Graph Neural Network Tutorial

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Content

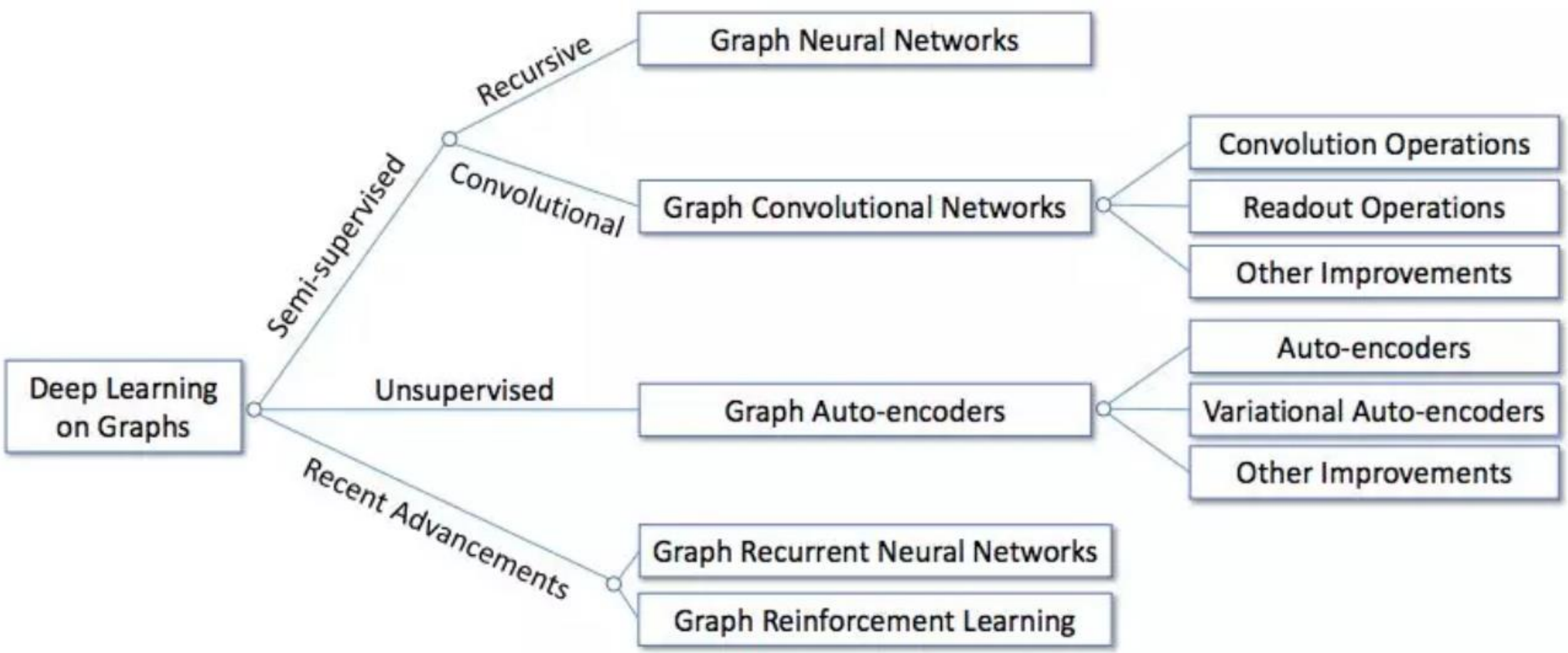
- 1. Survey：Graph Neural Network
- 2. GCN：图卷积神经网络
- 3. Application：工业界应用

Survey：Graph Neural Network

Background

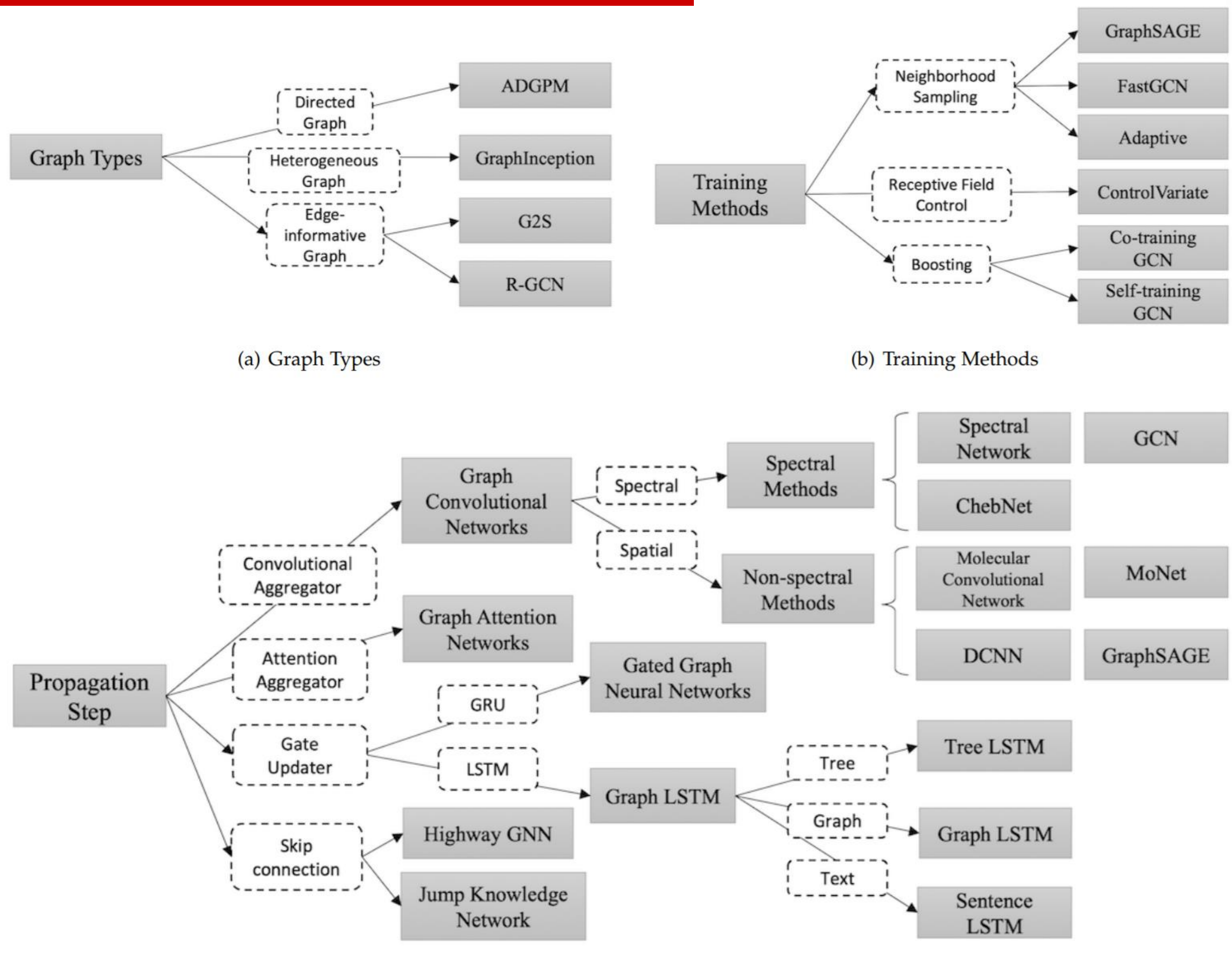
Event:	Graph Neural Network	CNN on Graph	Graph Networks
	Gori, 2005	LeCun, 2014	DeepMind, 2018
Framework:	Graph Nets	DGL	Euler
	DeepMind, 2018	NYU+AWS, 2018	Alibaba, 2019
Survey:	Deep learning on graphs: A survey	Graph Neural Networks: A Review of Methods and Applications	A Comprehensive Survey on Graph Neural Networks
	Zhu W, 2018	Sun M, 2018	Philip S. Yu, 2019

Survey 1: THU, 2018



Zhang Z, Cui P, Zhu W. Deep learning on graphs: A survey[J]. arXiv preprint arXiv:1812.04202, 2018.

Survey 2: THU, 2018



(c) Propagation Steps

Zhou J, Cui G, Zhang Z, et al. Graph Neural Networks: A Review of Methods and Applications[J]. arXiv preprint arXiv:1812.08434, 2018.

