Daniel Darabos

lynxanalytics

Intro to Graph Neural Networks

What neural networks eat


photo
network


photo
network
colorized

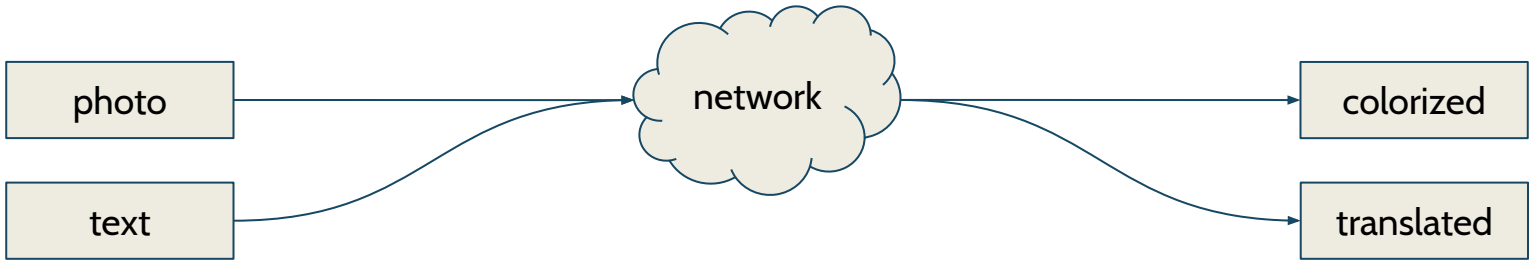


photo
text
network
colorized
translated

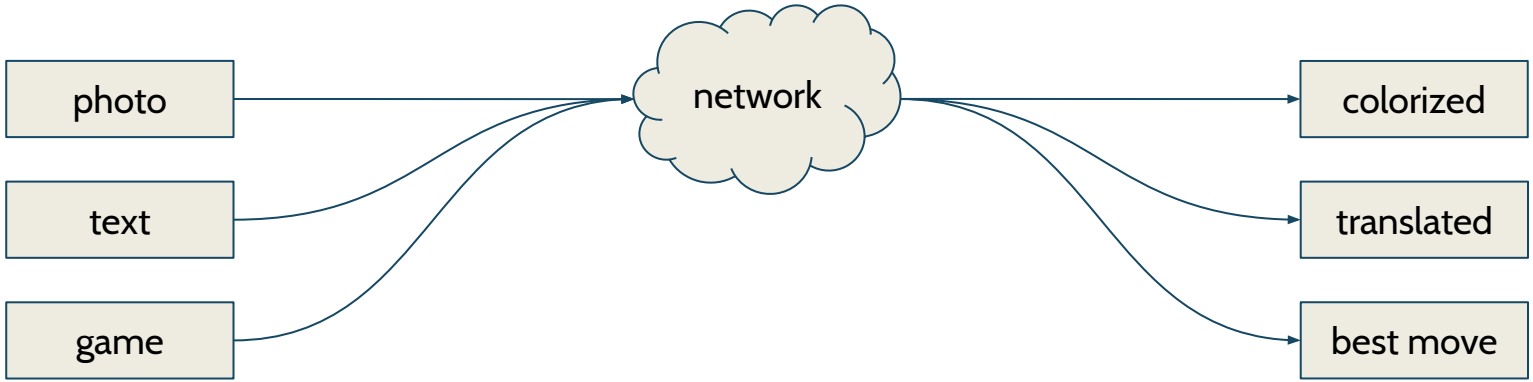


photo
text
game
network
colorized
