Graph neural networks and graph isomorphism

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Geometry of Deep Learning
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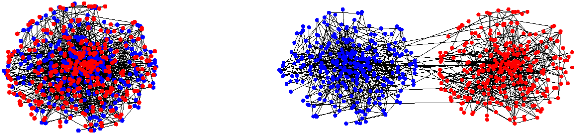
Motivating example 1

Clustering the stochastic block model

$A \sim SBM(p, q, n, 2)$ (two equal-sized communities):

$$\mathbb{P}(A_{ij} = 1) = \begin{cases} p & \text{if } i, j \text{ in the same community} \\ q & \text{if } i, j \text{ in different communities} \end{cases}$$



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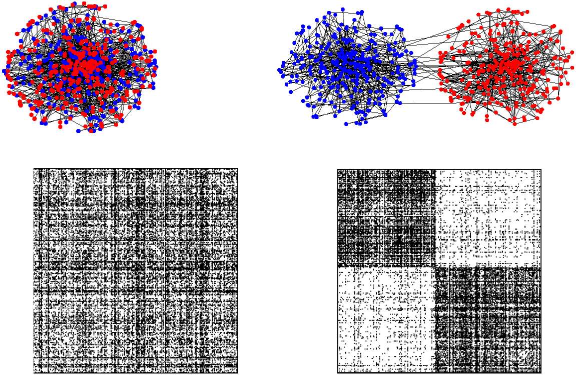
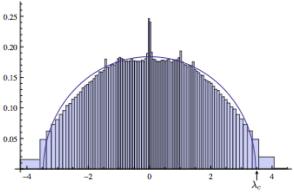


Clustering the stochastic block model

$A \sim SBM(a/n, b/n, n, 2)$ sparse.
Statistical threshold for detection: $(a-b)^2 > 2(a+b)$.

Spectrum doesn't concentrate (high degree vertices dominate it)
Laplacian is not useful for clustering



Other methods succeed. Example: semidefinite programming.

Krzakala, Moore, Mossel, Neeman, Sly, Zdeborová, Zhang, 2013

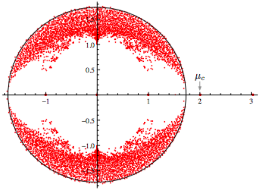
Deshpande, Abbe, Montanari, 2014

Abbe, Bandeira, Hall, 2014

Spectral redemption

Consider the non-backtracking operator (from linearized BP)

$$B_{(i\to j)(i'\to j')} = \begin{cases} 1 \text{ if } j = i' \text{ and } j' \neq i \\ 0 \text{ otherwise} \end{cases}$$



Second eigenvector of B reveals clustering structure

Krzakala, Moore, Mossel, Neeman, Sly, Zdeborová, Zhang, 2013

Bordenave, Lelarge, Massoulie, 2015

Bethe Hessian

$$BH(r) = (r^2 - 1)I - rA + D$$

Fixed points of BP $\longleftrightarrow$ Stationary points of Bethe free energy

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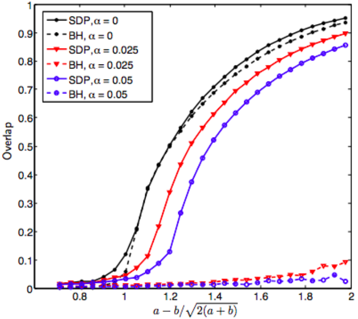
Pitfall: highly dependent in the model.



Saade, Krzakala, Zdeborová, 2014

Javanmard, Montanari, Ricci-Tersenghi, 2015

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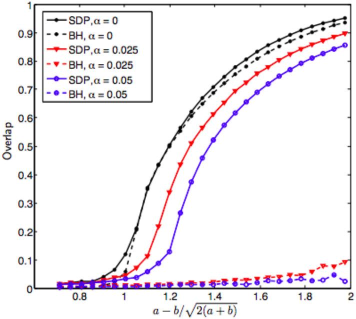

Goal: Combine graph operators $I, D, A, \ldots$ to generate robust "data-driven spectral methods" for problems in graphs

Saade, Krzakala, Zdeborová, 2014

Javanmard, Montanari, Ricci-Tersenghi, 2015

Graph neural networks

sGNN($\mathcal{M}$)

Power method: $v^{t+1} = Mv^t \qquad t = 1, \dots, T.$

Scarselli, Tsoi, Hagenbuchner, Monfardini, 2009

Chen, Li, Bruna, 2017

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Graph with adjacency matrix A. Set $\mathcal{M} = \{I_n, D, A, A^2, \ldots, A^{2^J}\}$,

$$v^{t+1} = \left(\sum_{M \in \mathcal{M}} M v^t \theta_M \right),$$

with $v^t \in \mathbb{R}^{n \times d_t}$,
$\Theta = \{\theta_1^t, \ldots, \theta_{|\mathcal{M}|}^t\}_t$, $\theta_M^t \in \mathbb{R}^{d_t \times d_{t+1}}$ trainable parameters.

