GNNs for Combinatorial Optimization and Traffic

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Graph Neural Networks and Applications

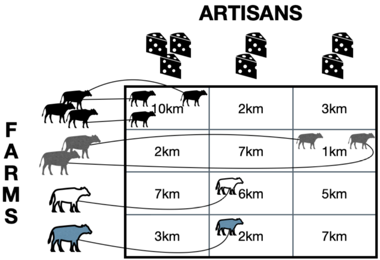
Topics

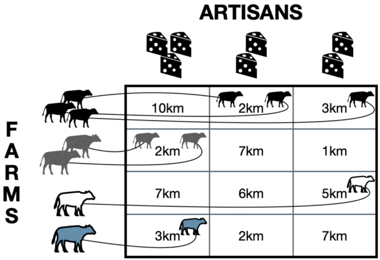
1. Combinatorial Optimization
2. Traffic Networks and ETA problem
3. Benchmarking & beyond

Combinatorial Optimization

Optimal transport

- How to optimize cost of production while maximizing profit?
- Monge-Kantorovich problems

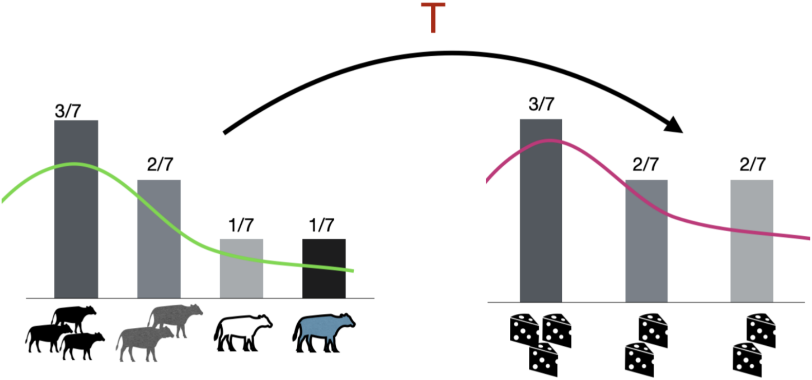




from `https://towardsdatascience.com/optimal-transport-a-hidden-gem-that-empowers-todays-machine-learning-2609bbf67e59`, 2020

Optimal transport

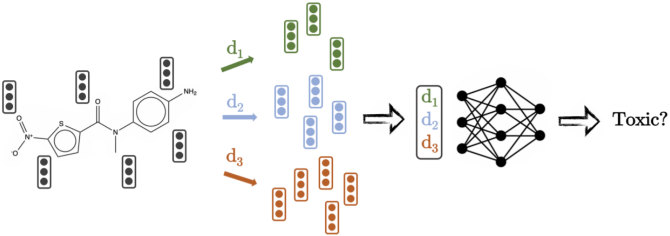
- Wasserstein distance for matching distributions
- Alternative pure generative models providing strong theoretical baselines for convergence and mapping properties



from `https://towardsdatascience.com/`

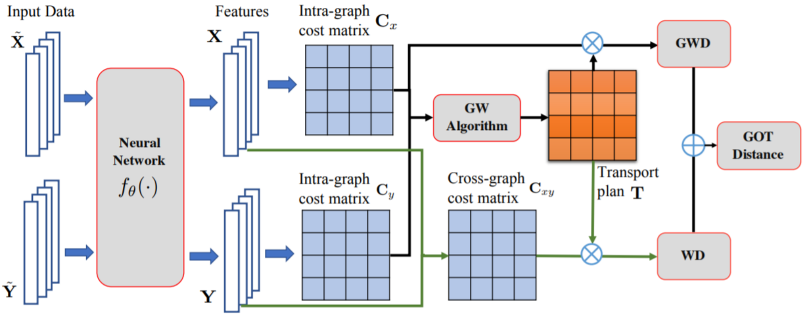
Optimal Transport Graph Neural Networks

- OT-GNN prototype model computes Wasserstein distances
- GNN node embeddings (left) vs. prototype embeddings (right)
- Molecular representation based on distances for supervised property prediction.



from Jaakkola et al., 2020

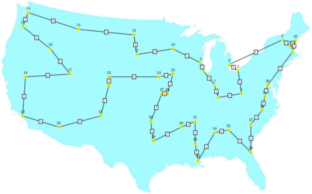
- Computation graph of the Graph Optimal Transport (GOT) distance used for cross-domain alignment.
- WD is short for Wasserstein Distance, and GWD is short for Gromov-Wasserstein Distance.

