# Graph Neural Networks on Large Random Graphs: Convergence, Stability, Universality

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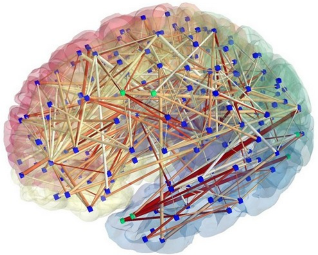
CNRS, GIPSA-lab

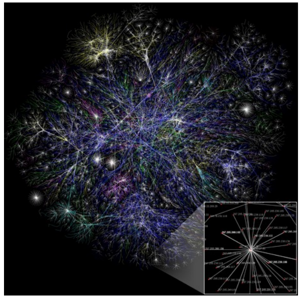
Joint work with Alberto Bietti (NYU) and Samuel Vaiter (CNRS, LJAD)

# Graph Machine Learning

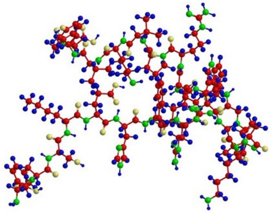
(Relatively) recent popularity of ML on graphs...



*Brain connectivity network*

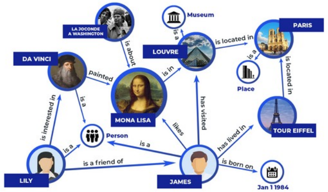


*Internet*

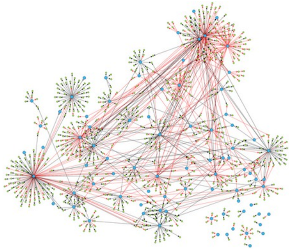


*Molecule*

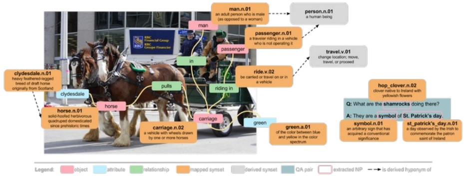
*Social network*



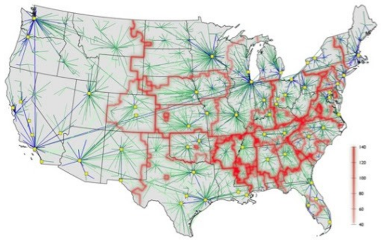

*Knowledge graph*



*Gene regulatory network*

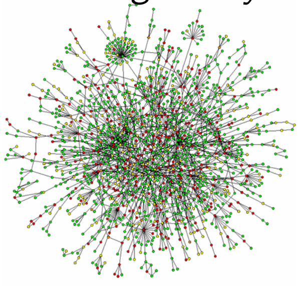


*Scene understanding network*



*Transportation network*

*Computer network*



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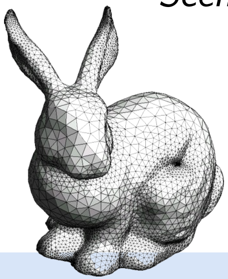

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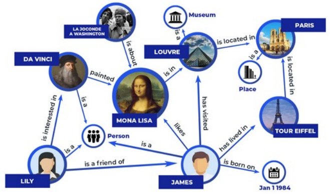


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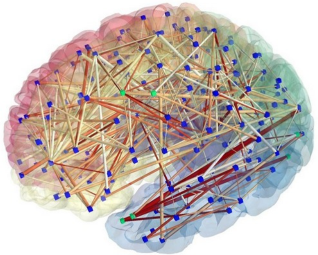

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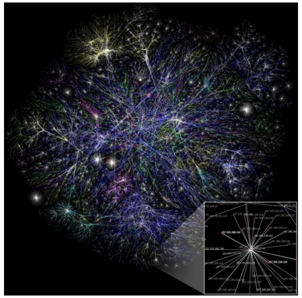

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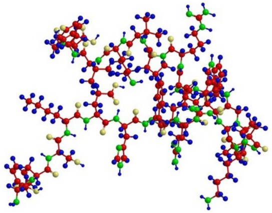

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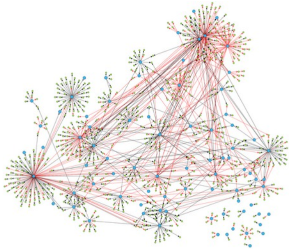

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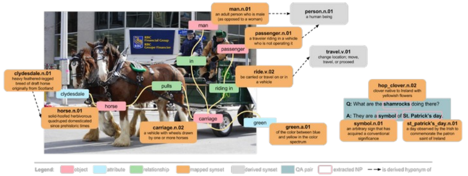

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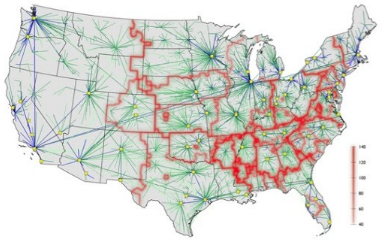

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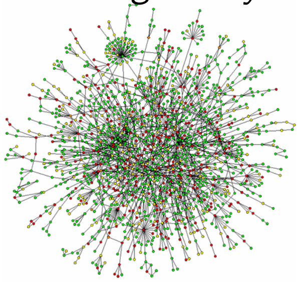

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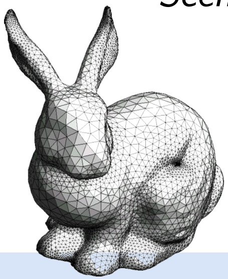

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*"if all you have is a hammer, everything looks like a nail"*

# ML on graphs: Graph Neural Networks

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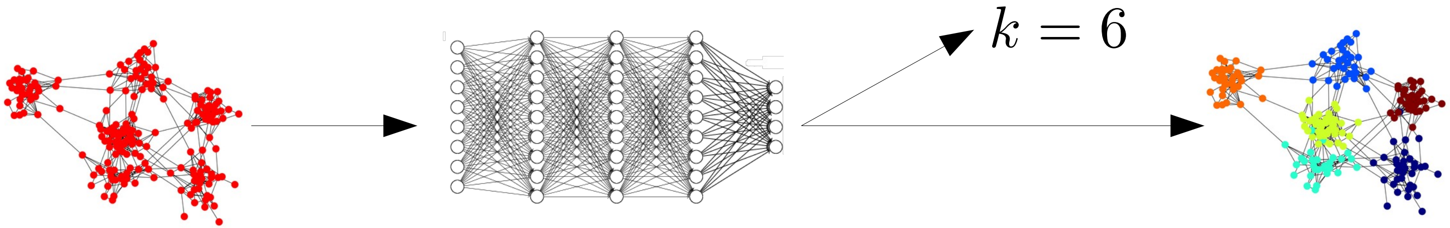


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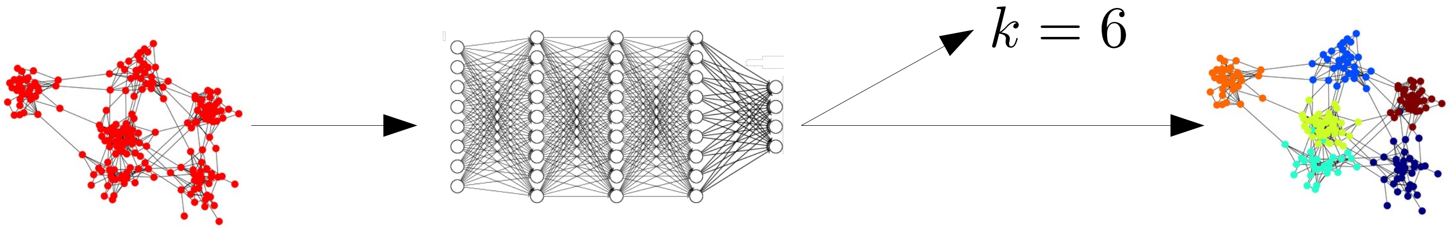


