Learning Discrete Structures for Graph Neural Networks

Luca Franceschi, Mathias Niepert, Massimilano Potil, Xiao He

Poster later: Pacific Ballroom # 177

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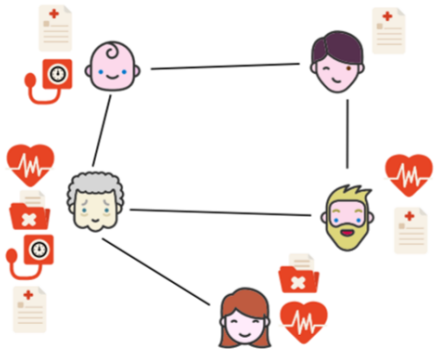
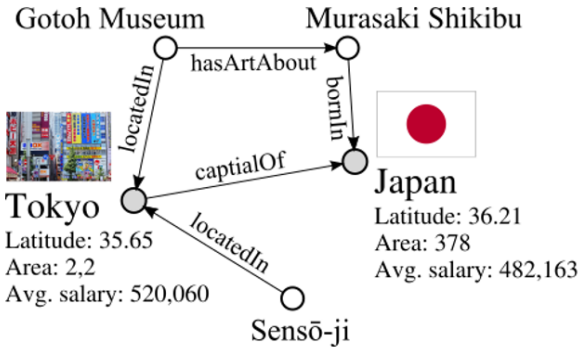
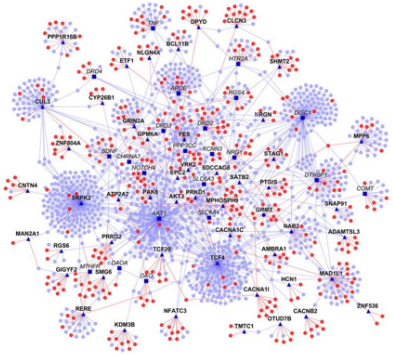
Introduction & Motivations