translated
best move

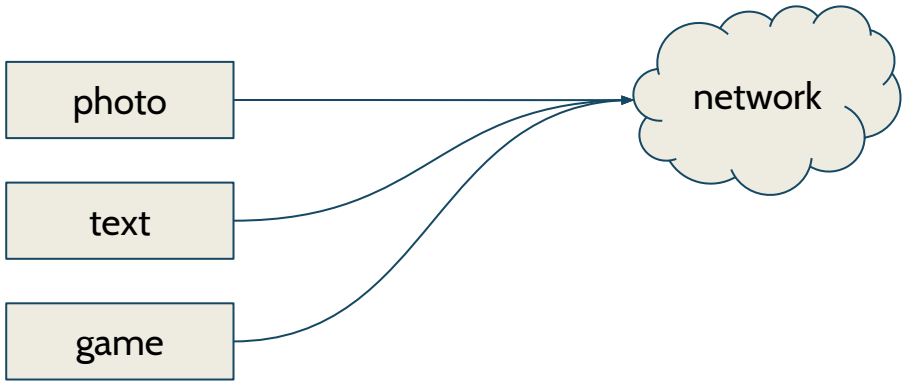


photo
text
game
network

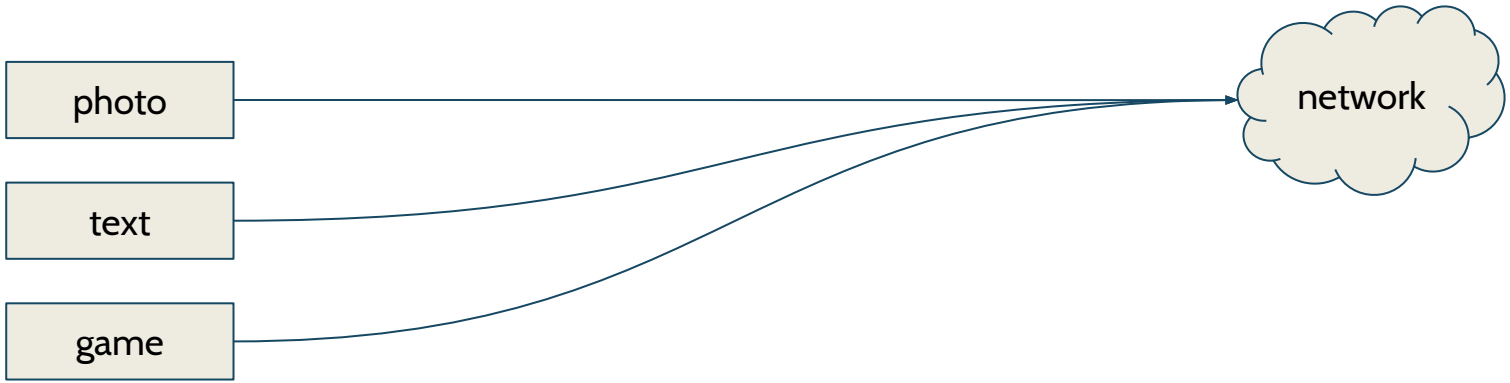