Survey 3: IEEE Fellow, 2019

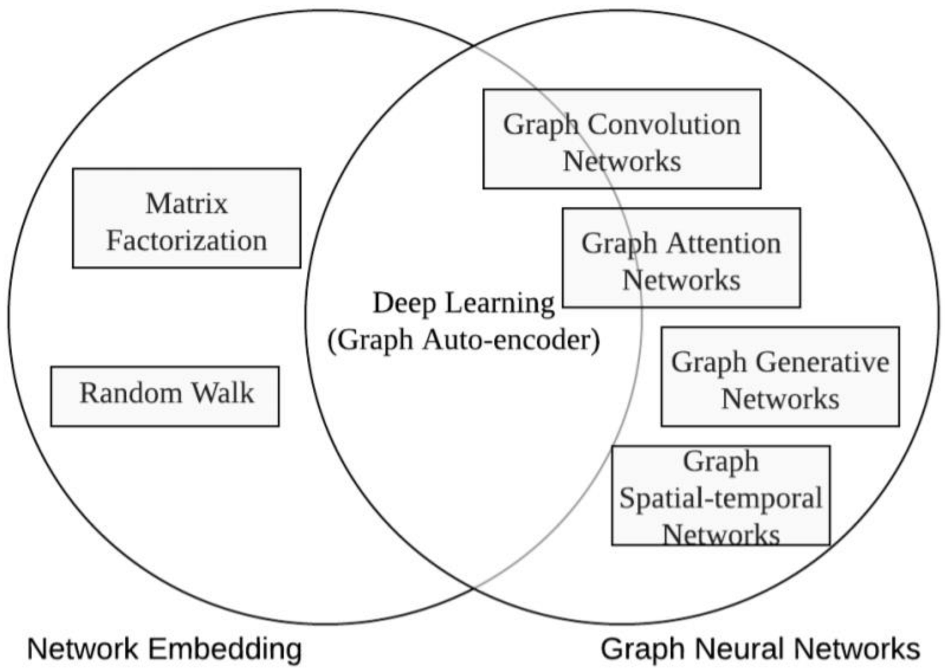
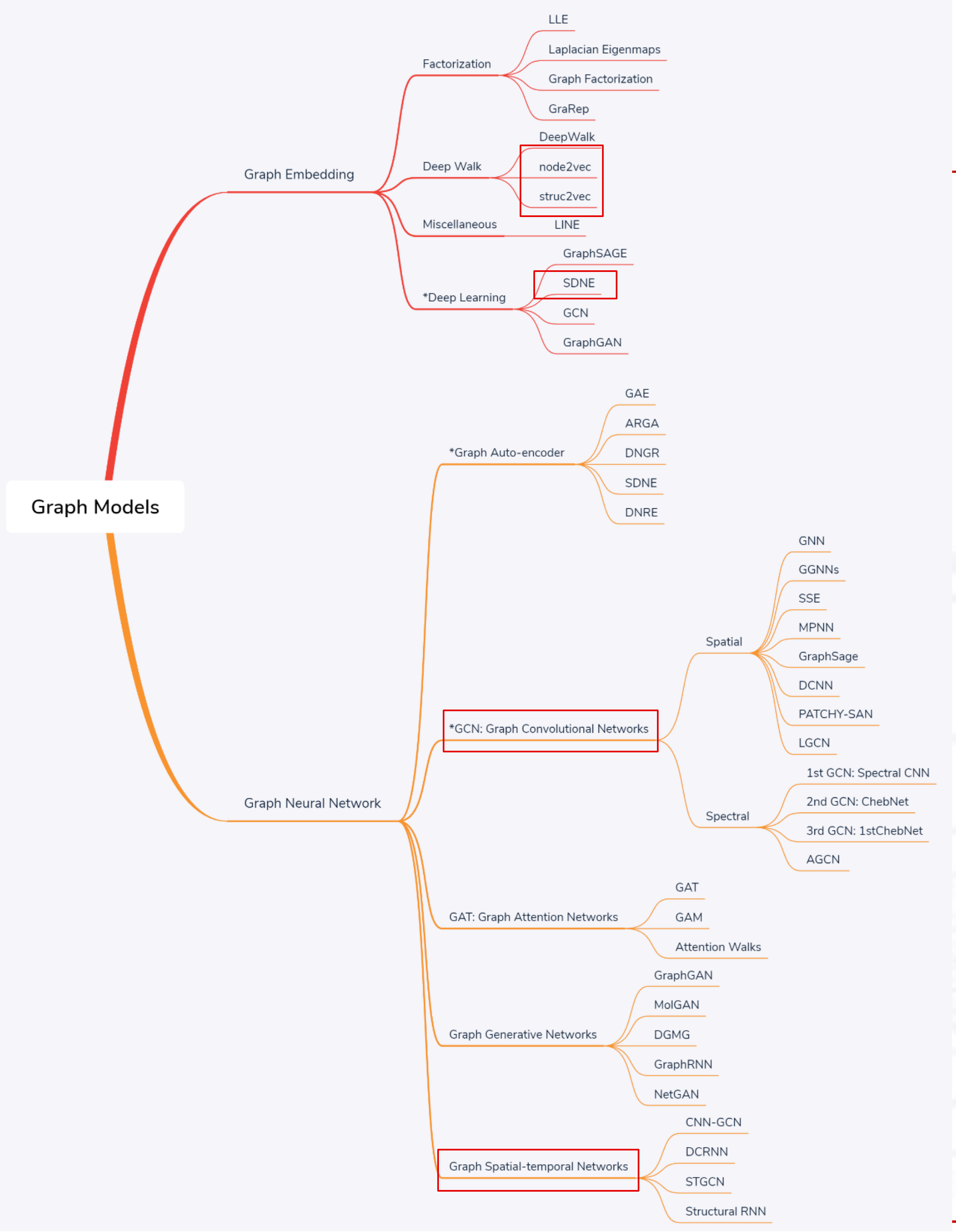


Fig. 2: Network Embedding v.s. Graph Neural Networks.

Wu Z, Pan S, Chen F, et al. A comprehensive survey on graph neural networks[J]. arXiv preprint arXiv:1901.00596, 2019.

XMind:


Graph Models
Graph Embedding
Factorization
LLE
Laplacian Eigenmaps
Graph Factorization
GraRep
Deep Walk
DeepWalk
node2vec
struc2vec
Miscellaneous
LINE
*Deep Learning
GraphSAGE
SDNE
GCN
GraphGAN
Graph Neural Network
*Graph Auto-encoder
GAE
ARGA
DNGR
SDNE
DNRE
*GCN: Graph Convolutional Networks
Spatial
GNN
GGNNs
SSE
MPNN
GraphSage
DCNN
PATCHY-SAN
LGCN
Spectral
1st GCN: Spectral CNN
2nd GCN: ChebNet
3rd GCN: 1stChebNet
AGCN
GAT: Graph Attention Networks
GAT
GAM
Attention Walks
Graph Generative Networks
GraphGAN
MolGAN
DGMG
GraphRNN
NetGAN
Graph Spatial-temporal Networks
CNN-GCN
DCRNN
STGCN
Structural RNN

