch," 28-Oct-2017.
- [77] M. Abadi et al., "Tensorflow: A system for large-scale machine learning," in 12th S{USENIX} Symposium on Operating Systems Design and Implementation ({OSDI} \$ 16), 2016, pp. 265–283.
- [78] M. Wang et al., "Deep graph library, 2018," URL http://dgl. ai.
- [79] Alibaba, "Euler," 2019.
- [80] M. Fey and J. E. Lenssen, "Fast Graph Representation Learning with PyTorch Geometric," arXiv [cs.LG], 06-Mar-2019.
- [81] D. Chai, L. Wang, and Q. Yang, "Bike Flow Prediction with Multi-graph Convolutional Networks," in Proceedings of the 26th ACM SIGSPATIAL International Conference on Advances in Geographic Information Systems, Seattle, Washington, 2018, pp. 397–400.
- [82] M. Wang et al., "Dynamic Spatio-temporal Graph-based CNNs for Traffic Prediction," arXiv [cs.CV], 05-Dec-2018.
- [83] Y. Li, R. Yu, C. Shahabi, and Y. Liu, "Diffusion Convolutional Recurrent Neural Network: Data-Driven Traffic Forecasting," arXiv [cs.LG], 06-Jul-2017.
- [84] Z. Wu, S. Pan, G. Long, J. Jiang, and C. Zhang, "Graph WaveNet for Deep Spatial-Temporal Graph Modeling," arXiv [cs.LG], 31-May-2019.
- [85] Y. Zhang, T. Cheng, and Y. Ren, "A graph deep learning method for short□ term traffic forecasting on large road networks," Computer-Aided Civil and Infrastructure Engineering, 2019.
- [86] F. L. Opolka, A. Solomon, C. Cangea, P. Veličković, P. Liò, and R. Devon Hjelm, "Spatio-Temporal Deep Graph Infomax," arXiv [cs.LG], 12-Apr-2019.
- [87] C. Chen et al., "Gated Residual Recurrent Graph Neural Networks for Traffic Prediction," in Proceedings of the AAAI Conference on Artificial Intelligence, 2019, vol. 33, pp. 485–492.
- [88] N. Zhang, X. Guan, J. Cao, X. Wang, and H. Wu, "A Hybrid Traffic Speed Forecasting Approach Integrating Wavelet Transform and Motif-based Graph Convolutional Recurrent Neural Network," arXiv [cs.CV], 14-Apr-2019.
- [89] X. Cheng, R. Zhang, J. Zhou, and W. Xu, "DeepTransport: Learning Spatial-Temporal Dependency for Traffic Condition Forecasting," in 2018 International Joint Conference on Neural Networks (IJCNN), 2018, pp. 1–8.
- [90] J. Sun, J. Zhang, Q. Li, X. Yi, and Y. Zheng, "Predicting Citywide Crowd Flows in Irregular Regions Using Multi-

- View Graph Convolutional Networks," arXiv [cs. CV], 19-Mar-2019.
- [91] B. Wang, X. Luo, F. Zhang, B. Yuan, A. L. Bertozzi, and P. Jeffrey Brantingham, "Graph-Based Deep Modeling and Real Time Forecasting of Sparse Spatio-Temporal Data," arXiv [cs.LG], 02-Apr-2018.
- [92] B. Yu, H. Yin, and Z. Zhu, "Spatio-Temporal Graph Convolutional Networks: A Deep Learning Framework for Traffic Forecasting," arXiv [cs.LG], 14-Sep-2017.
- [93] B. Yu, H. Yin, and Z. Zhu, "ST-UNet: A Spatio-Temporal U-Network for Graph-structured Time Series Modeling," arXiv [cs.LG], 13-Mar-2019.
- [94] L. Zhao et al., "T-GCN: A Temporal Graph ConvolutionalNetwork for Traffic Prediction," arXiv [cs.LG], 12-Nov-2018.
- [95] H. Yao, X. Tang, H. Wei, G. Zheng, and Z. Li, "Revisiting spatial-temporal similarity: A deep learning framework for traffic prediction," in AAAI Conference on Artificial Intelligence, 2019.
- [96] J. Atwood and D. Towsley, "Diffusion-convolutional neural networks," in Advances in Neural Information Processing Systems, 2016, pp. 1993–2001.
- [97] X. Zhou, Y. Shen, and L. Huang, "Revisiting Flow Information for Traffic Prediction," arXiv [eess.SP], 03-Jun-2019.
- [98] Y. Li and C. Shahabi, "A Brief Overview of Machine Learning Methods for Short-term Traffic Forecasting and Future Directions," SIGSPATIAL Special, vol. 10, no. 1, pp. 3–9, Jun. 2018.