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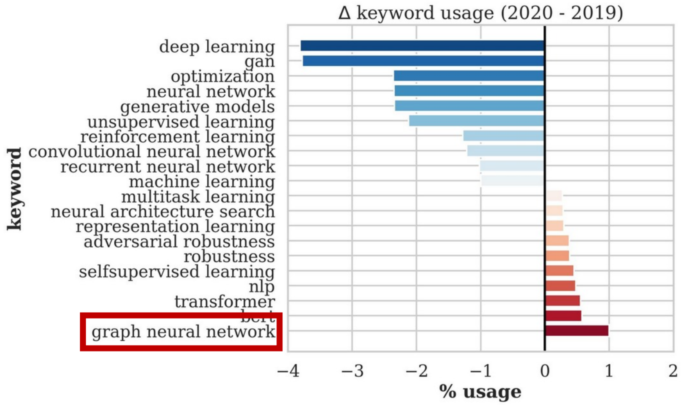

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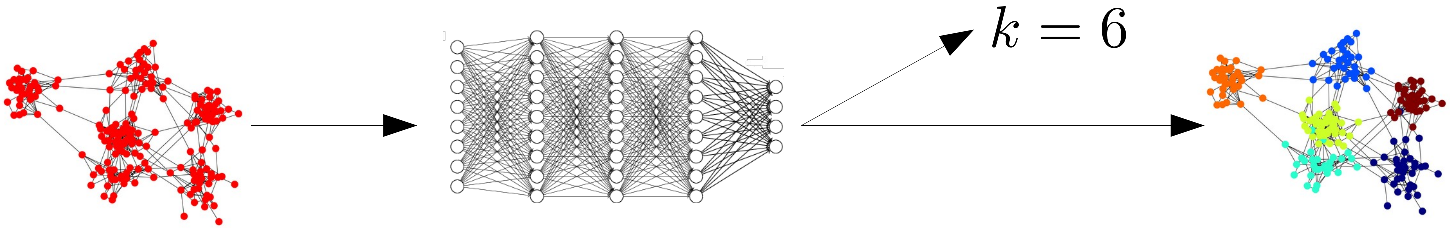
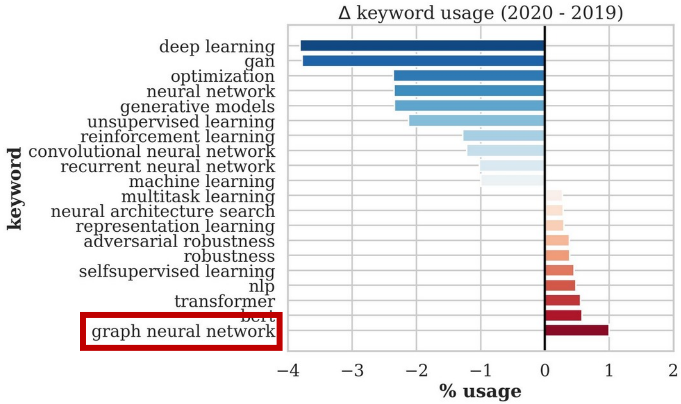



**Graph Neural Networks** (GNN) are "deep architectures" to do ML on graphs.

- Very (very) trendy right now!
- Work quite well, but...
  - Room for improvement! (compared to other "deep learning")
  - No "ImageNet moment" yet for GNNs (see *Open Graph Benchmark*)
  - The theory might be **actually useful** to design new architectures



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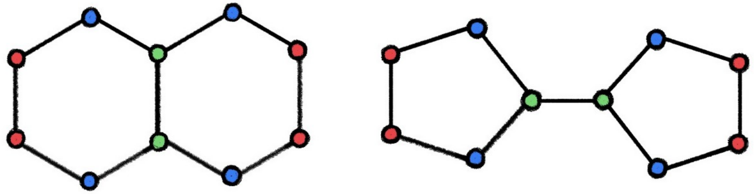

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  - *Can a GNN distinguish two non-isomorphic graphs?*
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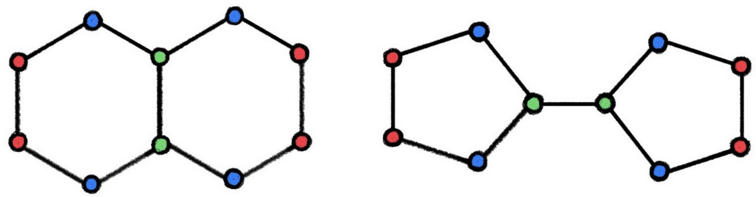
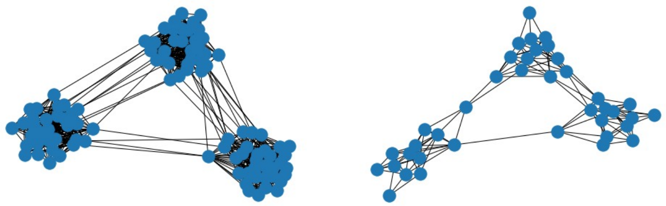


- Large graphs may "look the same", but are never isomorphic, of different size, etc.



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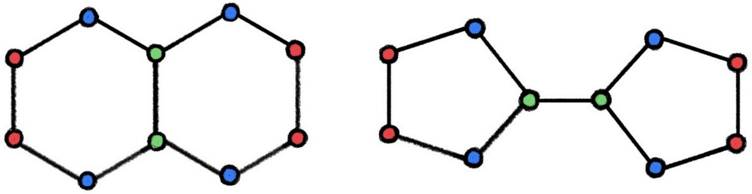

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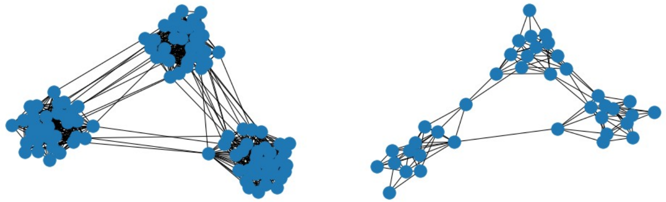

This talk: use random graph models to analyze GNN properties on large graphs

# Outline

1. Convergence of GNNs
2. Stability of c-GNNs
3. Universality of c-GNNs

# Random graphs models

Long history of modelling large graphs with **random generative models**

Chung and Lu. *Complex Graphs and Networks* (2004)
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**Latent position models** *(W-random graphs, kernel random graphs...)*

$$x_i \overset{iid}{\sim} P \in \mathbb{R}^d \qquad a_{ij} \sim \mathrm{Ber}(\alpha_n W(x_i, x_j))$$

***Unknown*** *latent variables* *Connectivity kernel*

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*Dense* $\alpha_n \sim 1$ $\quad$ *Sparse* $\alpha_n \sim 1/n$