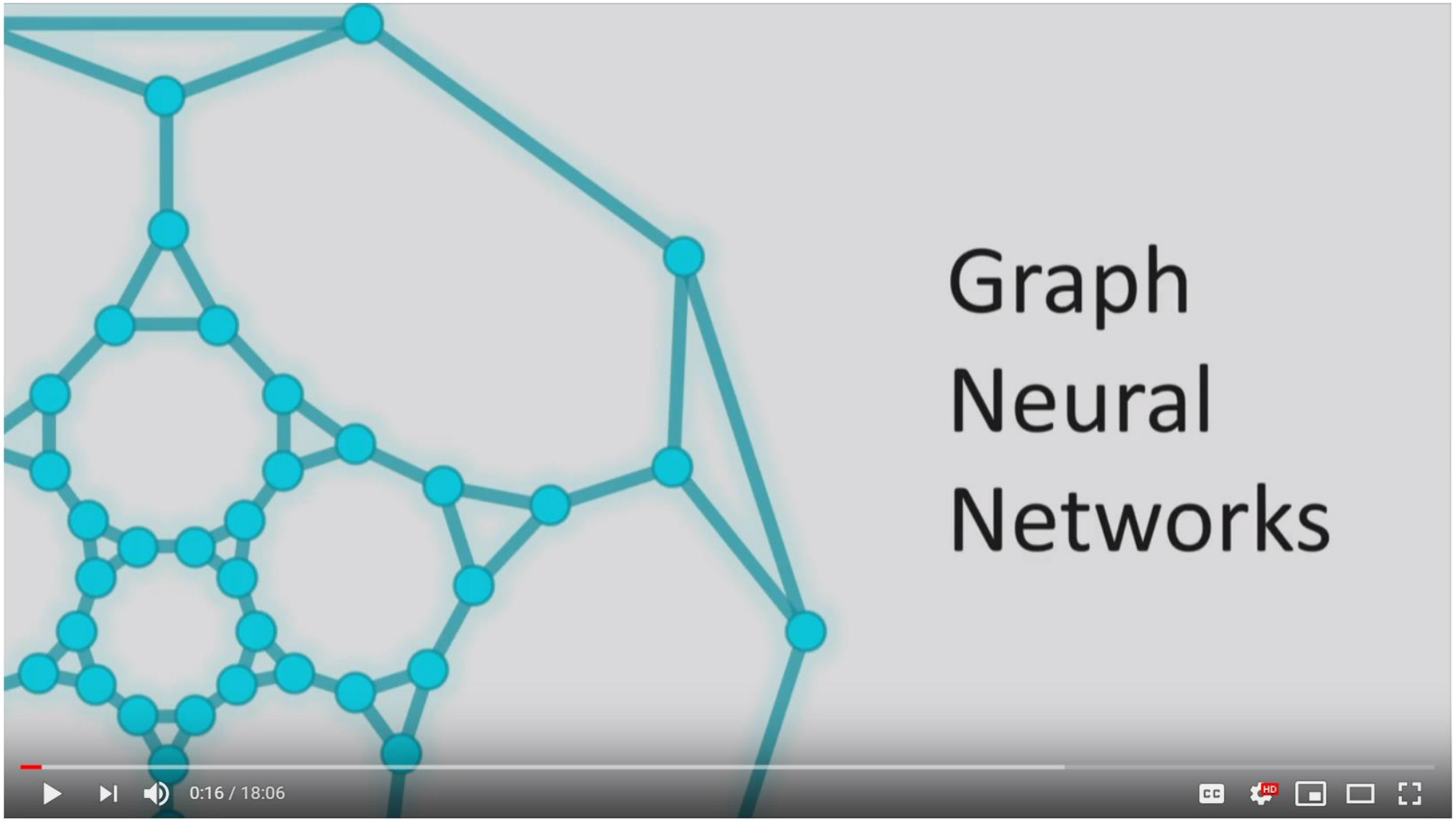
Applications

Tasks & Practical Applications

- Node classification
- Graph classification
- Network embedding
- Graph generation
- **Spatial-temporal sequence forecasting**
- **Point clouds classification and segmentation**
- **Action recognition**
- **Recommender Systems**
- **Chemistry&Biology&Medicine**

GCN：图卷积神经网络

Introduction



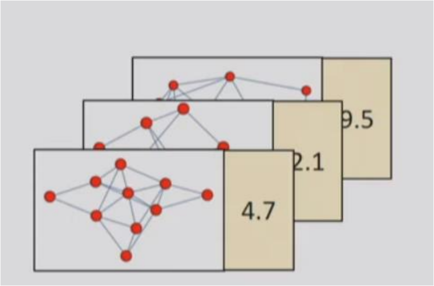
Graph neural networks: Variations and applications