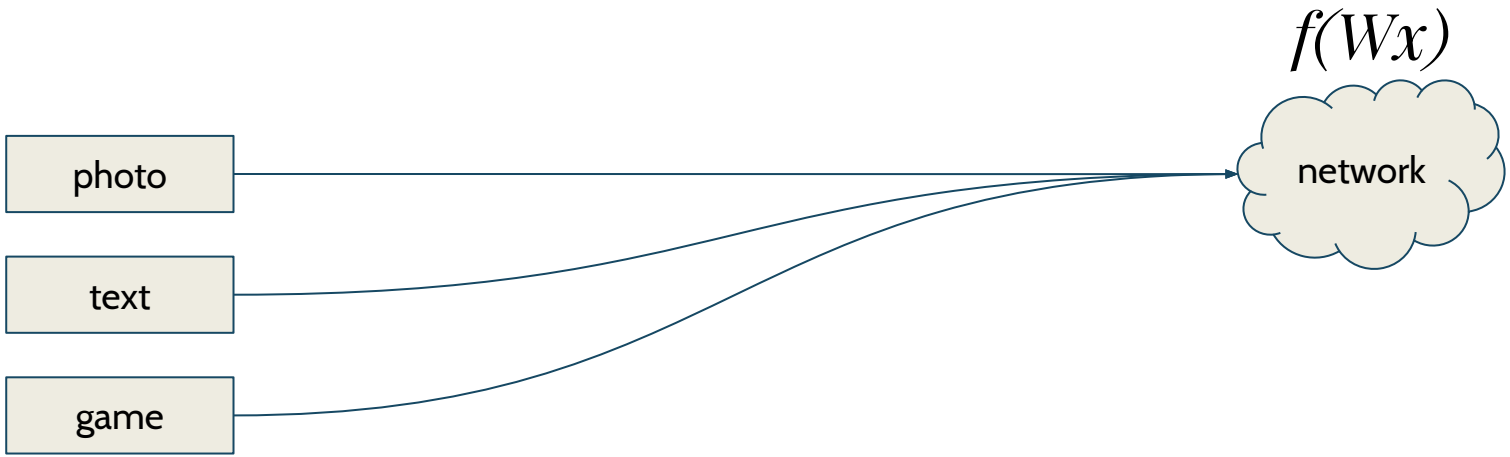
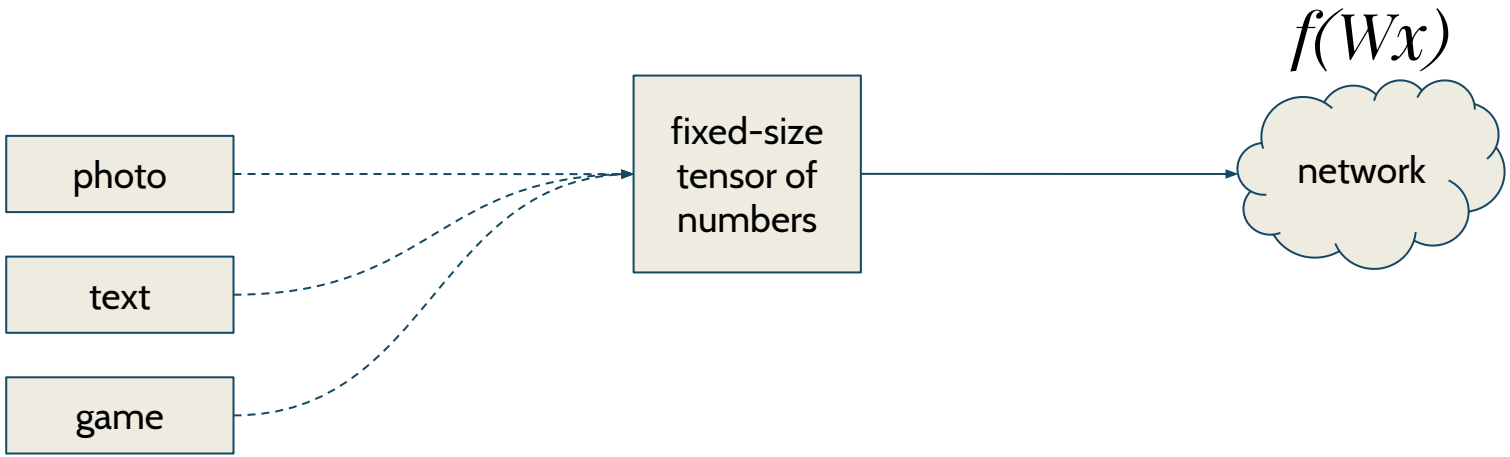
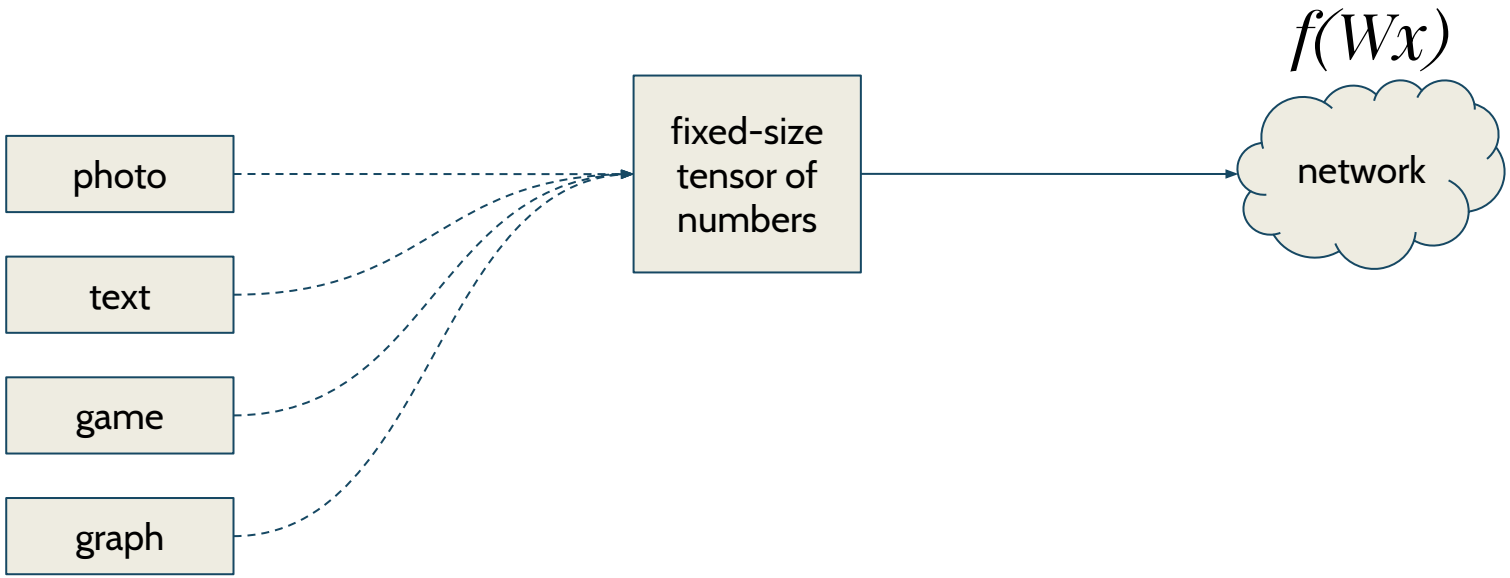
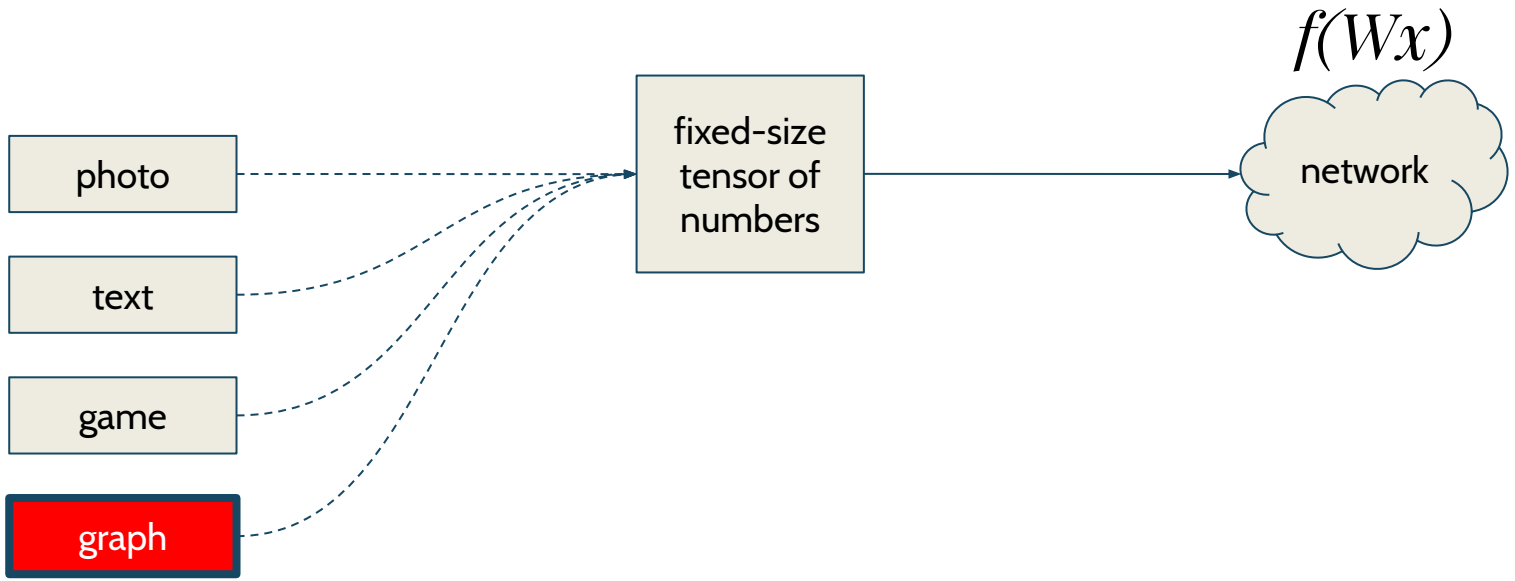