*Relatively sparse* $\alpha_n \sim (\log n)/n$

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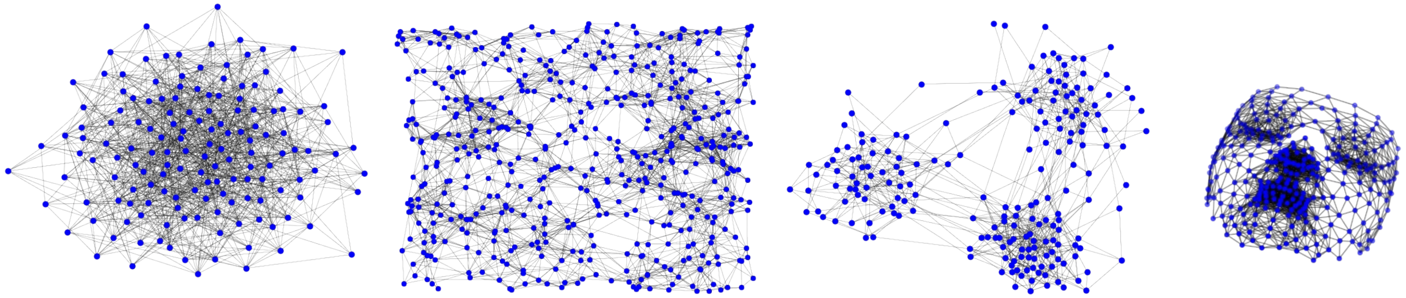

*Includes Erdös-Rényi, Stochastic Block Models, Gaussian kernel, epsilon-graphs...*

# Filtering on graphs

(Early-days) GNNs are based on **graph-convolutions** (filtering)

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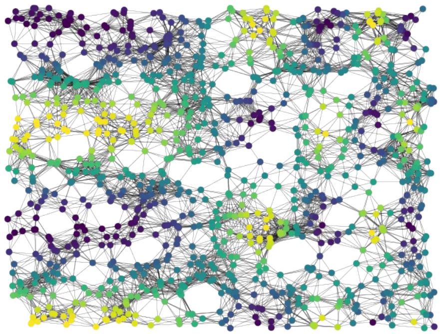

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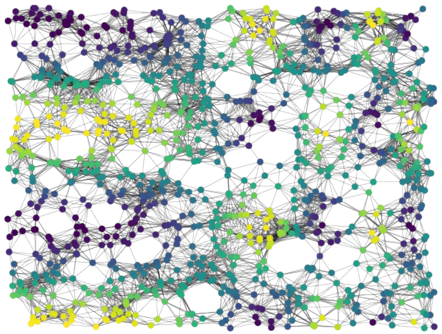

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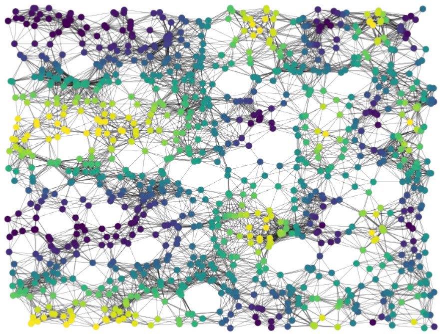

- Based on graph Fourier transform
- Defined by diagonalizing the graph Laplacian $L = Id - D^{-\frac{1}{2}} A D^{-\frac{1}{2}} = U^\top \Lambda U$

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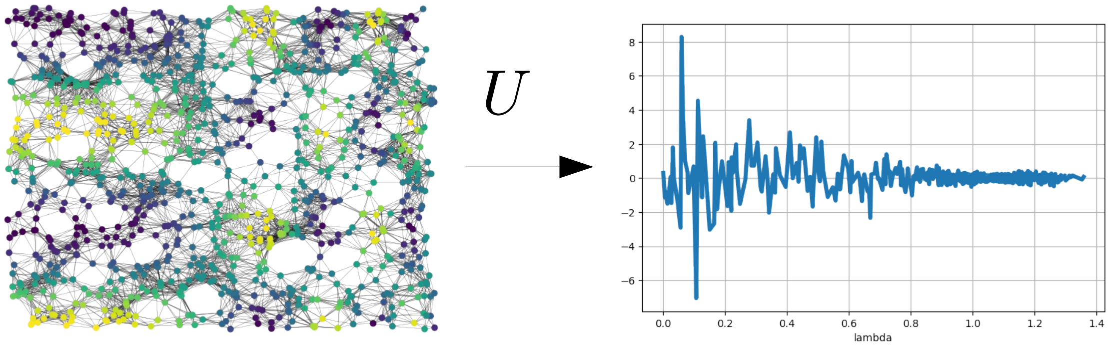

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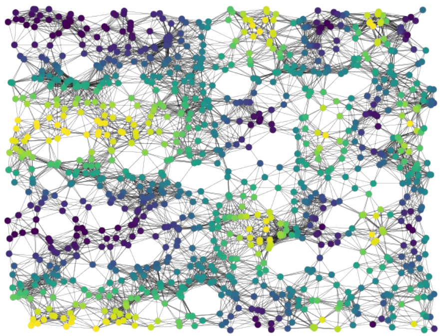

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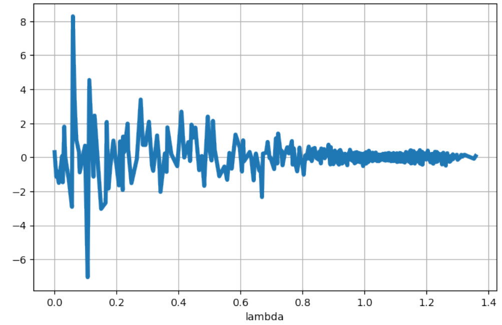


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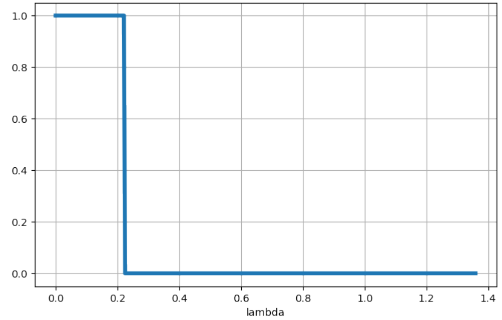

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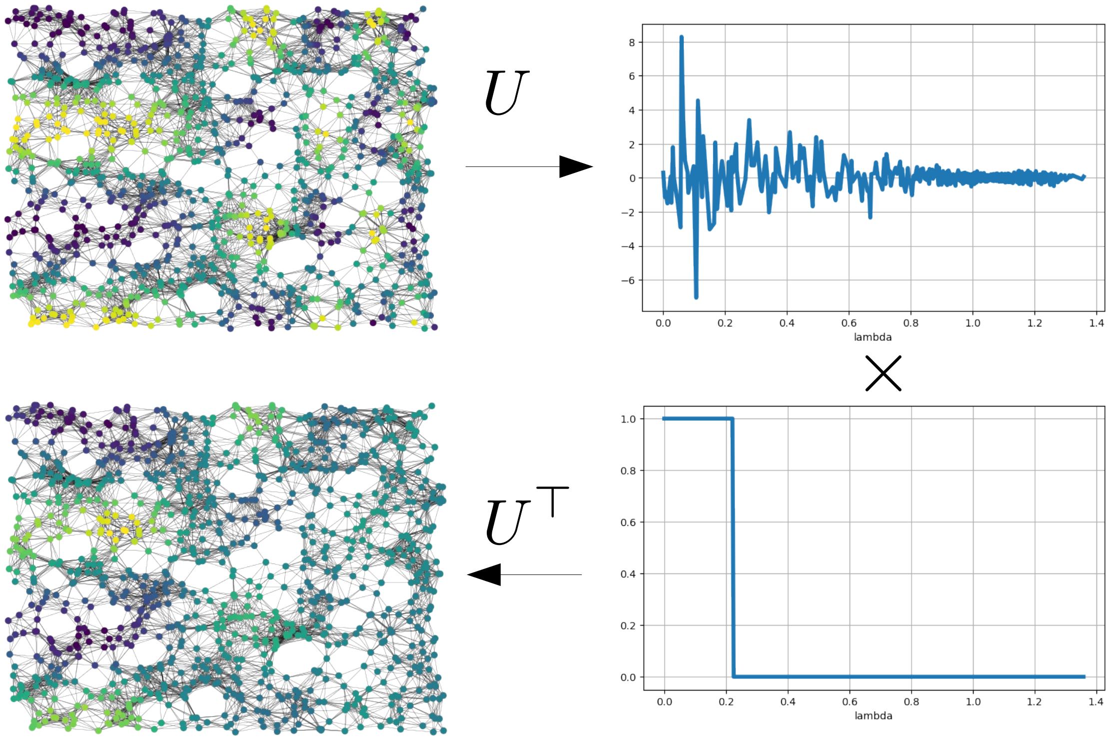