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- Extension to line graph (GNN with non-backtracking).
- Extension to power graph $\min(1, A^t)$

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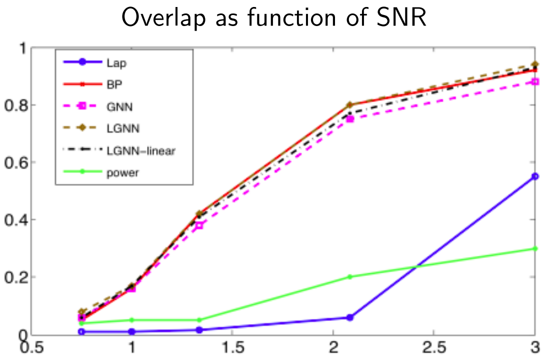
- Equivariant wrt permutations $G \mapsto \phi(G)$ then $G_\Pi \mapsto \Pi\phi(G)$.

Scarselli, Tsoi, Hagenbuchner, Monfardini, 2009

Chen, Li, Bruna, 2017

Numerical performance. SBM $k = 2$



Theoretical result: Under simplifications one can show that all local minima have small loss.

Chen, Li, Bruna, 2017

Yao, V., Bandeira, 2019

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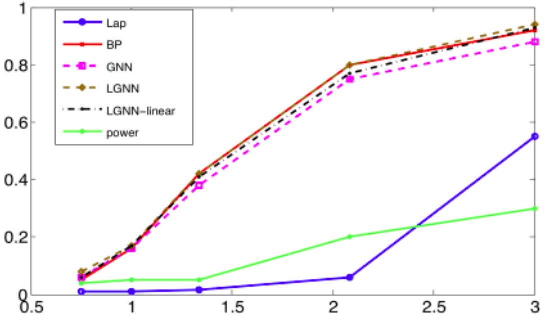
Overlap as function of SNR



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Extension to unsupervised setting: Max-cut on random regular graphs.

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Yao, V., Bandeira, 2019

Motivating example 2

Quadratic assignment problem

A, B $n \times n$ matrices. Π : set of $n \times n$ permutation matrices.

$$\text{Quadratic assignment} : \max_{X \in \Pi} \text{Trace}(AXBX^\top)$$

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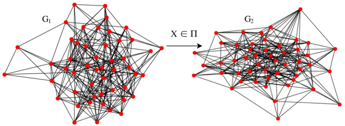

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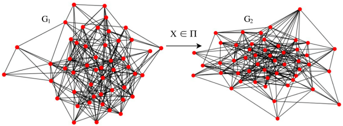

- Graph isomorphism

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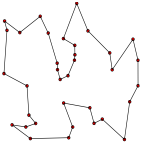
- Traveling salesman problem.



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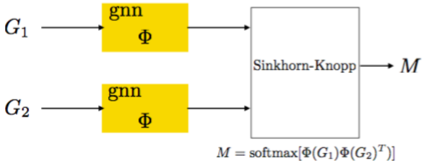
It includes many relevant problem as particular cases:

- Graph matching: $\min_{X \in \Pi} \|AX - XB\|_F^2$.
- Graph isomorphism.
- Traveling salesman problem.
- Gromov-Hausdorff distance of finite metric spaces.

It is NP-hard, even to approximate it.

GNN approach to quadratic assignment

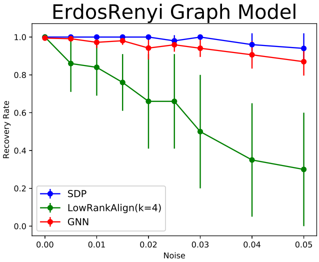
Siamese neural network:

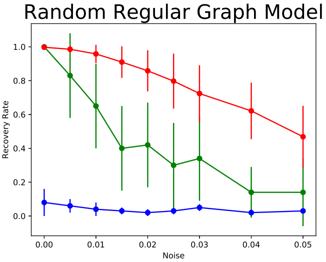


$G_2 = \pi \star G_1 \oplus N \qquad N \sim$ i.i.d. bit flip
$G_1 \sim$ Erdos-Renyi
$G_1 \sim$ Random regular