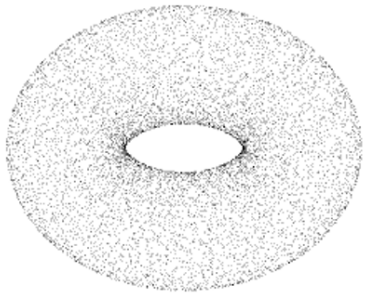
Patient network



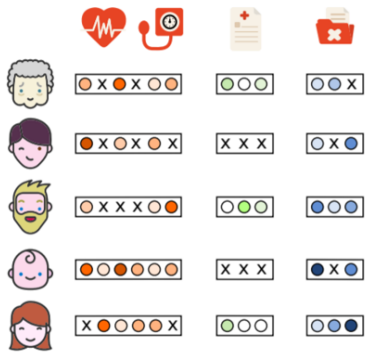
Knowledge graph



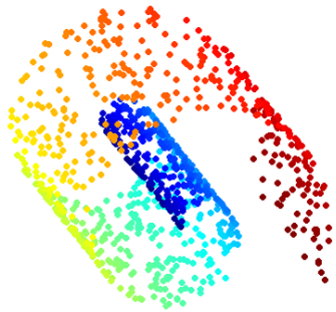
Schziophrenia protein interaction graph



Point cloud



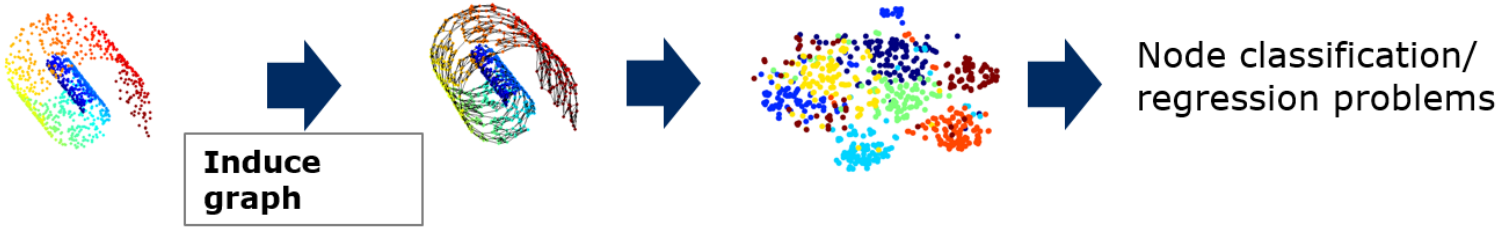
Tabular data



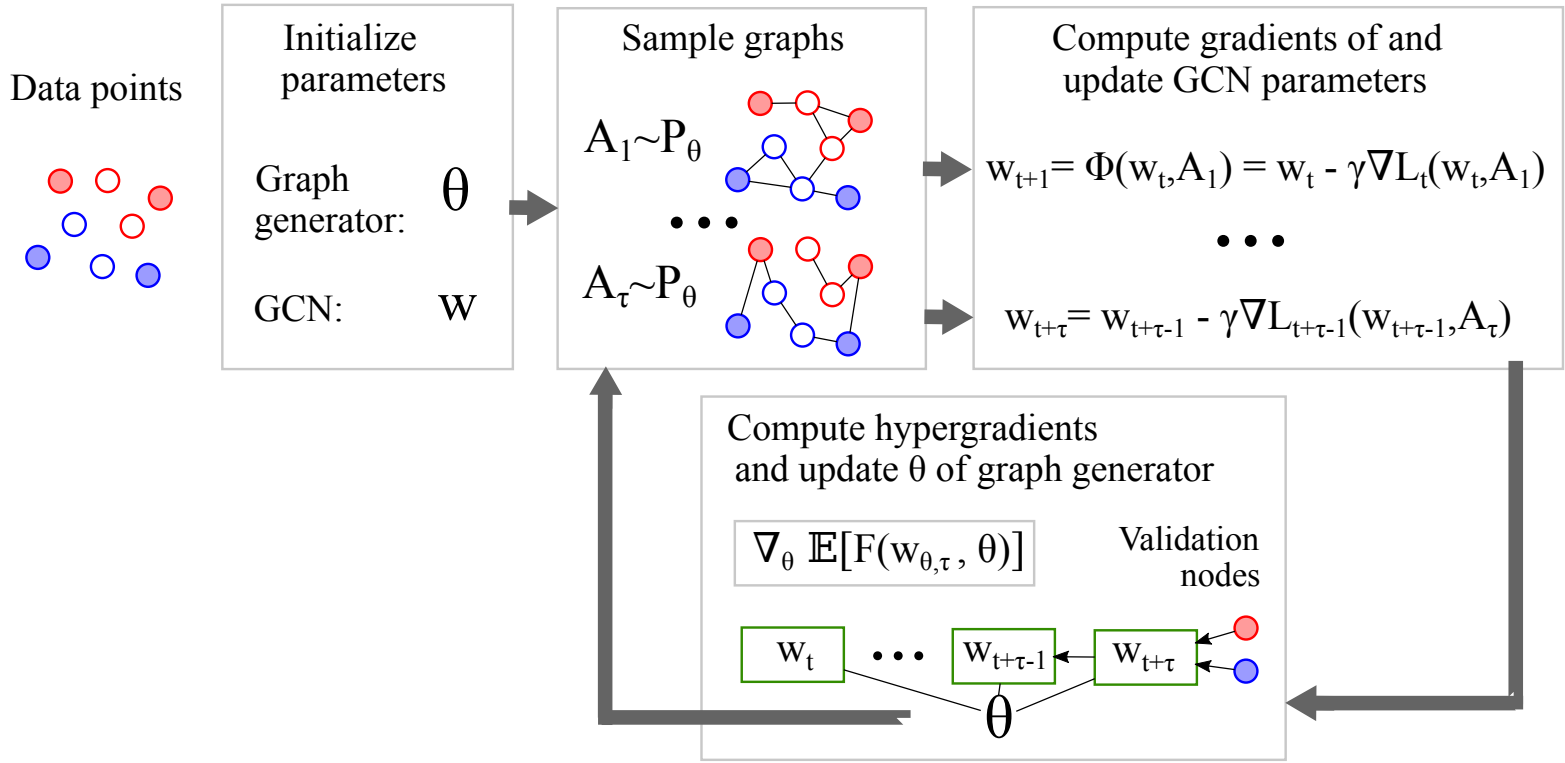
Data on a manifold

Aim: apply Graph Neural Networks (GNN) to settings in which an input graph is not available (or it is incomplete/nosiy)