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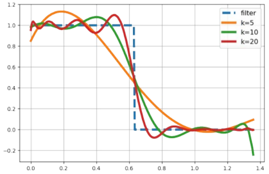
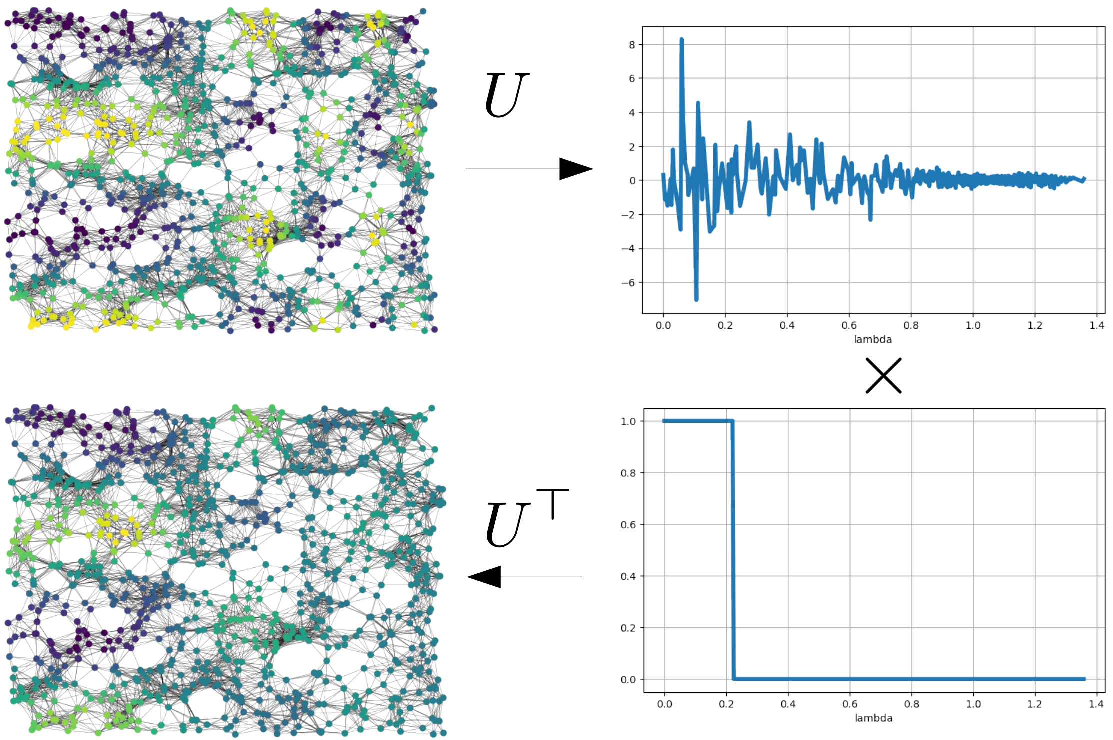
- Popular filters are polynomial filters

$$h \star z = (\textstyle\sum_k \beta_k L^k) z$$





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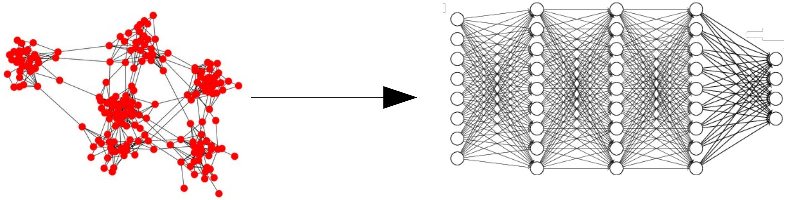

## (Spectral) Graph Neural Networks

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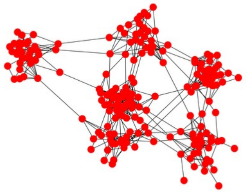

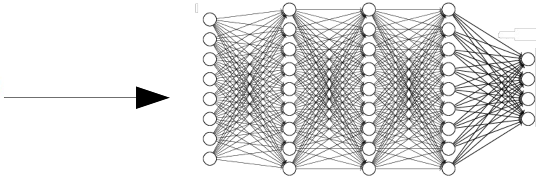

### (Spectral) Graph Neural Networks

- Propagate **signal over nodes**

$$z_j^{(\ell+1)} = \rho\left(\sum\nolimits_i h_{ij}^{(\ell)}(L) z_i^{(\ell)} + b_j^{(\ell)} 1_n\right)$$

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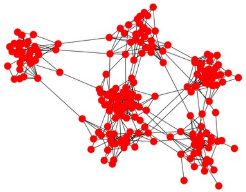

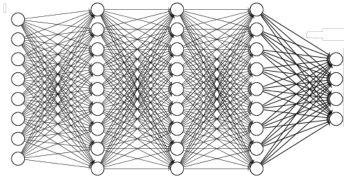

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*Non-lin.*

**Trainable** polynomial graph filters with normalized Laplacian

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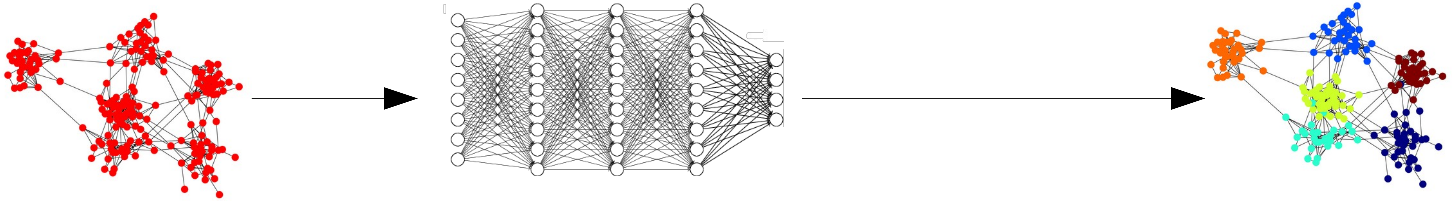

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**Trainable** polynomial graph filters with normalized Laplacian $h(L) = \sum_k \beta_k L^k$ $L = D^{-\frac{1}{2}} A D^{-\frac{1}{2}}$

Output

- Signal over nodes (permutation-equivariant)