photo
text
game
network

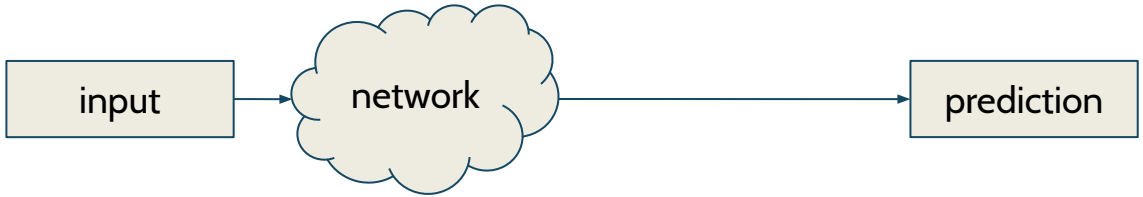

f(Wx)
photo
text
game
network

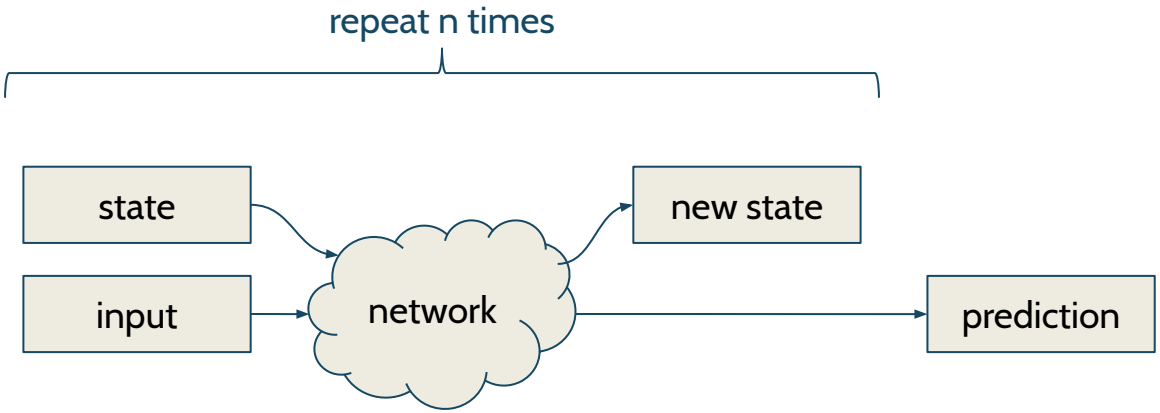

f(Wx)
photo
text
game
fixed-size tensor of numbers
network

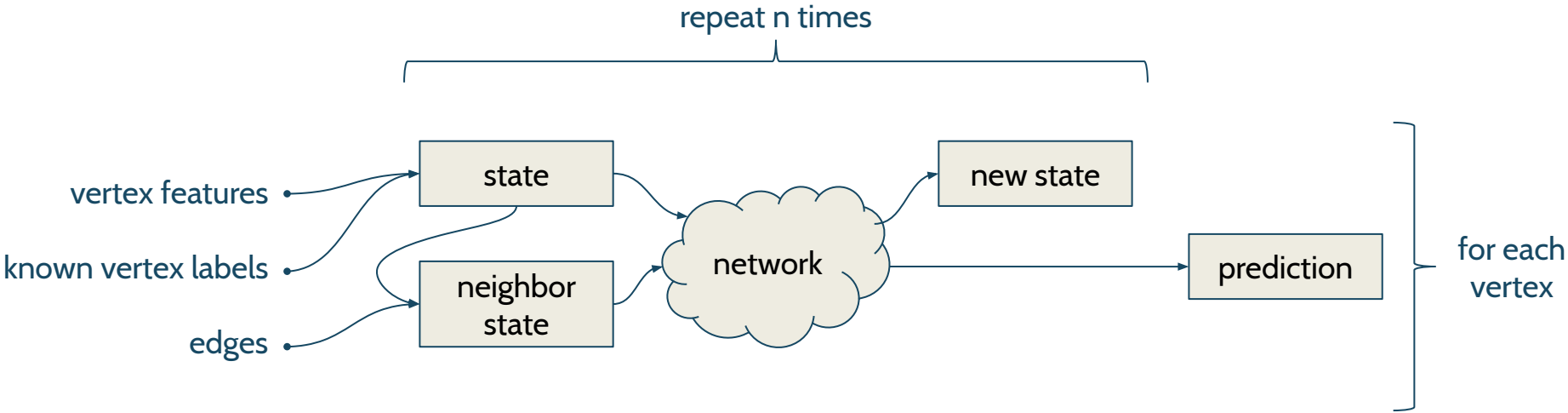

f(Wx)
photo
text
game
graph
fixed-size tensor of numbers
network

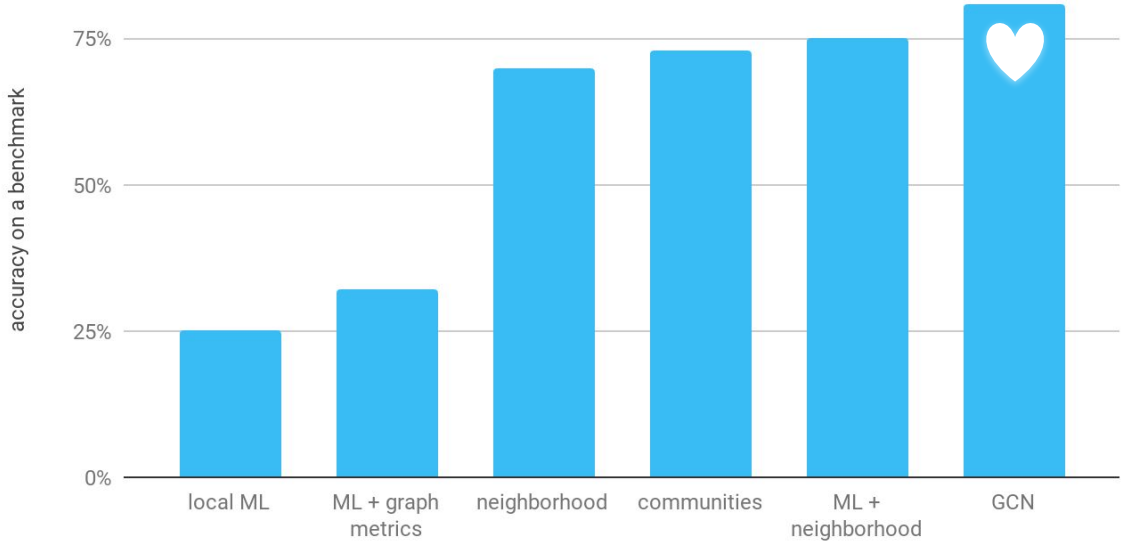

f(Wx)
photo
text
game
graph
fixed-size tensor of numbers
network

How to eat a graph


input
network
prediction


repeat n times
state
input
network
new state
prediction


repeat n times
vertex features
known vertex labels
edges
state
neighbor state
network
new state
prediction
for each vertex



“Neural Network That Learns From a Huge Graph”