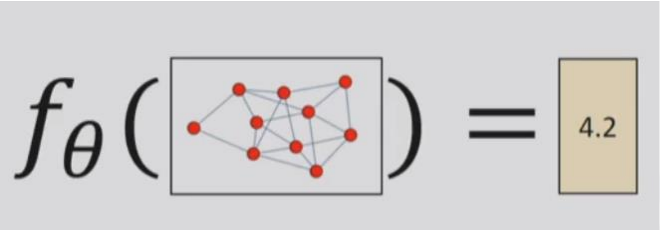
21,160 views

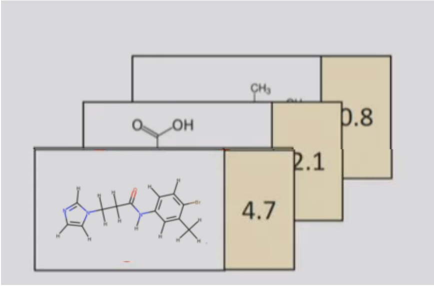
465 7 SHARE SAVE

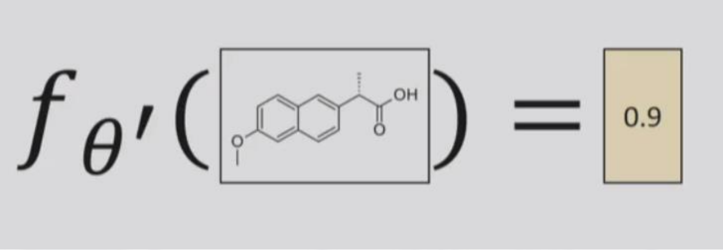
Introduction

- **Goal: Handle Graph Structured Data**

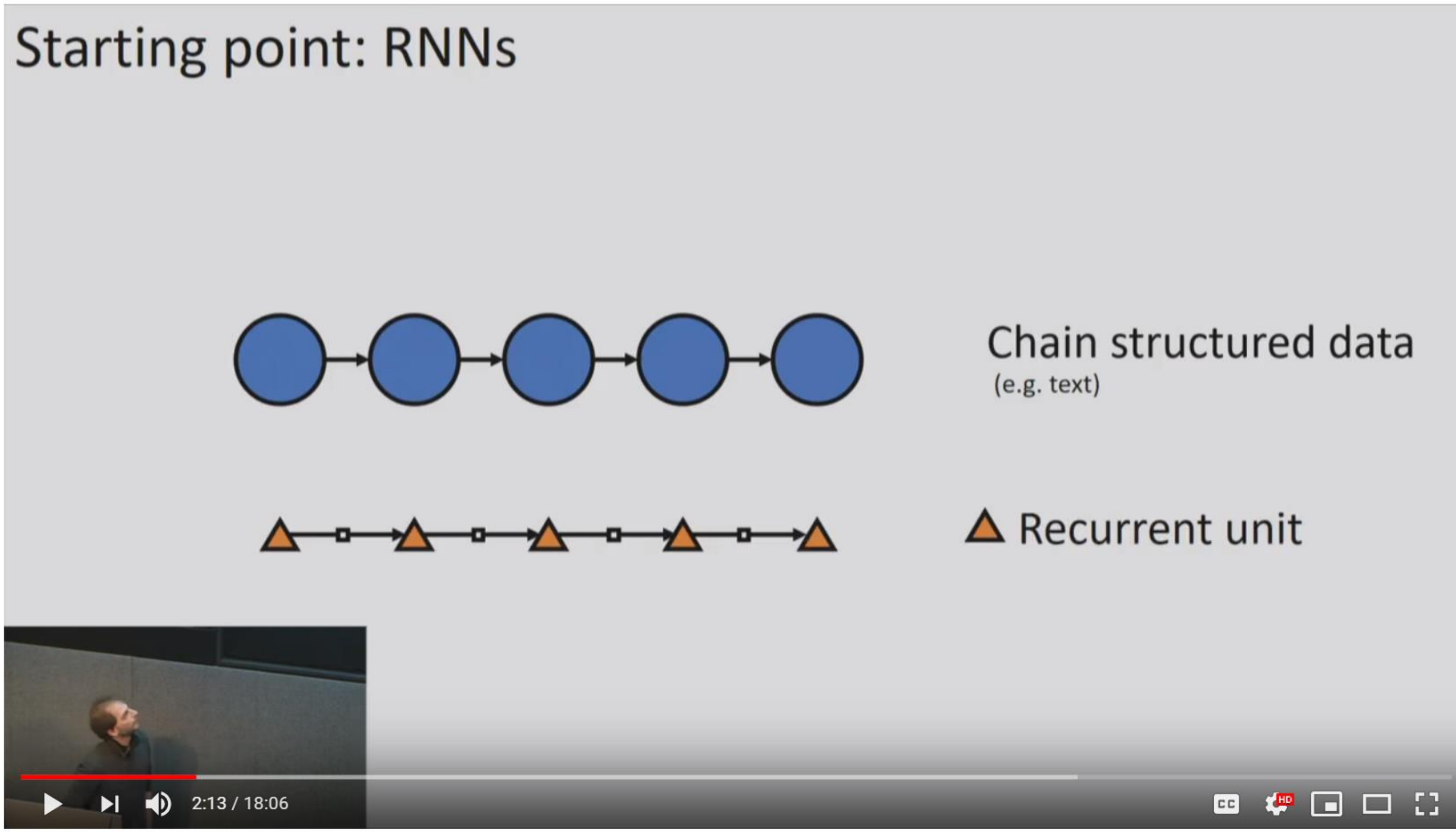




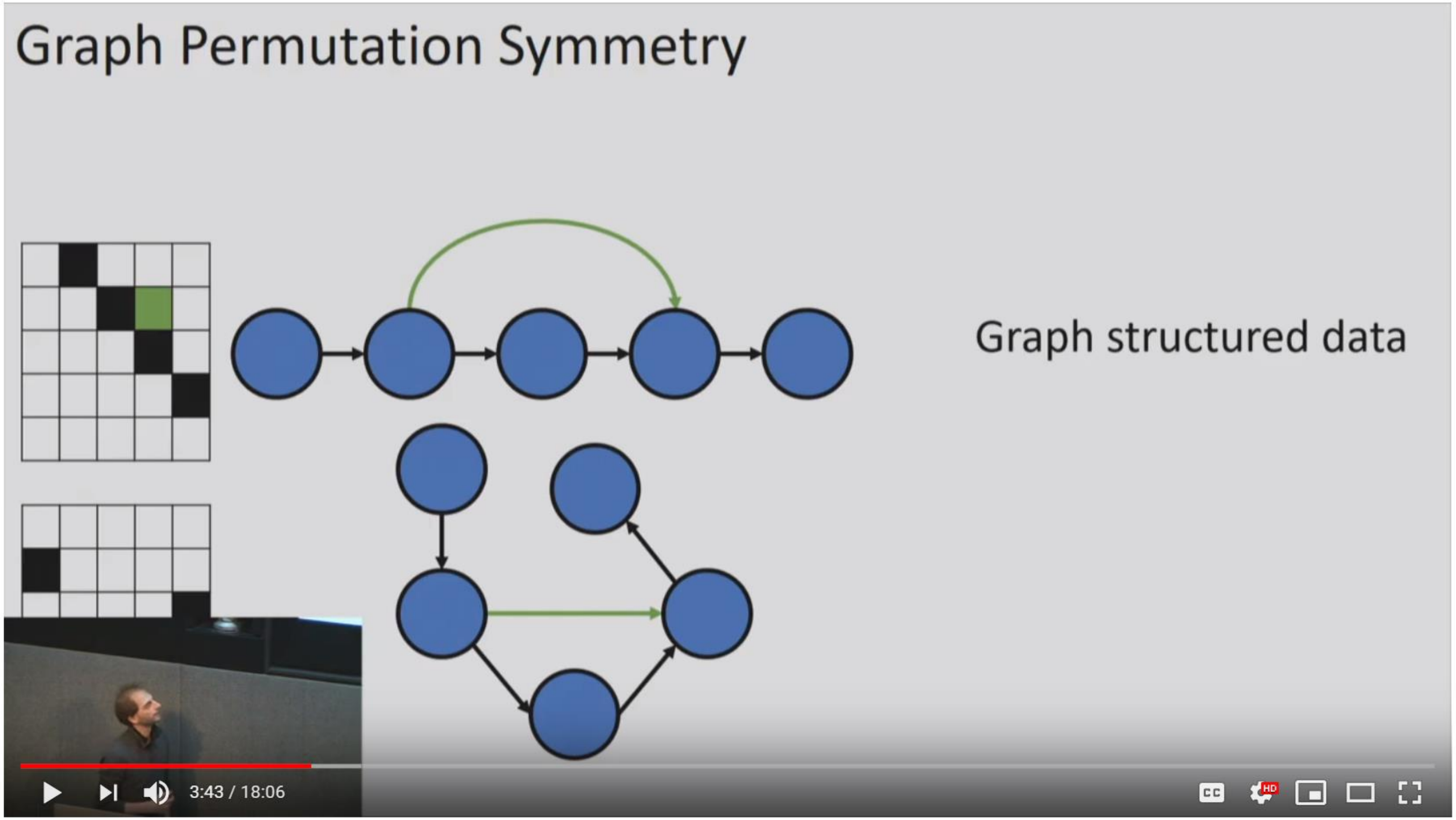




Introduction



Introduction



Graph neural networks: Variations and applications

21,160 views

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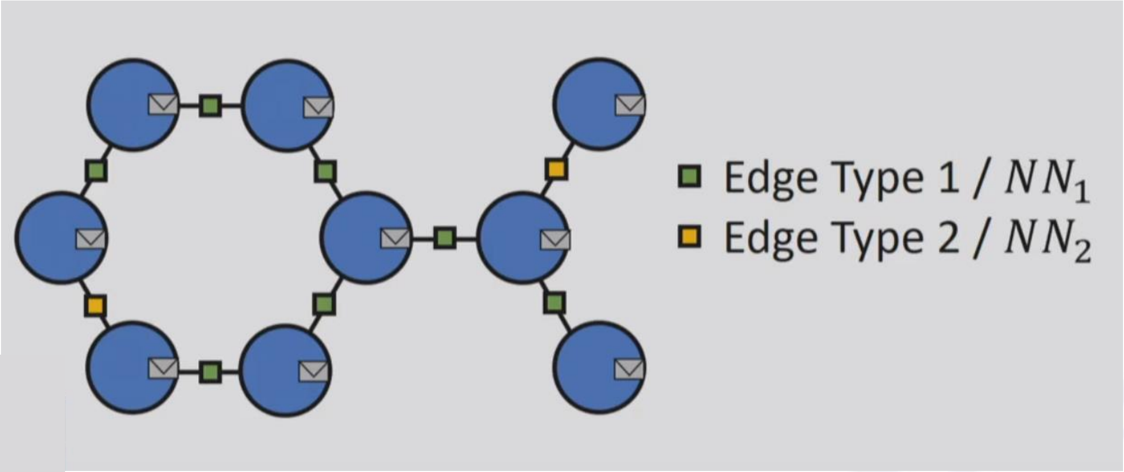
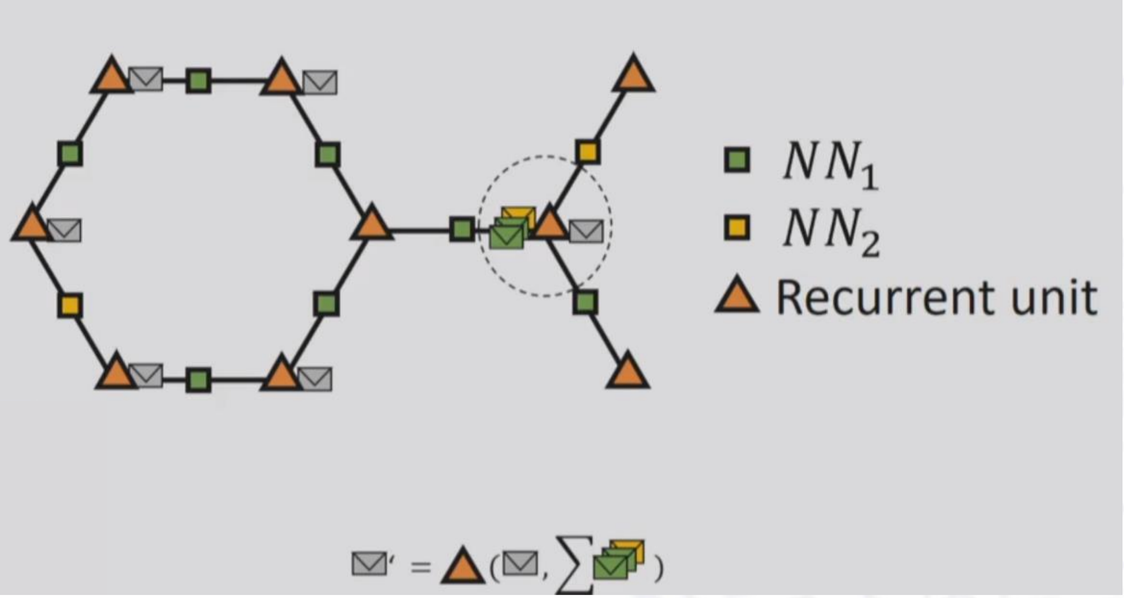
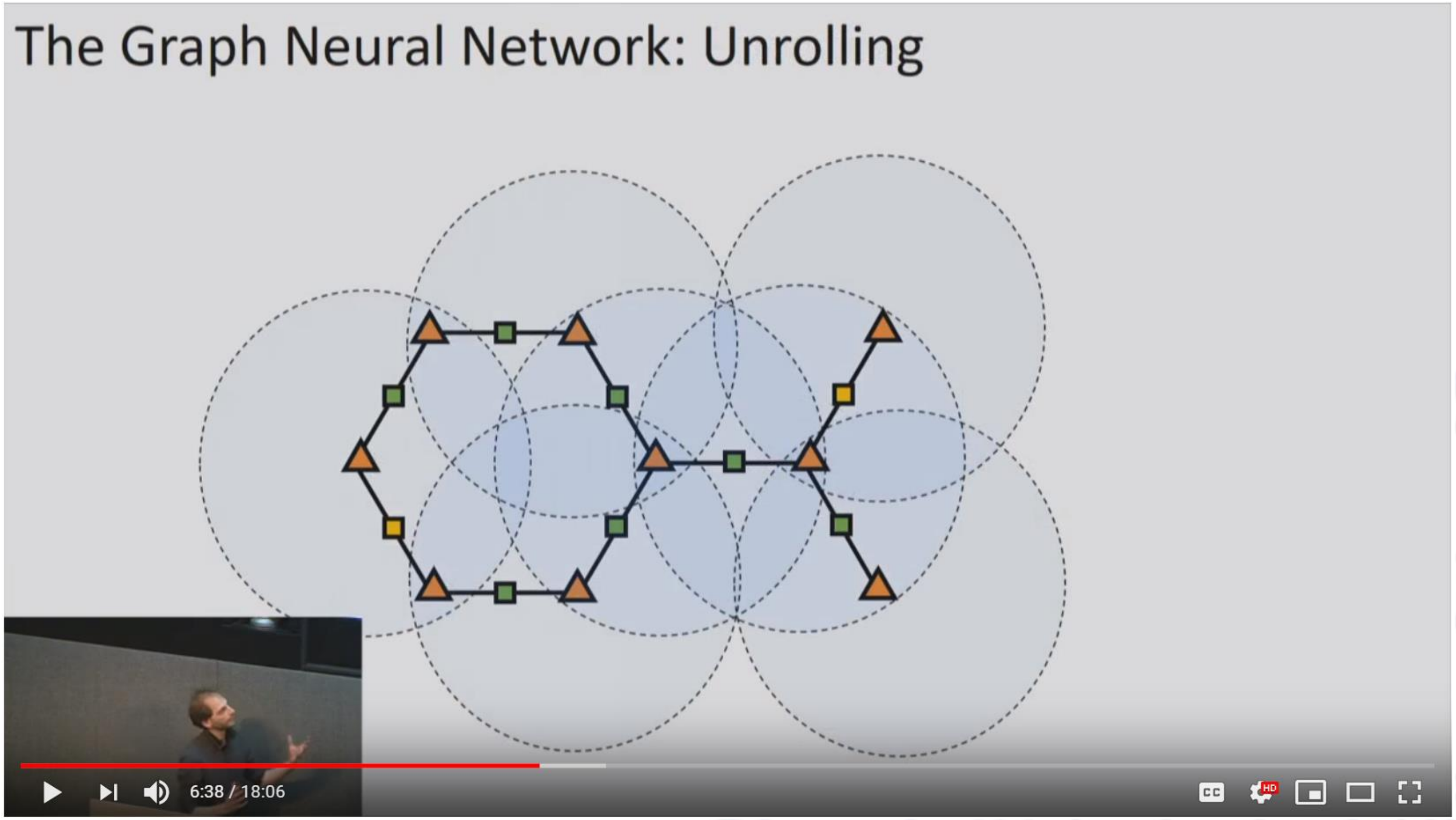
Introduction