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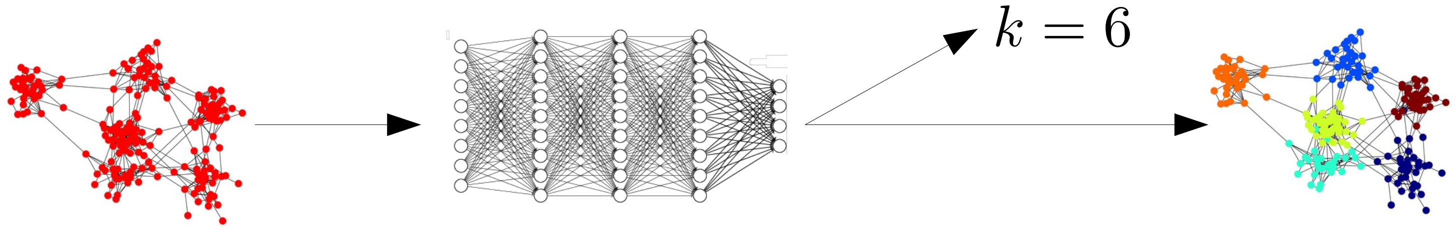


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$$z_j^{(\ell+1)} = \rho\left(\sum_i h_{ij}^{(\ell)}(L) z_i^{(\ell)} + b_j^{(\ell)} 1_n\right)$$

*Non-lin.*

**Trainable** polynomial graph filters with normalized Laplacian $h(L) = \sum_k \beta_k L^k$, $L = D^{-\frac{1}{2}} A D^{-\frac{1}{2}}$

Output

- Signal over nodes (permutation-equivariant)
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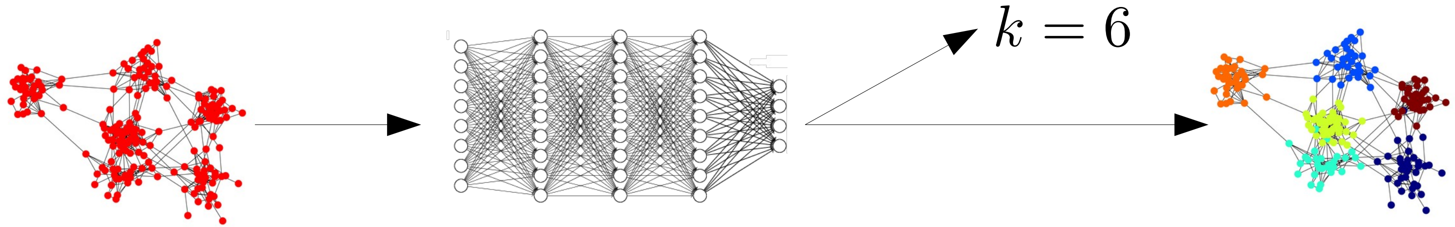
# Discrete vs. continuous

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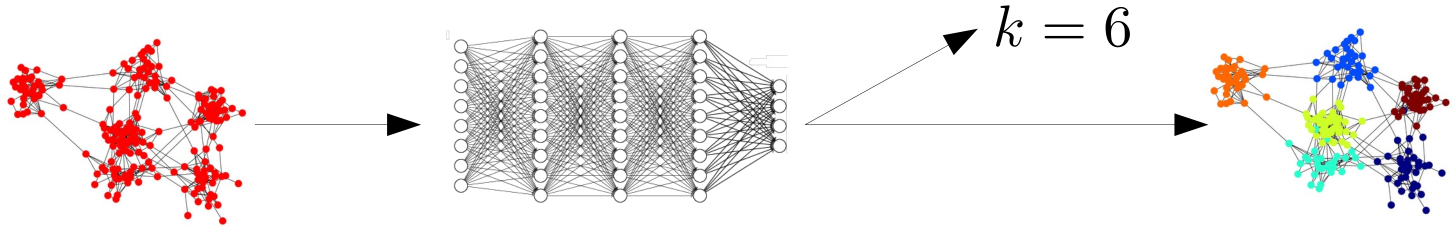


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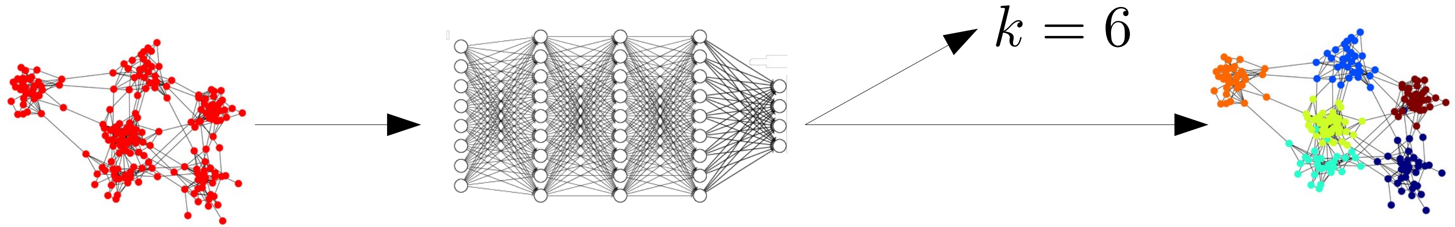


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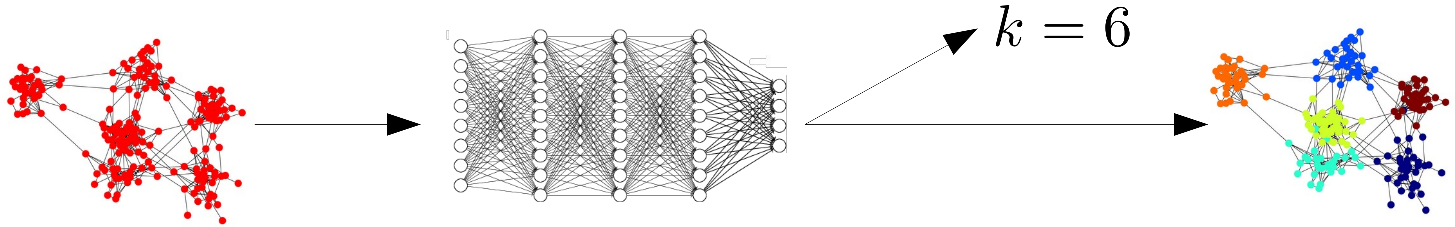


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**Thm (Non-asymptotic convergence)**

*If* $\alpha_n \gtrsim (\log n)/n$ *, with probability* $1 - n^{-r}$*, the deviation between the outputs of the discrete GNN and the continuous GNN is*

| | | |
|---|---|---|
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gipsa-lab

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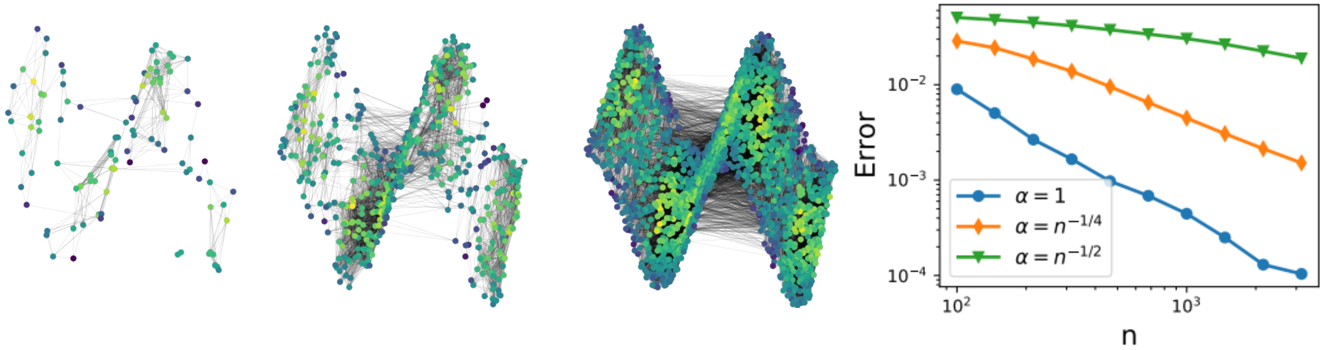