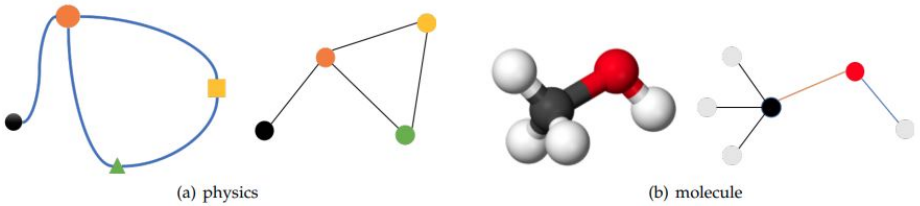
Spark Summit East 2017

Applications

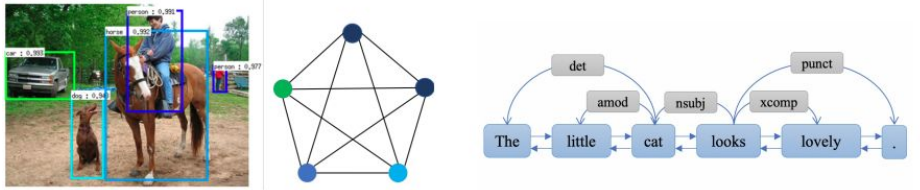
- Predict node attribute
- Predict edge attribute
- Predict edge
- Predict graph property
- Embed nodes
- Embed graph
- Generate similar graph

https://arxiv.org/abs/1812.08434

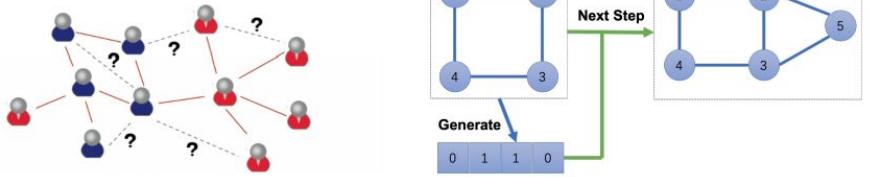
Zhou et al: Graph Neural Networks:
A Review of Methods and Applications
(Figure 4 below, Table 3 to the right)



(a) physics (b) molecule



(c) image (d) text



(e) social network (f) generation

Applications of graph neural networks.

Area	Application	Algorithm	Deep Learning Model	References
Text	Text classification	GCN	Graph Convolutional Network	[1], [23], [48] [2], [22], [46]
		GAT	Graph Attention Network	[68]
		DGCNN	Graph Convolutional Network	[106]
		Text GCN	Graph Convolutional Network	[107]
		Sentence LSTM	Graph LSTM	[62]
	Sequence Labeling (POS, NER)	Sentence LSTM	Graph LSTM	[62]
	Sentiment classification	Tree LSTM	Graph LSTM	[60]
	Semantic role labeling	Syntactic GCN	Graph Convolutional Network	[108]
	Neural machine translation	Syntactic GCN	Graph Convolutional Network	[109], [110]
		GGNN	Gated Graph Neural Network	[38]
	Relation extraction	Tree LSTM	Graph LSTM	[111]
		Graph LSTM	Graph LSTM	[44], [112]
		GCN	Graph Convolutional Network	[113]
	Event extraction	Syntactic GCN	Graph Convolutional Network	[114], [115]
	AMR to text generation	Sentence LSTM	Graph LSTM	[116]
		GGNN	Gated Graph Neural Network	[38]
	Multi-hop reading comprehension	Sentence LSTM	Graph LSTM	[117]
	Relational reasoning	RN	MLP	[96]
		Recurrent RN	Recurrent Neural Network	[118]
		IN	Graph Neural Network	[4]
Image	Social Relationship Understanding	GRM	Gated Graph Neural Network	[119]
	Image classification	GCN	Graph Convolutional Network	[120], [121]
		GGNN	Gated Graph Neural Network	[122]
		DGP	Graph Convolutional Network	[35]
		GSNN	Gated Graph Neural Network	[123]
	Visual Question Answering	GGNN	Gated Graph Neural Network	[119], [124], [125]
	Object Detection	RN	Graph Attention Network	[126], [127]
	Interaction Detection	GPNN	Graph Neural Network	[128]
		Structural-RNN	Graph Neural Network	[42]
	Region Classification	GCNN	Graph CNN	[129]
	Semantic Segmentation	Graph LSTM	Graph LSTM	[63], [130]
		GGNN	Gated Graph Neural Network	[131]
		DGCNN	Graph CNN	[132]
		3DGNN	Graph Neural Network	[133]
Science	Physics Systems	IN	Graph Neural Network	[4]
		VIN	Graph Neural Network	[91]
		GN	Graph Networks	[3]
	Molecular Fingerprints	NGF	Graph Convolutional Network	[51]
		GCN	Graph Convolutional Network	[99]
	Protein Interface Prediction	GCN	Graph Convolutional Network	[5]
	Side Effects Prediction	Decagon	Graph Convolutional Network	[134]
	Disease Classification	PPIN	Graph Convolutional Network	[135]
Knowledge Graph	KB Completion	GNN	Graph Neural Network	[6]
	KG Alignment	GCN	Graph Convolutional Network	[136]
Combinatorial Optimization		structure2vec	Graph Convolutional Network	[7]
		GNN	Graph Neural Network	[137]
		GCN	Graph Convolutional Network	[138]
		AM	Graph Attention Network	[139]
Graph Generation		NetGAN	Long short-term memory	[140]
		GraphRNN	Rucurrent Neural Network	[137]
		Regularizing VAE	Variational Autoencoder	[141]
		GCPN	Graph Convolutional Network	[142]
		MolGAN	Relational-GCN	[143]