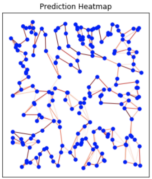


from Liu et al., 2020

Combinatorial Optimization and Reasoning with Graph Neural Networks

- Travelling Salesperson Problem (TSP)
- GNNs have been used to search for approximate solutions
- Probabilities are assigned to each node for belonging to the solution set, either independent of one-another (Non-autoregressive) or conditionally through graph traversal (Autoregressive).
- The predicted probabilities are converted into discrete decisions through classical graph search such as greedy or beam search.

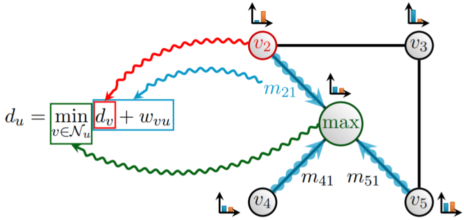




from Veliˇckovi´c et al., 2021; Joshi et al., 2020

Combinatorial Optimization and Reasoning with Graph Neural Networks

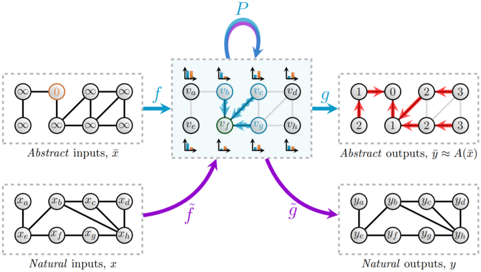
- Bellman-Ford shortest pathfinding algorithm.
- Node features align with intermediate computed values (red)
- Message functions align with the candidate solutions from each neighbor (blue)
- Aggregation function (max) aligns with the optimization across neighbours (green) for path-finding



from Veli ˇ ckovi ´c et al., 2021

Combinatorial Optimization and Reasoning with Graph Neural Networks

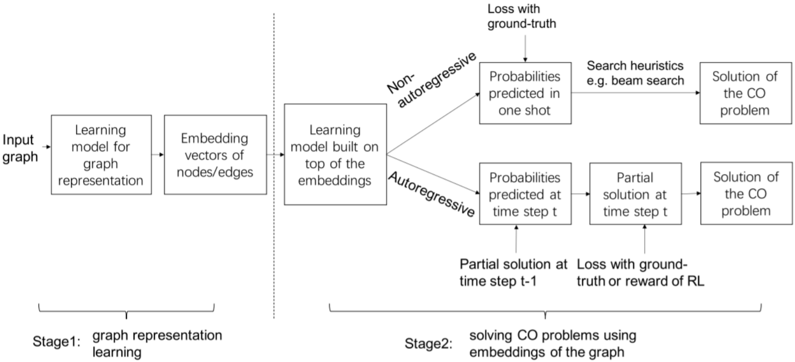
- Algorithmic reasoner is trained in the encode-process-decode fashion, learning P under $g(P(f(x))) \approx A(x)$, for a target algorithm A (BFS)
- Once trained, the processor network P is frozen and stitched into a pipeline over natural inputs with new encoder and decoder f and g.
- End-to-end differentiable function that has no explicit information loss, while retaining alignment with BFS.



from Veliˇckovi´c et al., 2021

Graph Learning for Combinatorial Optimization: A Survey of State-of-the-Art

- Taxonomy of optimization methods using GNNs



from Xu et al., 2020

Graph Learning for Combinatorial Optimization: A Survey of State-of-the-Art

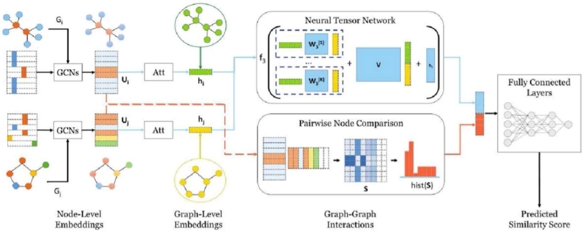
- List of models and optimization problems