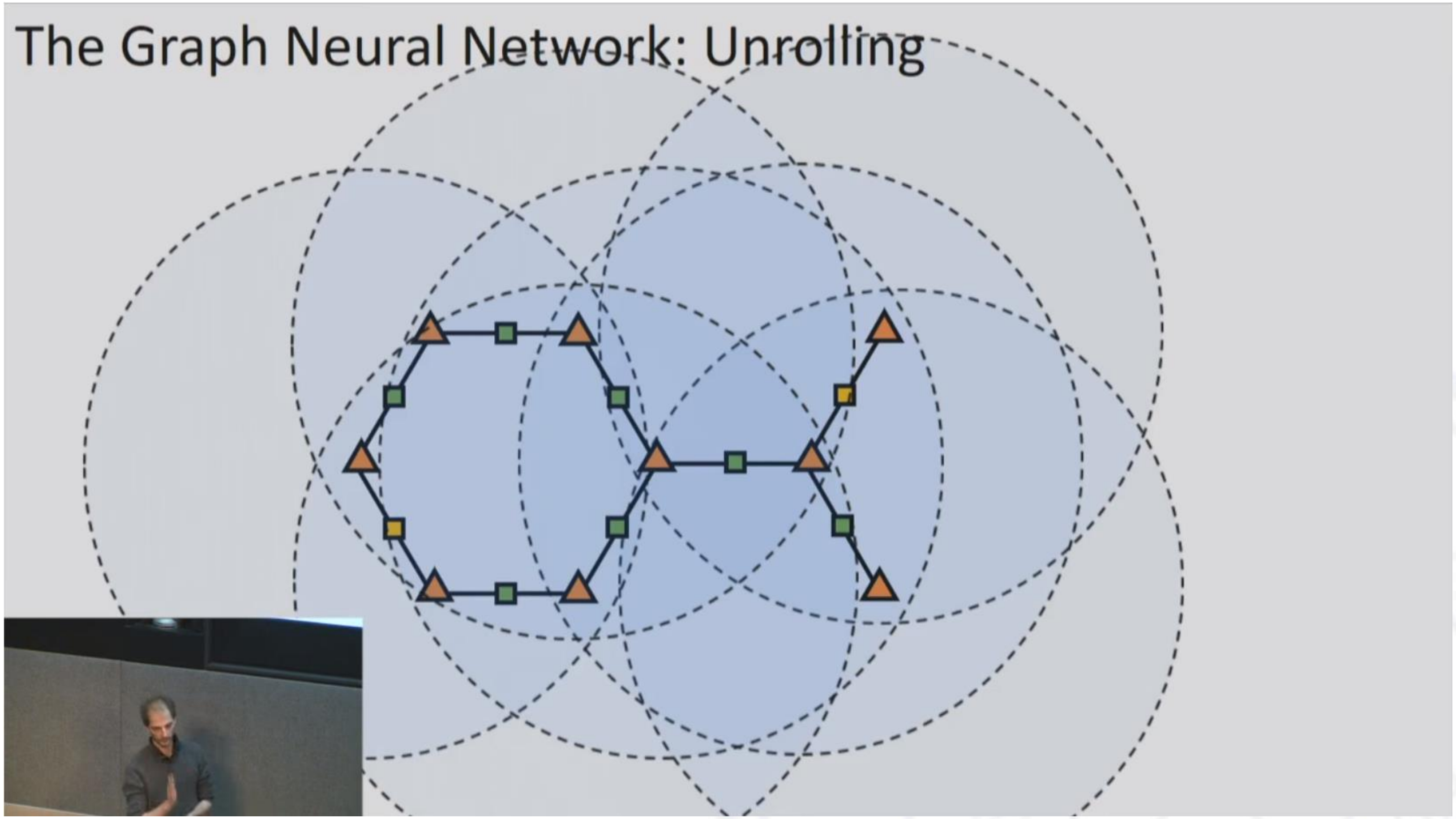




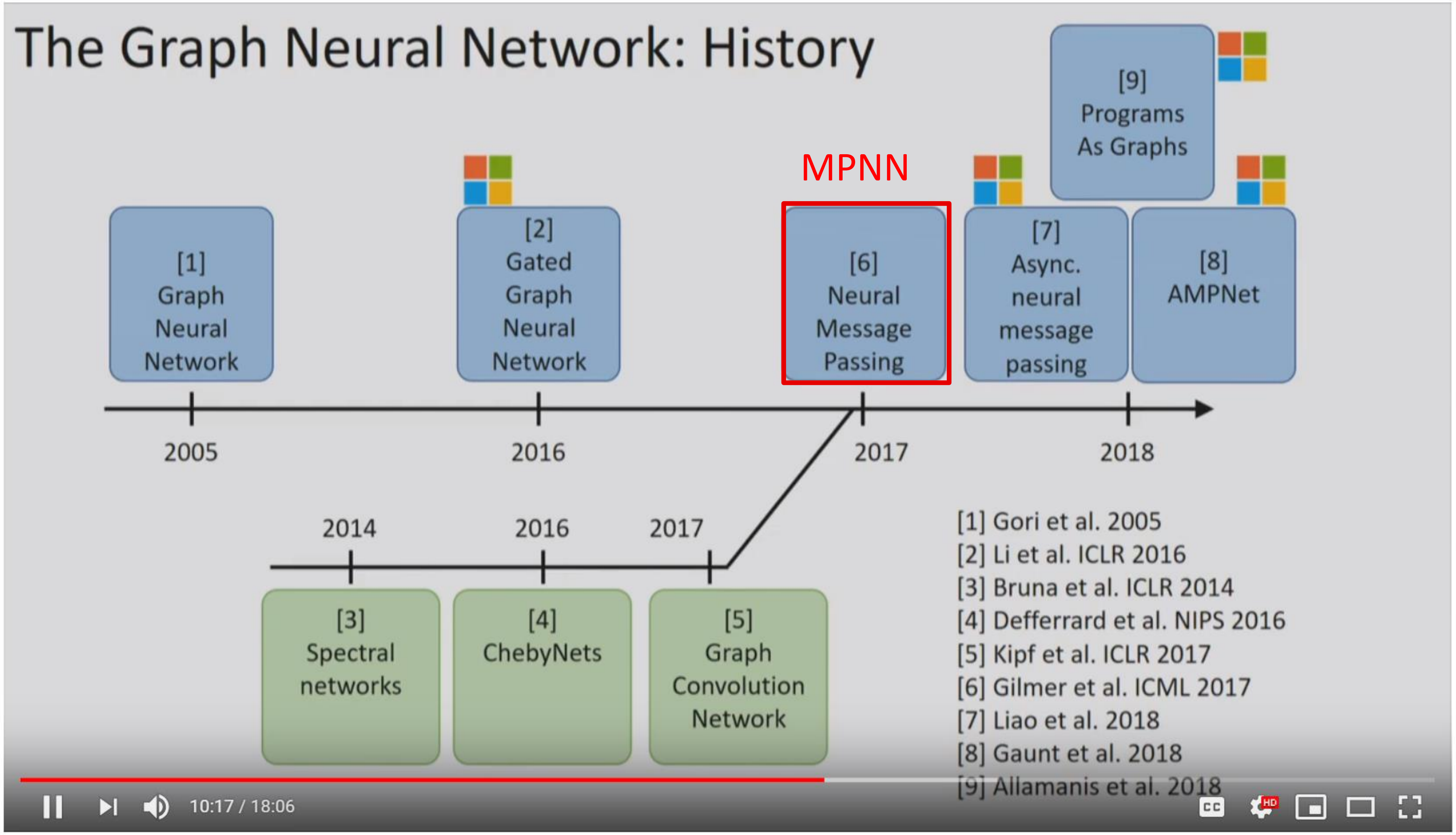
Introduction



Introduction



History



Graph neural networks: Variations and applications

21,160 views 465 7 SHARE SAVE

Spectral Conv.