Nowak, V., Bandeira, Bruna, 2017

Numerical experiments





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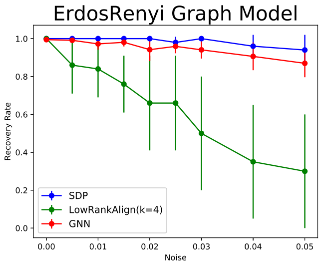

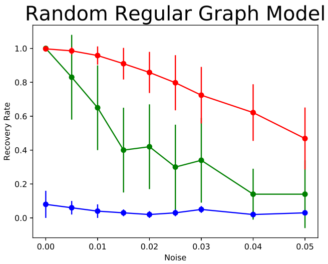

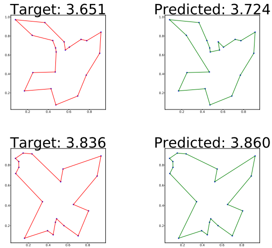

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Other GNN formulation

Message passing neural network

$$a_v^{(k)} = \mathrm{AGGREGATE}^{(k)}\left(\{h_u^{(k-1)} : u \in \mathcal{N}(u)\}\right)$$

$$h_v^{(k)} = \mathrm{COMBINE}^{(k)}\left(h_v^{(k-1)}, a_v^{(k)}\right)$$

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- There exist many formulations of GNN
- All satisfy one essential property:
  - invariance or equivariance with respect to permutations
  - node labels are not intrinsic

Hamilton, Ying, Leskovec, 2017

How powerful are graph neural networks?

Q: How good are they at distinguishing non-isomorphic graphs?

Xu, Hu, Leskovec, Jekelga 2019

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A: MPNN can be as powerful as the Weisfeler-Lehman test (1968).
W-L test is as powerful as the LP relaxation (Ullman et al 1994).

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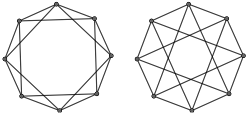
In particular MPNN cannot distinguish between non-isomorphic regular graphs with the same degree.



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Invariant functions on graphs

- Linear case:
  - If $L : \mathbb{R}^{n^k} \to \mathbb{R}$ invariant, then $vec(L) = \pi^{\otimes k} vec(L)$.
  - If $L : \mathbb{R}^{n^k} \to \mathbb{R}^{n^k}$ equivariant, then $vec(L) = \pi^{\otimes 2k} vec(L)$

  - The space of invariant [equivariant] linear functions on k-tensors has dimension $b(k)$ [$b(2k)$].

    ($b(k)$ denotes Bell Number: number of partitions of a size k set).

Maron, Ben-Hamu, Shamir, Lipman, 2019

Maron, Fetaya, Segol, Lipman, 2019

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- Universal approximation:
  - Invariant networks constructed by composition of linear invariant layers $L_t : \mathbb{R}^{n^k \times a} \to \mathbb{R}^b$ with ReLU or sigmoid activation functions universally approximate the space of invariant functions.
  - Extension to equivariant functions.

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    Arbitrary high order tensors are needed.

    Rates of convergence are not known.

Maron, Ben-Hamu, Shamir, Lipman, 2019

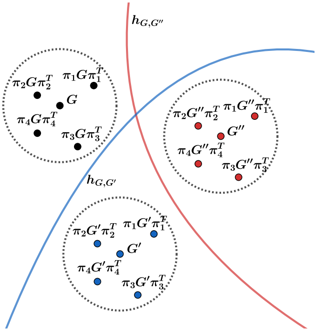
Maron, Fetaya, Segol, Lipman, 2019

Keriven, Peyré, 2019

Graph isomorphism equivalence to universal approximation

GIso-discriminating class of functions

A class $\mathcal{C}$ of permutation-invariant functions from $\mathcal{X}^{n\times n}$ to $\mathbb{R}$ so that for all pairs $G_1 \not\simeq G_2 \in \mathcal{X}^{n\times n}$, there exists $h \in \mathcal{C}$ such that $h(G_1) \neq h(G_2)$.



Chen, V., Chen, Bruna, 2019

Graph isomorphism equivalence to universal approximation

Universally approximating

A class $\mathcal{C}$ of permutation-invariant functions from $\mathcal{X}^{n\times n}$ to $\mathbb{R}$ so that for all permutation-invariant function f from $\mathcal{X}^{n\times n}$ to $\mathbb{R}$, and for all $\epsilon > 0$, there exists $h_{f,\epsilon} \in \mathcal{C}$ such that $\|f - h_{f,\epsilon}\|_\infty := \sup_{G\in\mathcal{X}^{n\times n}} |f(G) - h_{f,\epsilon}(G)| < \epsilon$

Remark

Universally approximating classes of functions are also GIso-discriminating.