Method	CO problem	Model
ConvNet [34]	TSP	GNN, non-autoregressive
DTSPGNN [57]	TSP	GNN, non-autoregressive
CPNGNN [59]	MDS, MM, MVC	GNN, non-autoregressive
GAP [49]	Graph partition	GNN, non-autoregressive
GMN [41]	GED	GNN, non-autoregressive
SimGNN [2]	GED	GNN, non-autoregressive
GRAPHSIM [3]	GED	GNN, non-autoregressive
GNNGC [40]	GColor	GNN, non-autogressive
SiameseGNN [51]	Graph matching, TSP	GNN, non-autogressive
PCAGM [69]	Graph matching	GNN, non-autogressive
IsoNN [44]	Graph Iso.	AutoEncoder, non-autogressive
GNNTS [42]	MIS, MVC, MC	GNN, non-autoregressive
Ptr-Net [67]	TSP	AutoEncoder, autoregressive
LSTMGMatching [46]	Graph matching	AutoEncoder, autogressive
S2V-DQN [14]	MVC, MaxCut, TSP	GNN, autoregressive
CombOptZero [1]	MVC, MaxCut, MC	GNN, autoregressive
RLMCS [4]	MCS	GNN, autoregressive
CENALP [19]	Graph alignment	SkipGram, autoregressive
TSPImprove [71]	TSP	AutoEncoder, autoregressive
AM [37]	TSP	AutoEncoder, autoregressive

from Xu et al., 2020

Graph Learning for Combinatorial Optimization: A Survey of State-of-the-Art

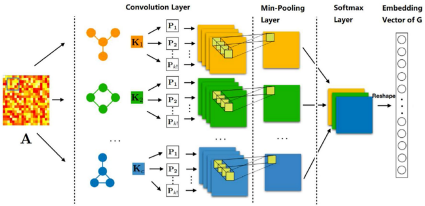
- SimGNN model for graph comparison
- The blue solid line illustrates the first strategy of comparing graphs using their global summaries
- The orange dashed line indicates the second strategy of the pair-wise node comparison



from Xu et al., 2020; Wang et al., 2019

Graph Learning for Combinatorial Optimization: A Survey of State-of-the-Art

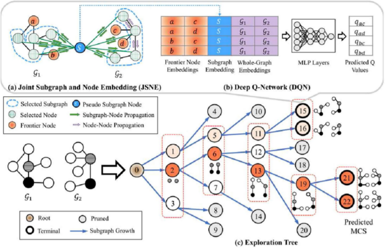
- Given a set of motifs, the convolution layer of IsoNN encoder extracts a set of isomorphism features from G for each motif
- IsoNN examines $k!$ permutations for motifs, smallest one is regarded as the optimal isomorphism feature from MinPooling
- Softmax layer is used to normalize them different features.
- Normalized features are concatenated as the embedding of G
- Decoder is an MLP to predict the binary class of graph



from Xu et al., 2020; Zhang et al., 2019

Graph Learning for Combinatorial Optimization: A Survey of State-of-the-Art

- RLMCS model for optimizing MVC (minimum vertex cover) problem
- Each step, RL agent transits to at most k best next states
- Beam search builds an exploration tree, where each node of the tree is a state and each edge of the tree is an action.
- The partial solution is returned as a maximal independent set
- The largest among the computed candidate sets is outputted