谱图卷积

- 由谱图概念引出图拉普拉斯矩阵L，然后根据特征分解得到 $L=U\Lambda U^{-1}=U\Lambda U^{T}$。由傅里叶变换推广到图傅里叶变换，再由卷积定理得到谱图卷积。
- 谱图：图拉普拉斯矩阵的特征值
- 图拉普拉斯矩阵：L=D−A（D是度矩阵，A是邻接矩阵）
- 特征分解：$L=U\Lambda U^{-1}$ 矩阵分解为特征值和特征向量的乘积
- 傅里叶变换：时域信号与拉普拉斯算子特征函数的积分
- 图傅里叶变换：$\hat{f}=U^{T}f$ 时域信号与图拉普拉斯算子特征值的求和
- 图傅里叶逆变换：$f=U\hat{f}$

Spectral Conv.

谱图卷积

- 卷积定理：函数卷积的傅里叶变换就是函数傅里叶变换的乘积

$$f * h = F^{-1}(\hat{f(w)} \cdot \hat{h(w)})$$

- 谱图卷积：

$$(f * h)_G = U((U^T f) \odot (U^T h)) \qquad \hat{f} = U^T f, \hat{h} = U^T h$$

$$(f * h)_G = U \begin{pmatrix} \hat{h}(\lambda_1) & & \\ & \ddots & \\ & & \hat{h}(\lambda_n) \end{pmatrix} U^T f$$

Spectral Conv.

GCN

- 第一代GCN (ICLR 2014)

$$y_{output} = \sigma\left(U\begin{pmatrix}\theta_1 & & \\ & \ddots & \\ & & \theta_n\end{pmatrix}U^T x\right)$$

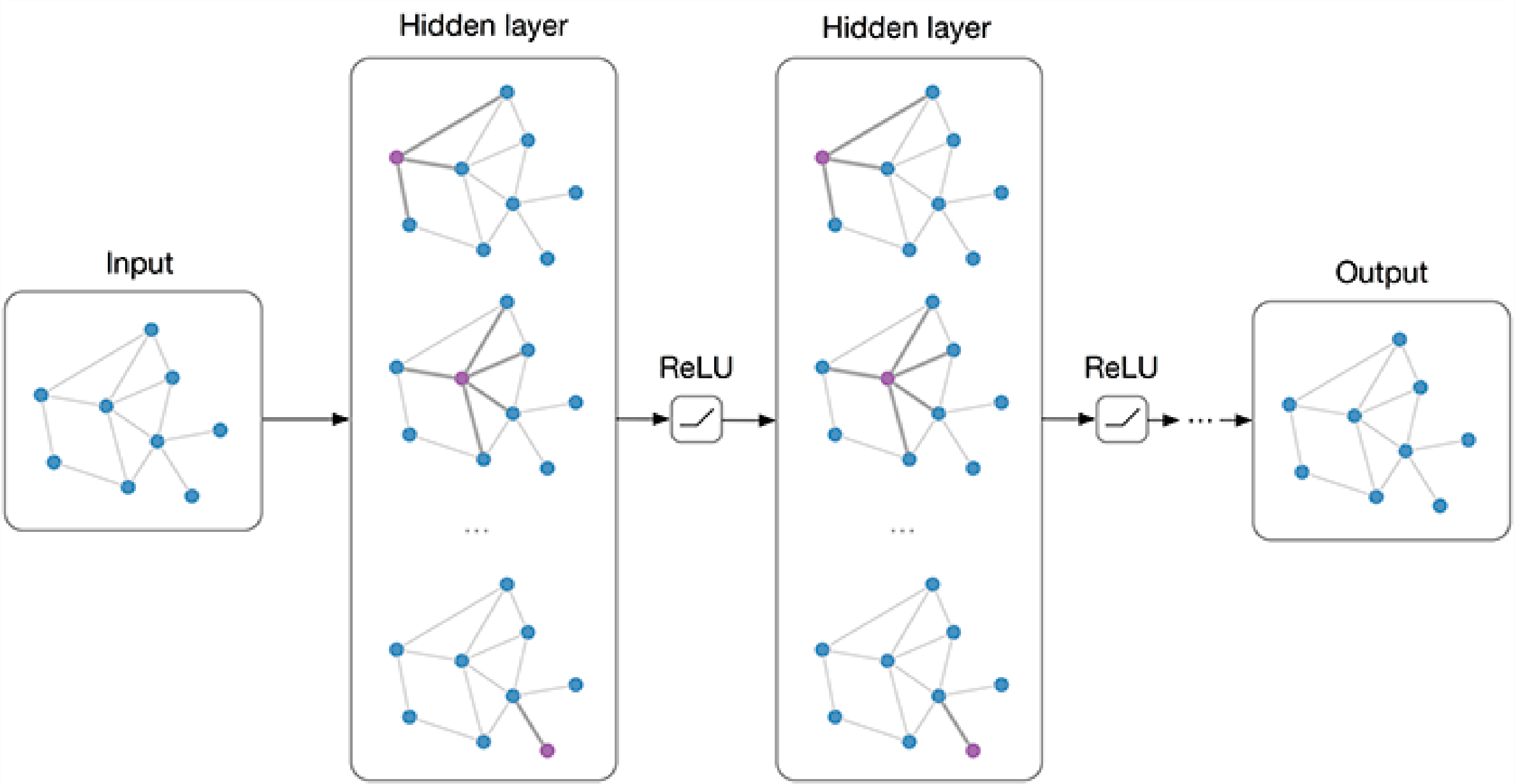
- 第二代GCN (NIPS 2016)

$$y_{output} = \sigma\left(U\begin{pmatrix}\sum_{j=0}^{K}\alpha_j\lambda_1^j & & \\ & \ddots & \\ & & \sum_{j=0}^{K}\alpha_j\lambda_n^j\end{pmatrix}U^T x\right)$$

- 第三代GCN (ICLR 2017)
  1. 令K=1，每层卷积只考虑直接领域，类似CNN3*3的Kernel
  2. 深度加深，宽度减少（DL经验：深度>宽度）