Chen, V., Chen, Bruna, 2019

Graph isomorphism equivalence to universal approximation

$\mathcal{C}^{+L}$

If $\mathcal{C}$ is a collection of functions from $\mathcal{X}^{n \times n}$ to $\mathbb{R}$, consider the set of functions from graphs G to $\mathcal{NN}([h_1(G), ..., h_d(G)])$ for some finite d and $h_1, ..., h_d \in \mathcal{C}$, where $\mathcal{NN}$ is a feed-forward neural network with ReLU and L layers.

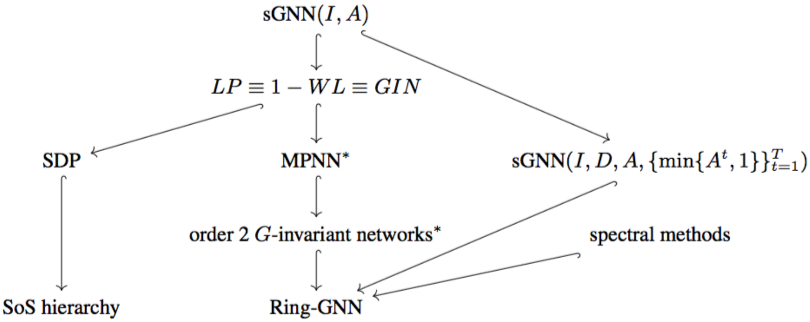
Theorem

If $\mathcal{C}$ is GIso-discriminating $\mathcal{C}^{+2}$ is universally approximating.

Chen, V., Chen, Bruna, 2019

Comparison of classes of functions through GIso

$\mathcal{C} \subseteq \mathcal{C}'$ if for all pairs of non-isomorphic graphs G_1, G_2, if there exists $h \in \mathcal{C}$ so that $h(G_1) \neq h(G_2)$ then there exists $h' \in \mathcal{C}'$ so that $h'(G_1) \neq h'(G_2)$.



Ring GNN

Input: Graph with n nodes and d features: $A \in \mathbb{R}^{n \times n \times d}$.

Equivariant linear layer from $\mathbb{R}^{n \times n \times d}$ to $\mathbb{R}^{n \times n \times d'}$. For $\theta \in \mathbb{R}^{d \times d' \times 17}$:
$L_\theta(A)_{\cdot,\cdot,k'} = \sum_{k=1}^{d} \sum_{i=1}^{15} \theta_{k,k',i} L_i(A_{\cdot,\cdot,i}) + \sum_{i=16}^{17} \theta_{k,k',i} \overline{L}_i$.
Set $A^{(0)} = A$.

$$\begin{aligned} B_1^{(t)} &= \rho(L_{\alpha^{(t)}}(A^{(t)})) \\ B_2^{(t)} &= \rho(L_{\beta^{(t)}}(A^{(t)}) \cdot L_{\gamma^{(t)}}(A^{(t)})) \\ A^{(t+1)} &= k_1^{(t)} B_1^{(t)} + k_2^{(t)} B_2^{(t)} \end{aligned}$$

where $k_1^{(t)}, k_2^{(t)} \in \mathbb{R}$, $\alpha^{(t)}, \beta^{(t)}, \gamma^{(t)} \in \mathbb{R}^{d^{(t)} \times d'^{(t)} \times 17}$ are learnable parameters.
Scalar output: $\theta_S \sum_{i,j} A_{ij}^{(T)} + \theta_D \sum_{i,i} A_{ii}^{(T)} + \sum_i \theta_i \lambda_i(A^{(T)})$, where $\theta_S, \theta_D, \theta_1, \ldots, \theta_n \in \mathbb{R}$ are trainable parameters, and $\lambda_i(A^{(T)})$ is the i-th eigenvalue of $A^{(T)}$.

Extensions - Future work

- Explicit rates:
  Connect GNN depth/architecture with classes of graphs they separate.

- Optimization landscape of GNNs:
  Current analysis of optimization landscape relies in simplified models to show that all local minima are confined in low-energy configurations.

- Connection with SoS:
  For some classes of "detecting hidden structures problems" existence of degree-d SoS refutations implies success of certain (typically non-explicit) spectral methods.
  - Can we express such class of spectral methods with GNNs.
  - Can we learn them?

Hopkins, Kothari, Potechin, Raghavendra, Schramm, Steurer, 2017

References

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