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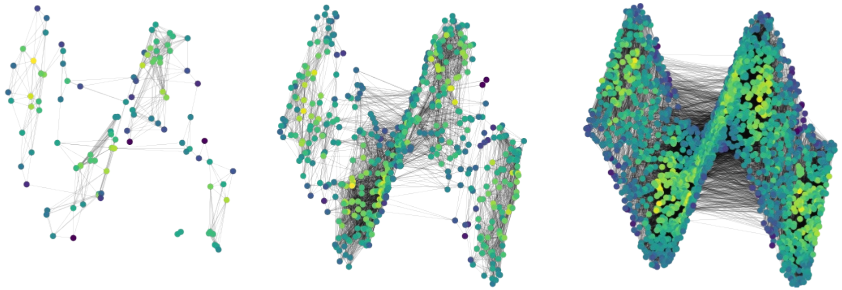

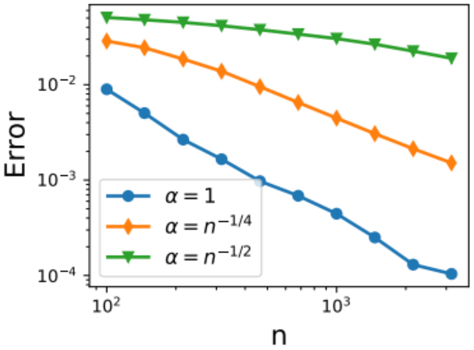


- Thanks to normalized Laplacian, the limit does ***not*** depend on $\alpha_n$ but the rate of convergence does...
- Could have used normalized adjacency $A/(n\alpha_n)$ with operator $\int W(x,y)f(y)dP(y)$

# Outline

1. Convergence of GNNs
2. Stability of c-GNNs
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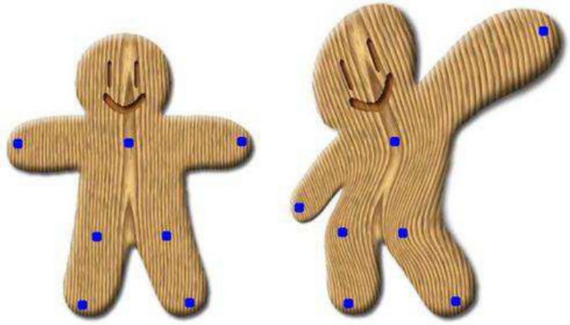
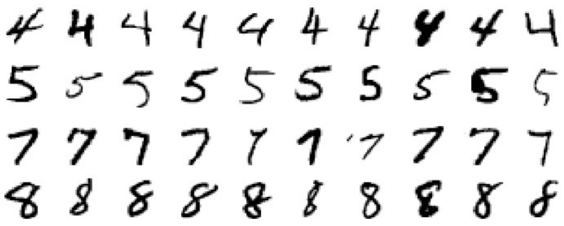
$$\|\Phi(f) - \Phi(f \circ (Id - \tau))\| \leq \|\nabla\tau\|_\infty$$





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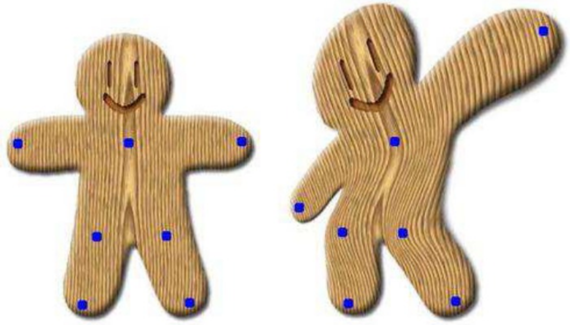

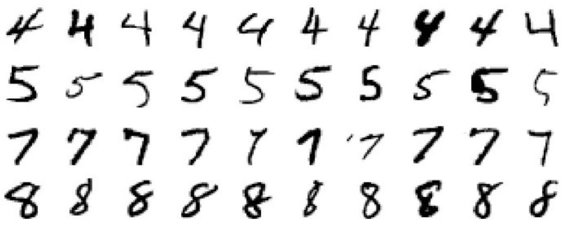


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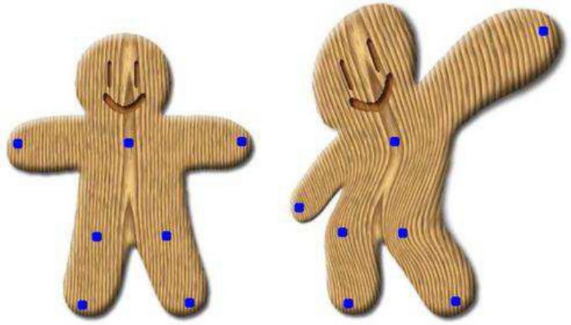

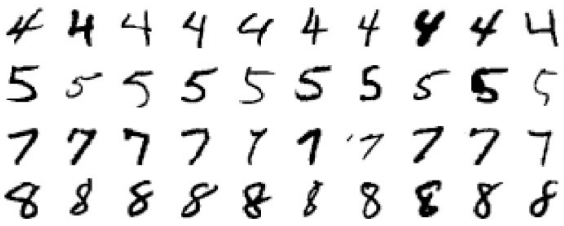

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  - *Difficult to interpret, difficult to define for different-sized graphs*
  - *What's a meaningful notion of deformation for a graph?*

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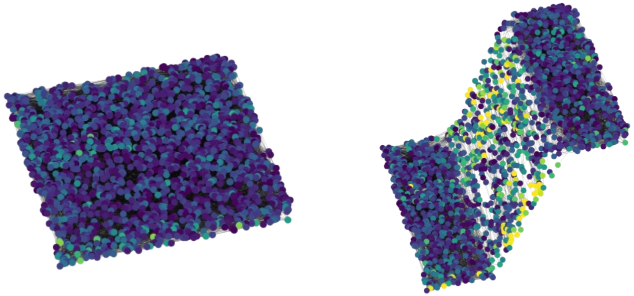

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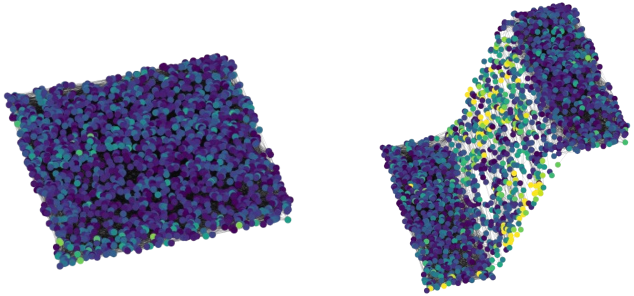

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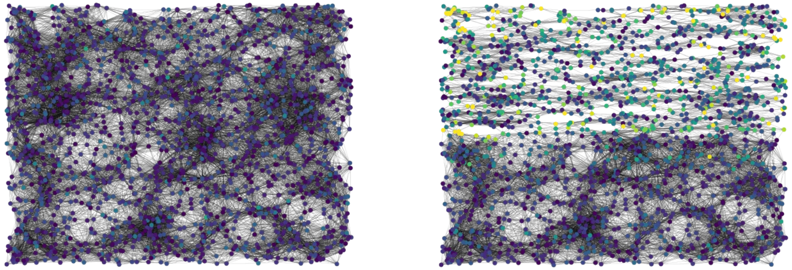