GCN

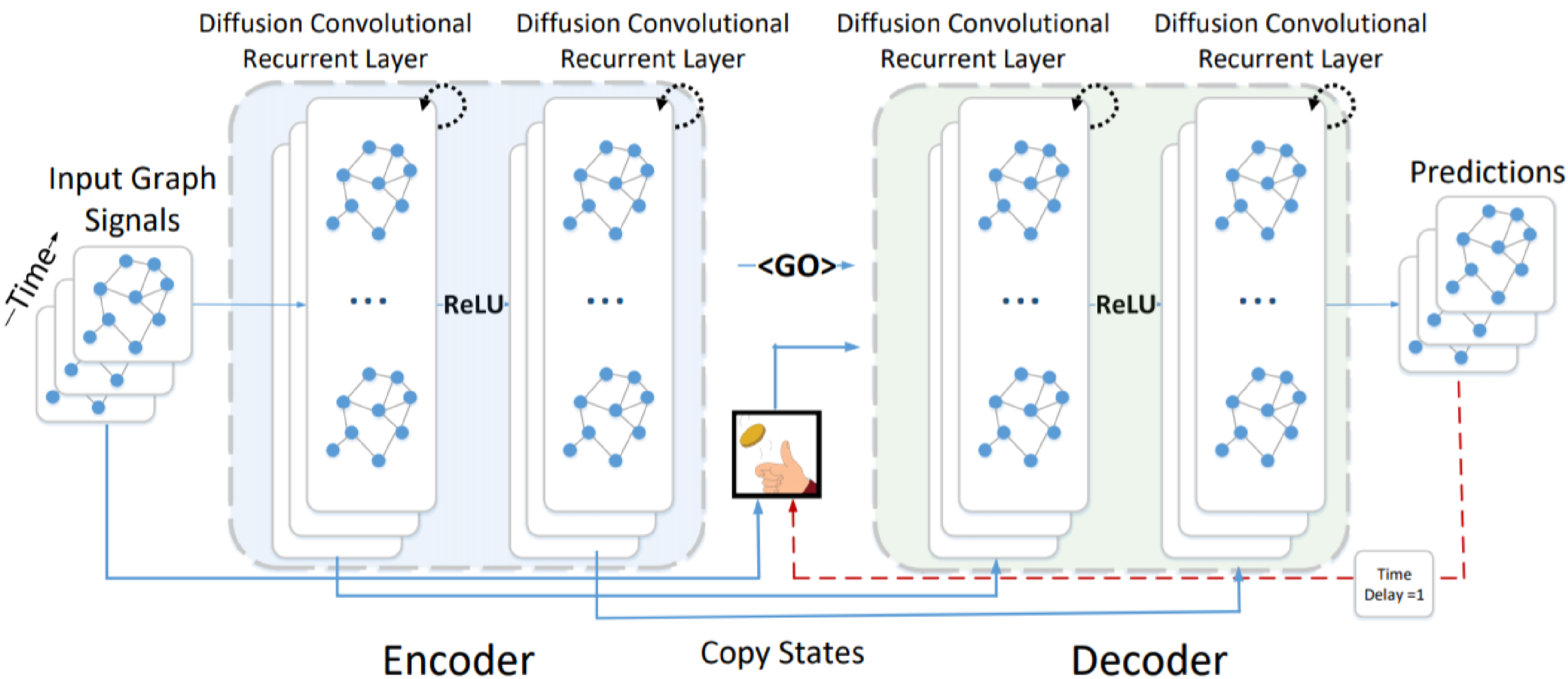
GCN



Kipf T N, Welling M. Semi-supervised classification with graph convolutional networks[J]. arXiv preprint arXiv:1609.02907, 2016.