LDS: Jointly Learning Structure and Parameters



Formulation: bilevel programming problem (gradient-based HPO) with discrete random variables $\Rightarrow$ discrete and sparse graph



See Franceschi et al. *Forward and Reverse Gradient-based Hyperparameter Optimization*, ICML 2017

Experiments: Semi-supervised Learning

	Wine	Cancer	Digits	Citeseer	Cora	20news	FMA
LogReg	92.1 (1.3)	**93.3 (0.5)**	85.5 (1.5)	62.2 (0.0)	60.8 (0.0)	42.7 (1.7)	37.3 (0.7)
Linear SVM	93.9 (1.6)	**90.6 (4.5)**	87.1 (1.8)	58.3 (0.0)	58.9 (0.0)	40.3 (1.4)	35.7 (1.5)
RBF SVM	**94.1 (2.9)**	**91.7 (3.1)**	86.9 (3.2)	60.2 (0.0)	59.7 (0.0)	41.0 (1.1)	**38.3 (1.0)**
RF	93.7 (1.6)	**92.1 (1.7)**	83.1 (2.6)	60.7 (0.7)	58.7 (0.4)	40.0 (1.1)	**37.9 (0.6)**
FFNN	89.7 (1.9)	**92.9 (1.2)**	36.3 (10.3)	56.7 (1.7)	56.1 (1.6)	38.6 (1.4)	33.2 (1.3)
LP	89.8 (3.7)	76.6 (0.5)	**91.9 (3.1)**	23.2 (6.7)	37.8 (0.2)	35.3 (0.9)	14.1 (2.1)
ManiReg	90.5 (0.1)	81.8 (0.1)	83.9 (0.1)	67.7 (1.6)	62.3 (0.9)	**46.6 (1.5)**	34.2 (1.1)
SemiEmb	91.9 (0.1)	89.7 (0.1)	**90.9 (0.1)**	68.1 (0.1)	63.1 (0.1)	**46.9 (0.1)**	34.1 (1.9)
Sparse-GCN	63.5 (6.6)	72.5 (2.9)	13.4 (1.5)	33.1 (0.9)	30.6 (2.1)	24.7 (1.2)	23.4 (1.4)
Dense-GCN	90.6 (2.8)	90.5 (2.7)	35.6 (21.8)	58.4 (1.1)	59.1 (0.6)	40.1 (1.5)	34.5 (0.9)
RBF-GCN	90.6 (2.3)	**92.6 (2.2)**	70.8 (5.5)	58.1 (1.2)	57.1 (1.9)	39.3 (1.4)	33.7 (1.4)
kNN-GCN	93.2 (3.1)	**93.8 (1.4)**	**91.3 (0.5)**	68.3 (1.3)	66.5 (0.4)	41.3 (0.6)	**37.8 (0.9)**
kNN-LDS	**97.3 (0.4)**	**94.4 (1.9)**	**92.5 (0.7)**	**71.5 (1.1)**	**71.5 (0.8)**	**46.4 (1.6)**	**39.7 (1.4)**