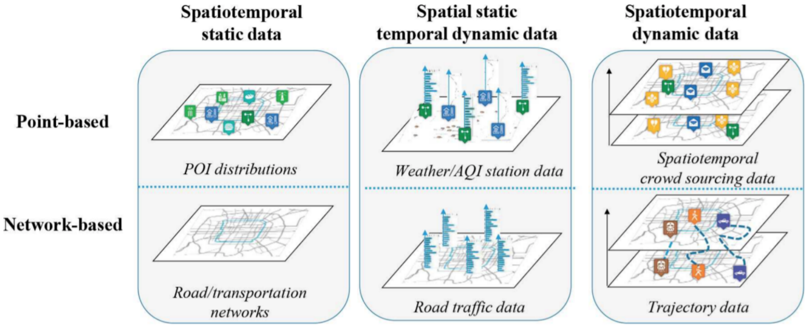


from Xu et al., 2020; Wang et al., 2020

Traffic Network & GNNs

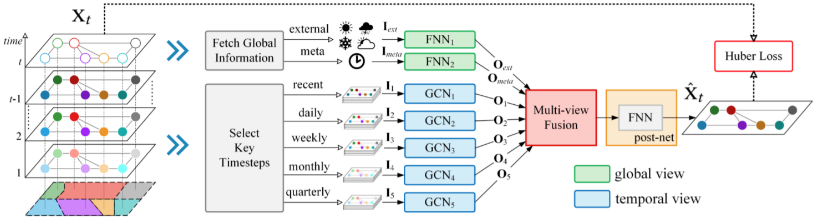
Graph Neural Networks for Traffic Forecasting

- Different traffic data representations



from Oliveira et al., 2021; Zheng, Y., 2019

- MVGCN uses late fusion for different time scales dependencies



from Oliveira et al., 2021; Zheng, Y., 2020

Graph Neural Networks for Traffic Forecasting

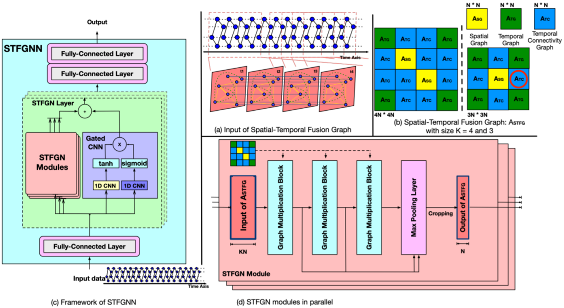
- Ur: urban, Fw: freeway
- S: speed, F: flow, V: volume
- L: loop counters, FCD: floating car data

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

from Oliveira et al., 2021

Spatial-Temporal Fusion Graph Neural Networks for Traffic Flow Forecasting

- STFGNN processes (a) input of Spatial-Temporal Fusion Graph (b).
- Graphs: Spatial ASG, temporal ATG, temporal connectivity ATC.
- STFGNN (c) as Gated CNN module and STFGNN modules in parallel.
- Spatial-Temporal Fusion Graph Modules (d) are independently trained for input iteratively generated from (a) in parallel as well.

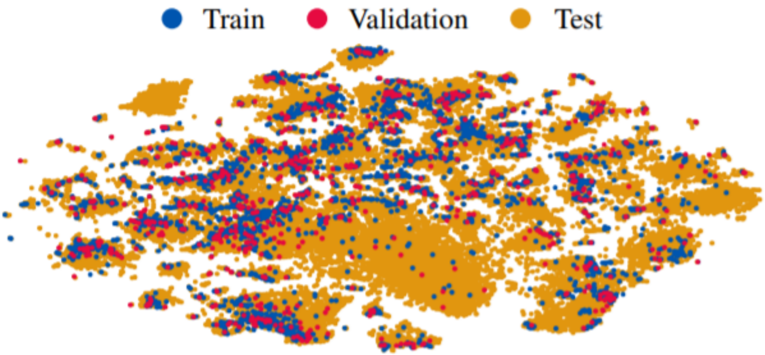


from Zhu et al., 2021; Xu et al., 2020

GNN benchmarking

Open Graph Benchmark: Datasets for Machine Learning on Graphs

- OPEN GRAPH BENCHMARK (OGB)
- Large scale graph machine learning
- Automated end-to-end graph ML pipeline



from Leskovec et al., 2020; `https://ogb.stanford.edu`

Other Benchmarks

- Dgl-lifesci: An open-source toolkit for deep learning on graphs in life science
- Biological structure and function emerge from scaling unsupervised learning to 250 million protein sequences
- Open Catalyst 2020 (OC20) Dataset and Community Challenges
- Train on Small, Play the Large: Scaling Up Board Games with AlphaZero and GNN
- Discovering Symbolic Models from Deep Learning with Inductive Biases
- Learning to simulate complex physics with graph networks

from Karypis et al., 2021; `https://github.com/awslabs/dgl-lifesci`

from Fergus et al., 2021; `https://github.com/facebookresearch/esm`

from Palizhati et al., 2021; `https://opencatalystproject.org/`

from El-Yaniv et al., 2021; Ho et al., 2020; Battaglia t al., 2020

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