*Deformation of kernel*

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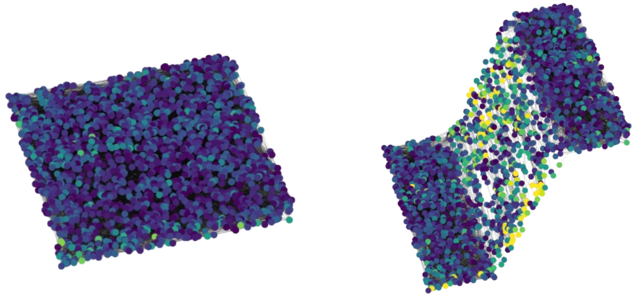

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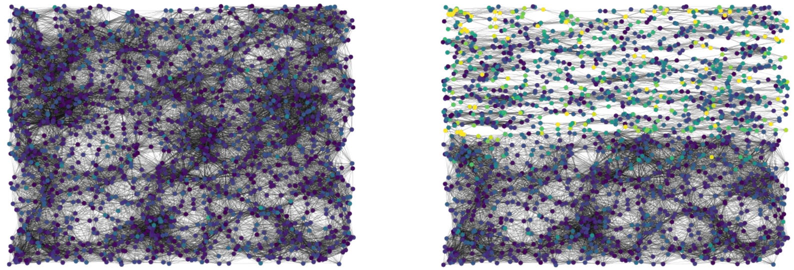


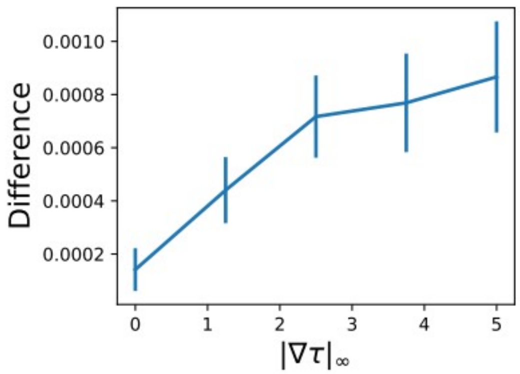
*Deformation of kernel*

**Thm (Stability, simplified)**

For *translation-invariant* kernels, if:

- $W$ is replaced by $W(x - \tau(x), x' - \tau(x'))$
- $P$ is replaced by $(Id - \tau)\sharp P$ (and $f$ is translated)
- $f$ is replaced by $f \circ (Id - \tau)$

Then, the deviation of c-GNN is bounded by $\|\nabla\tau\|_\infty$



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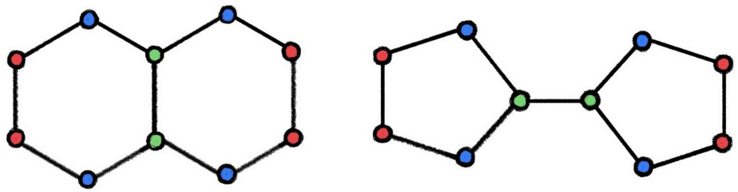

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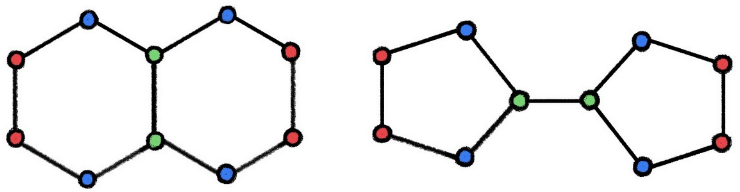

*By construction*, message-passing GNNs are not more powerful than WL test, and can be as powerful if the message-passing function is injective (sufficient number of neurons).

Xu et al. *How Powerful are Graph Neural Networks?* (2019)

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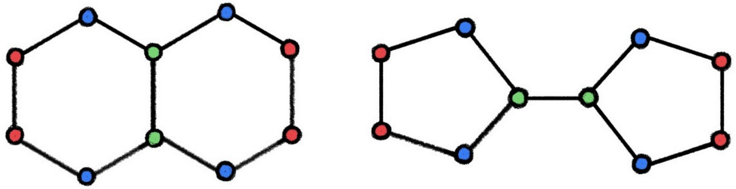

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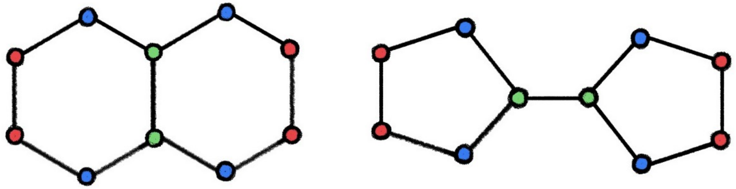

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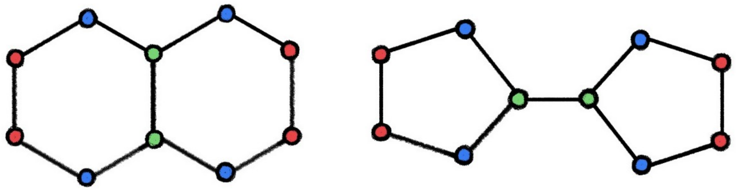

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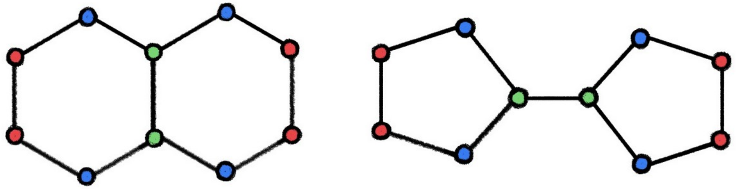

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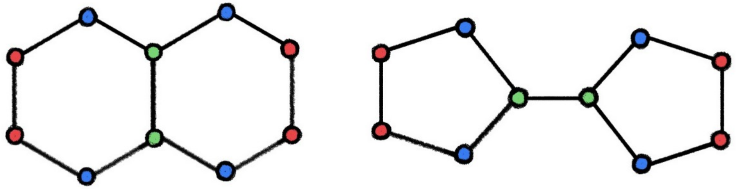

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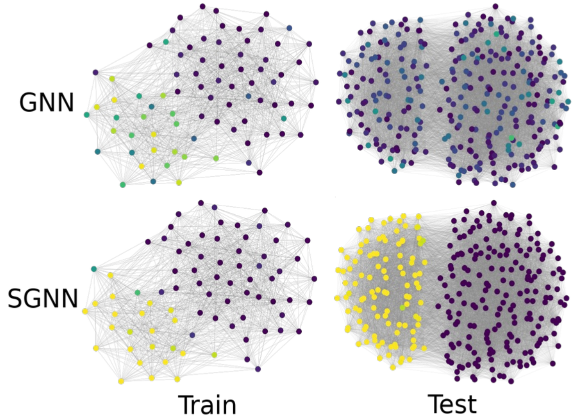

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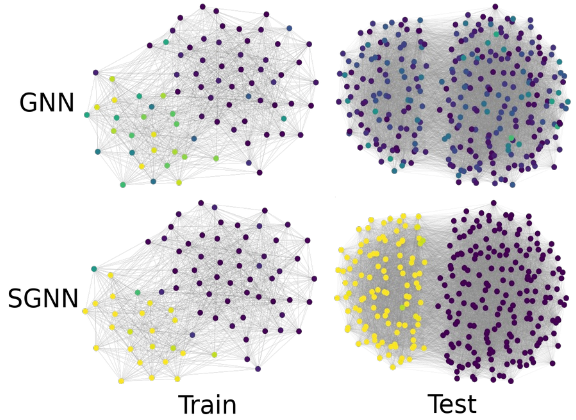