You can do it!

Libraries

- Graph Nets
- Deep Graph Library
- PyTorch Geometric

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Matthias Fey
rusty1s

Libraries

- Graph Nets
- Deep Graph Library
- PyTorch Geometric

Google DeepMind

4.4k★

aws

4.4k★

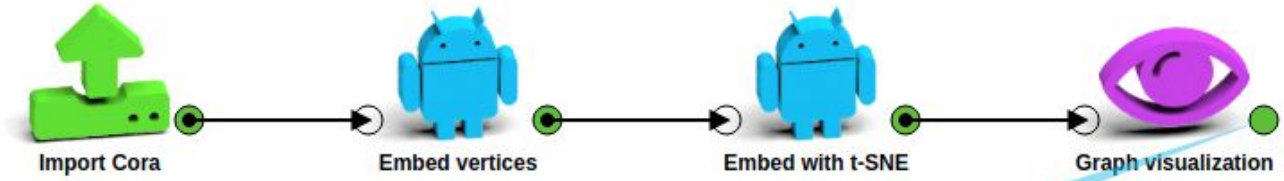
6.6k★

Matthias Fey
rusty1s

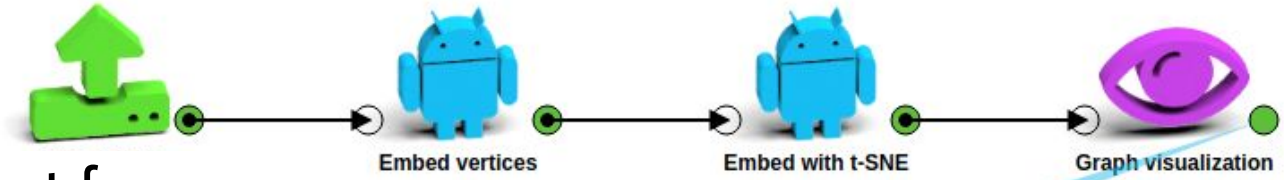
PyTorch Geometric in action

```
from torch_geometric.nn import Node2Vec
model = Node2Vec(
    num_nodes, embedding_dim, walk_length,
    context_size, walks_per_node)
optimizer = torch.optim.Adam(model.parameters())
for i in range(10):
    model.train()
    optimizer.zero_grad()
    loss = model.loss(edges)
    loss.backward()
    optimizer.step()
model.eval()
z = model(torch.arange(num_nodes)
```

LynxKite in action



LynxKite in action



Import from Neo4j

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Intro to Graph Neural Networks

https://arxiv.org/abs/1812.08434
https://github.com/rusty1s/pytorch_geometric
https://lynxkite.com/