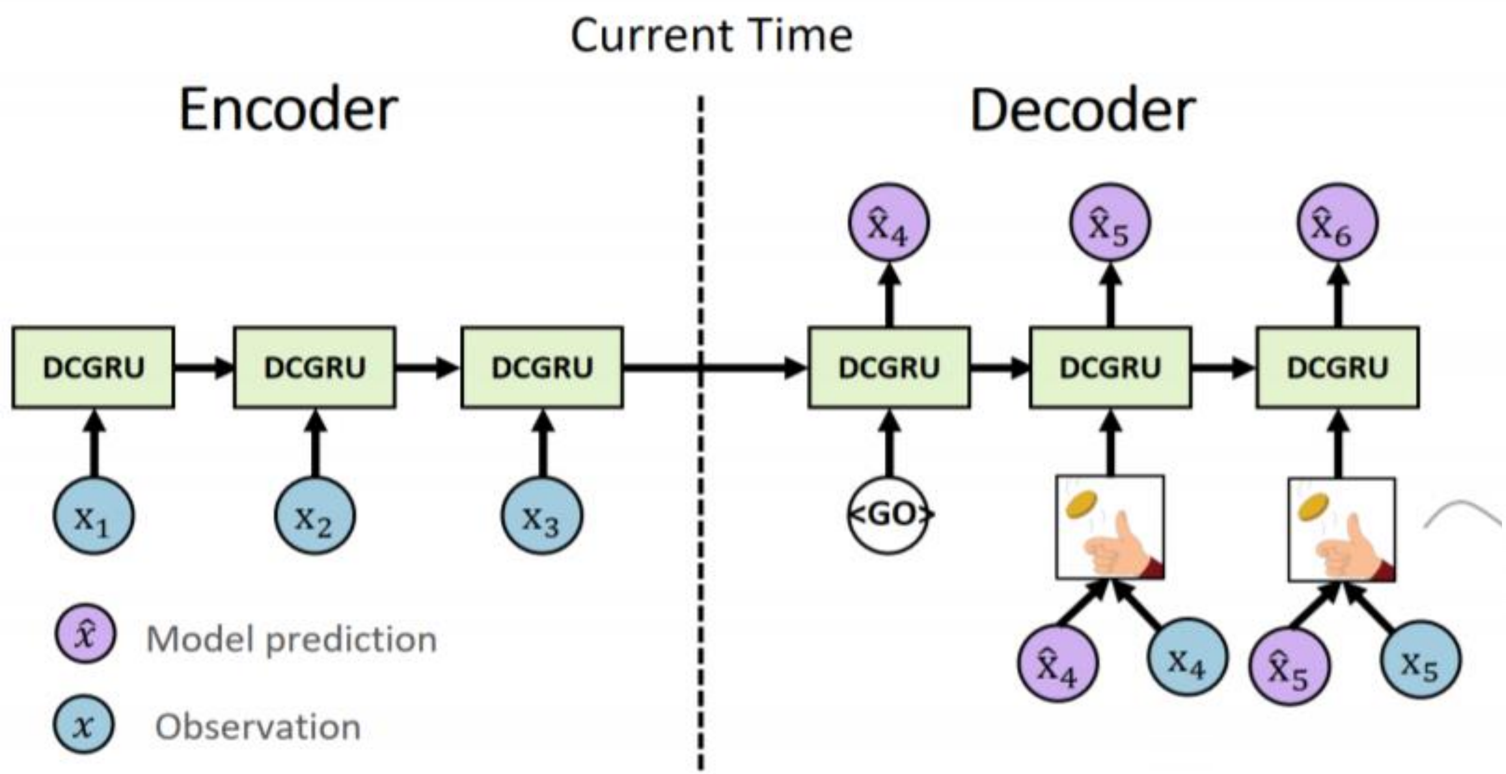
Spatiotemporal GCN

DCRNN



Spatiotemporal GCN

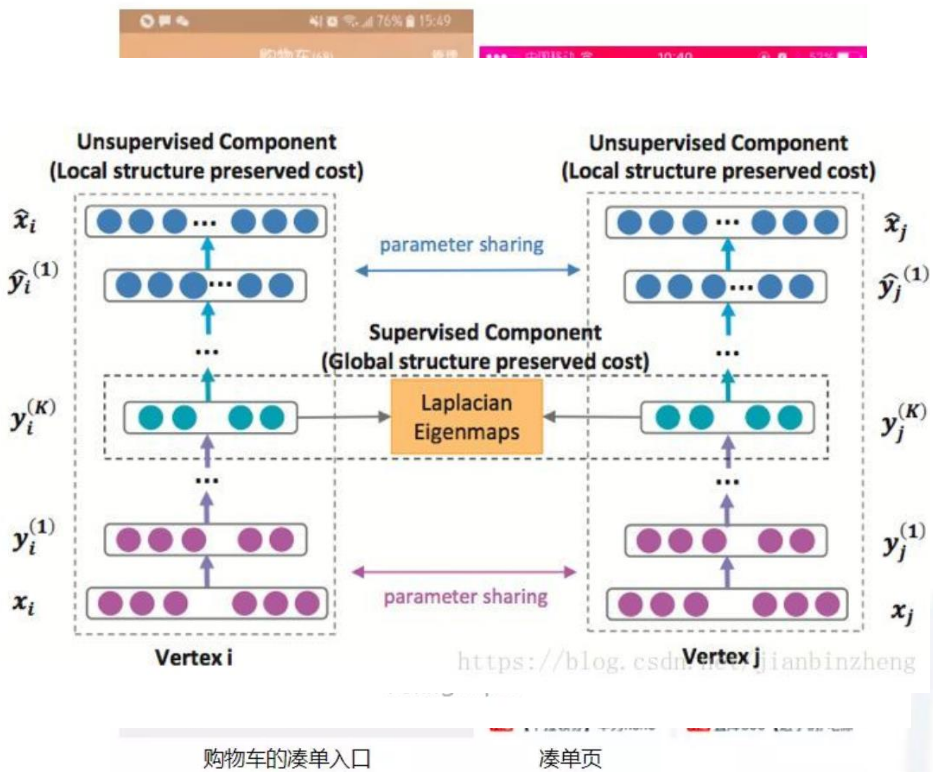
- DCRNN



Application：工业界应用

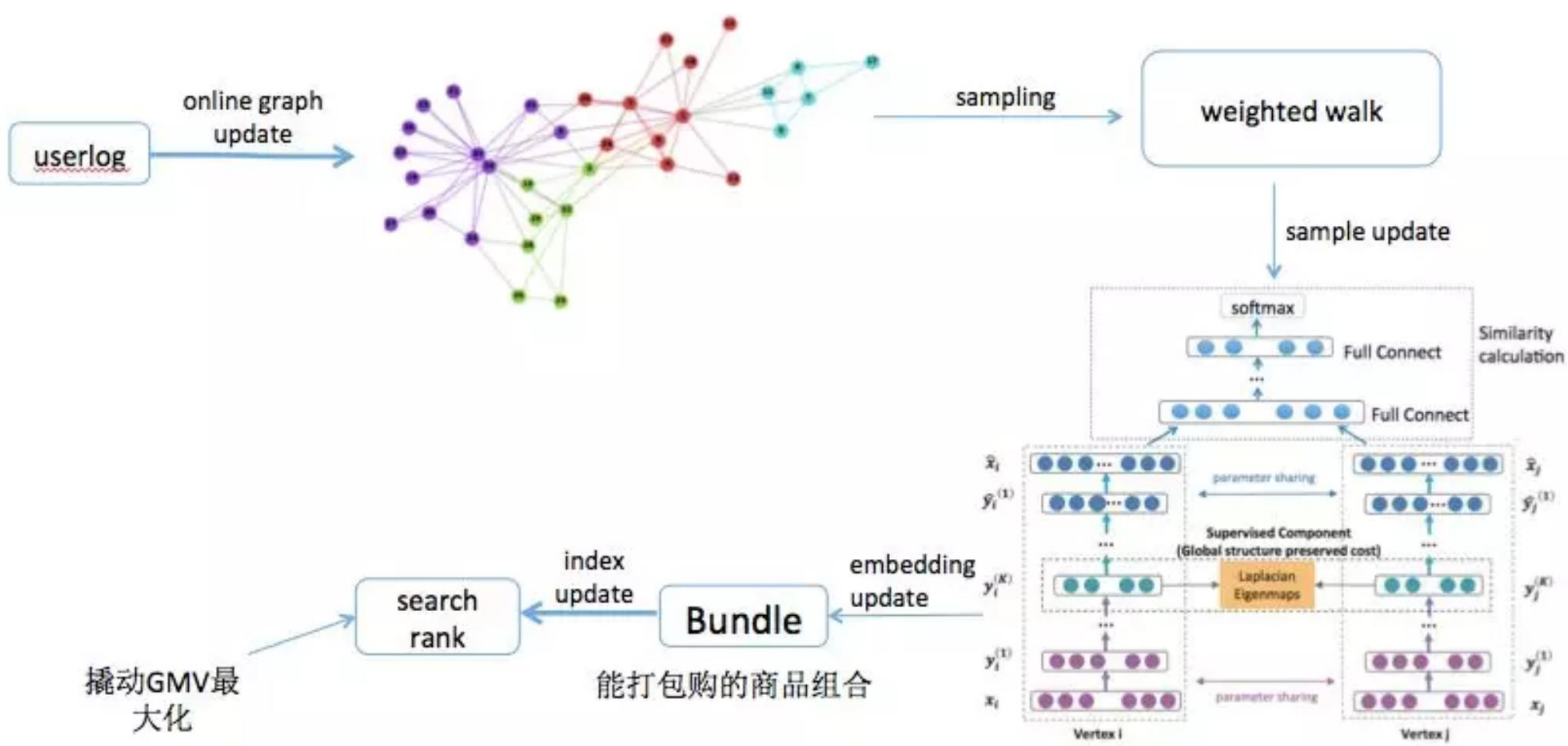
SDNE

阿里凑单算法



- 基于用户购买行为构建graph，节点：商品，边：商品间同时购买的行为，权重：同时购买的比重，可以是购买次数、购买时间、金额等feature；
- 基于权重Sampling（weighted walk）作为正样本的候选，负样本从用户非购买行为中随机抽样
- embedding部分将无监督模型升级成有监督模型，将基于weighted walk采出来的序，构造成item-item的pair对，送给有监督模型（SDNE）训练

SDNE



userlog
online graph update
sampling
weighted walk
sample update
softmax
Full Connect
Full Connect
Similarity calculation
Supervised Component
(Global structure preserved cost)
Laplacian Eigenmaps
Vertex i
Vertex j
embedding update
Bundle
能打包购的商品组合
index update
search rank
撬动GMV最大化

node2vec

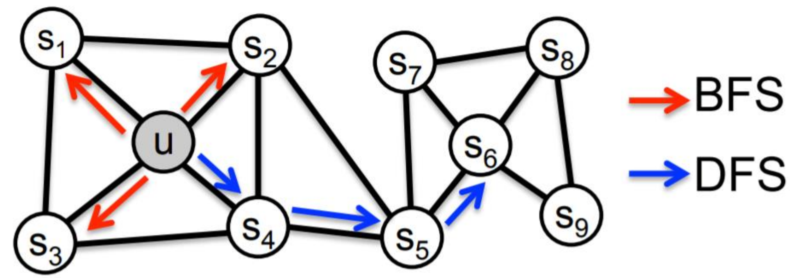
□ 计算广告：微信朋友圈 Lookalike 算法

- 业务场景：怎么给广告主挖掘潜在用户？
- 基本思想：基于广告主给出的客户名单，是不是可以做一个这样的尝试：找这批广告主的好友作为潜在用户，一就是社交相似性，二在微信朋友圈这样一个投放平台，同用户之间的行为会因为社会影响而形成传播，即微信社交Lookalike的基本思想。
- 具体而言：我们通过历史投放的广告采集到学习样本，比如说我的好友有400多个，对于有一部分好友我跟他历史上有同时曝光到一些广告，这些好友我可以计算出我跟他的广告相似度，就等于共同点击的广告数除以共同曝光的广告数。而剩余的好友，历史上没有共同曝光过广告。那我们有其他领域的数据，比如说我跟他的亲密关系，浏览或者阅读文章等兴趣相同点，能否通过这些社交的行为数据，预测到我跟他在广告上的喜好度？

node2vec

计算广告：微信朋友圈 Lookalike 算法

- 如何把图结构切入一个向量输入到机器学习模型中？

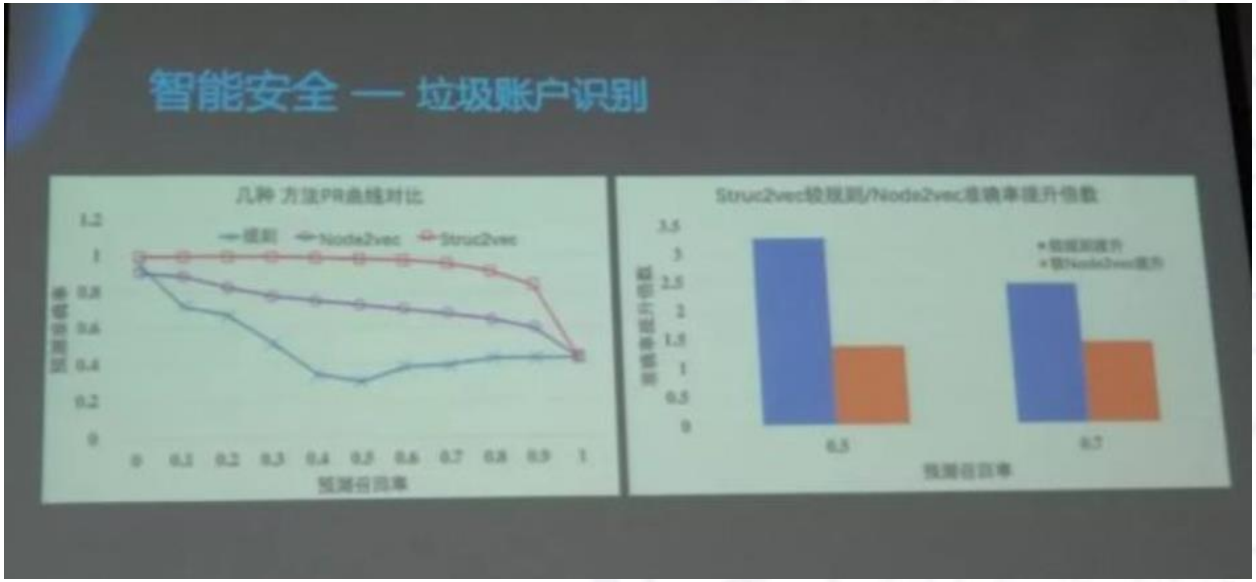


- 机器学习模型框架：

struc2vec

垃圾账户识别

- 业务场景：对于新注册用户，怎么来判定这是不是一个垃圾用户？
- 大概思路：从系统的角度来考虑人和这个社会之间的关联，然后构造网络，从网络结构来思考，一个人的信息不会很多，那么可以借整个网络的信息来一起分析
- 结果对比：**struc2vec** vs. **node2vec**



Summary

- 1. Survey：Graph Neural Network
  - Background, Graph Models, Applications
- 2. GCN：图卷积神经网络
  - Introduction, Spectral Conv.,
- 3. Application：工业界应用
  - SDNE, node2vec, struc2vec

谢 谢！

团队主页：**http://scsc.xmu.edu.cn/~longbiao**