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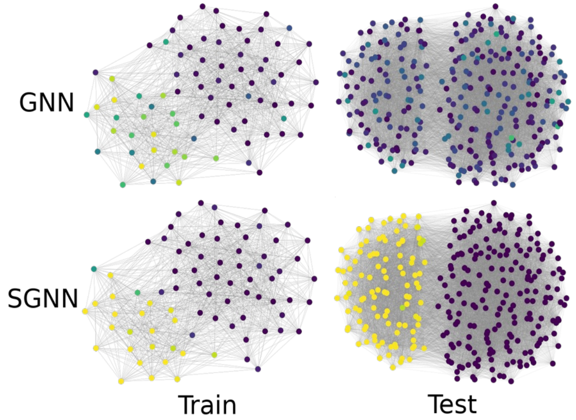

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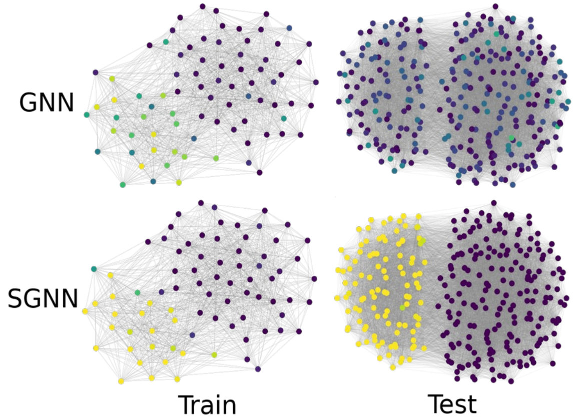

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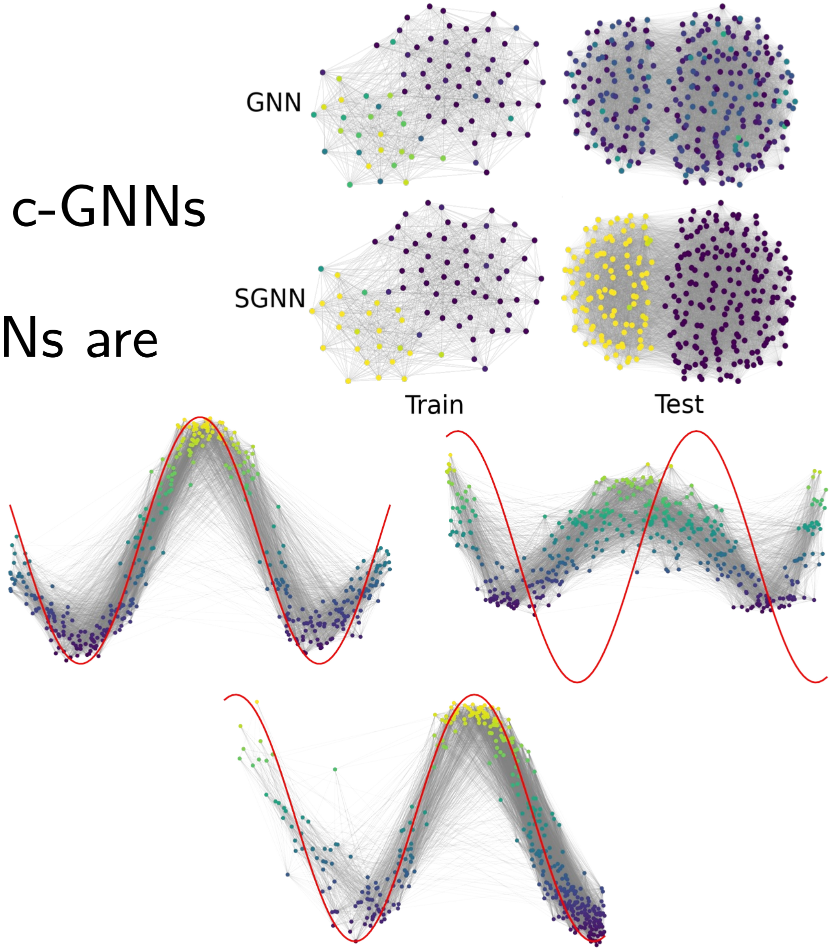
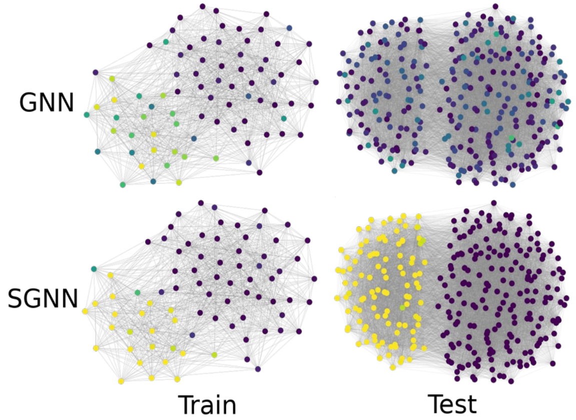
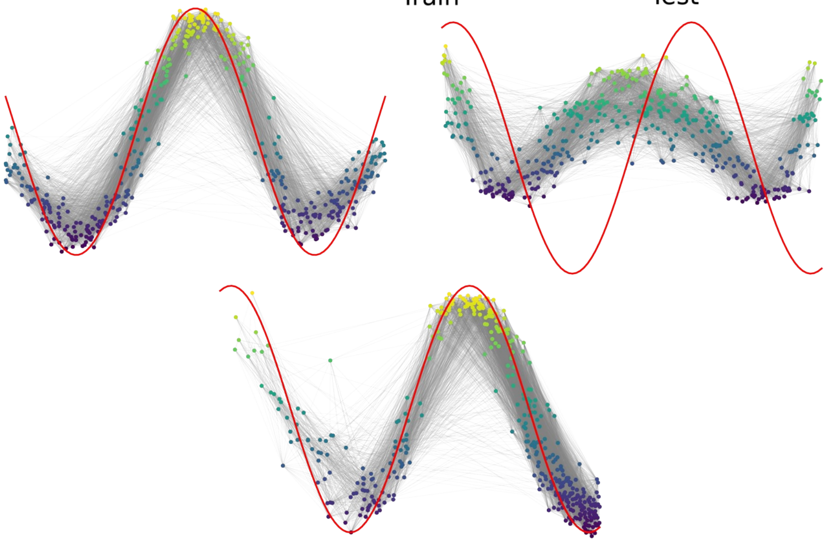


# Continuous SGNN and universality

- Thm. SGNNs converge toward c-SGNN.
- Thm. c-SGNNs are *strictly more powerful* than c-GNNs
- Thm. Using Stone-Weierstrass theorem, c-SGNNs are universal (both permutation-invariant/equivariant):
  - On most SBMs
  - Many "additive" kernels $W(x,y) = w(v(x) + v(y))$
  - 1D radial kernels *(w/ symmetry)* $W(x,y) = w(|x-y|)$
  - Most dot-product kernels... $W(x,y) = w(x^\top y)$



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- Message-passing GNNs, high-order tensors...
- Generalization, optimization...

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Keriven, Bietti, Vaiter. *Convergence and Stability of Graphs Convolutional Networks on Large Random Graphs.* NeurIPS 2020 (Spotlight)

Keriven, Bietti, Vaiter. *On the Universality of Graph Neural Networks on Large Random Graphs.* NeurIPS 2021

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