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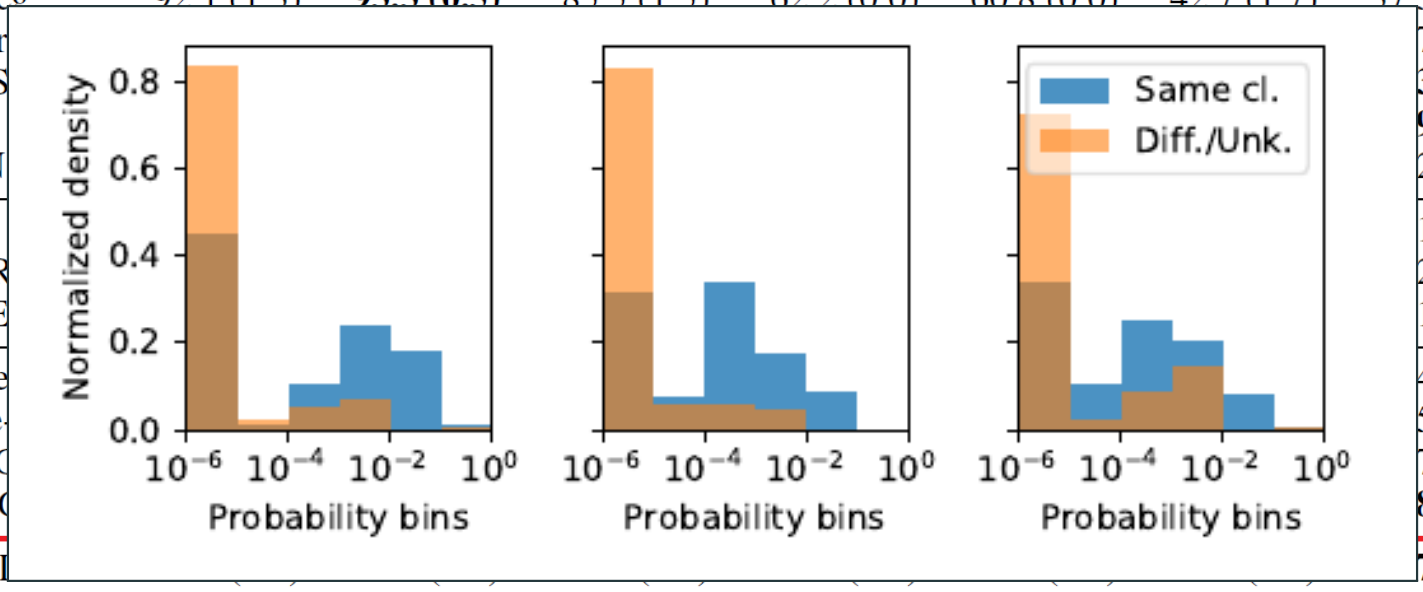
RBF S							**3 (1.0)**
RF							**9 (0.6)**
FFNN							2 (1.3)
LP							1 (2.1)
ManiR							2 (1.1)
SemiE							1 (1.9)
Sparse							4 (1.4)
Dense-							5 (0.9)
RBF-C							7 (1.4)
kNN-C							**8 (0.9)**
kNN-I							**7 (1.4)**

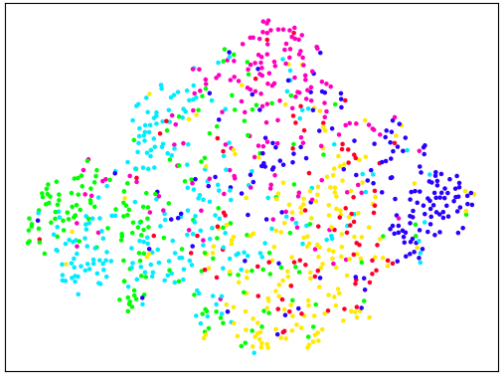


Many Thanks!

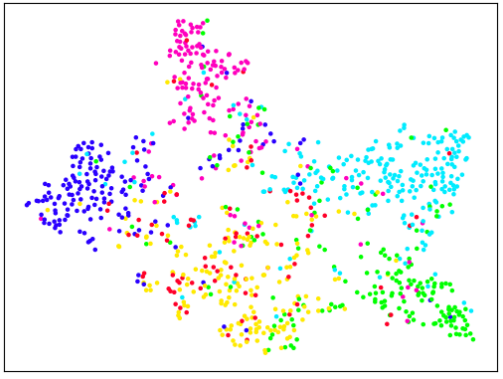
Poster # 177

Github page: `https://github.com/lucfra/LDS`

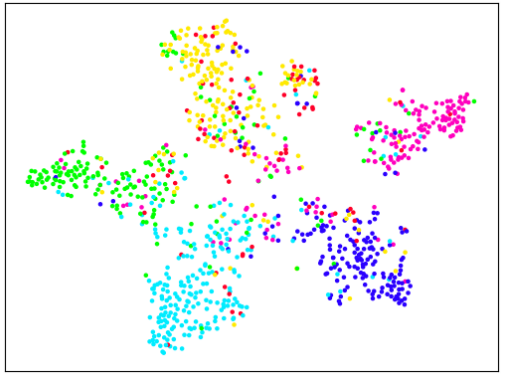
Some learned representations by a GCN on Citeseer



Dense Graph



kNN Graph



LDS graph