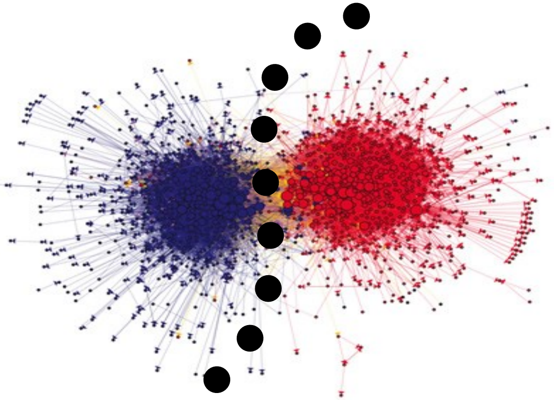
Part III: Dynamics on graphs

Summary of part 2

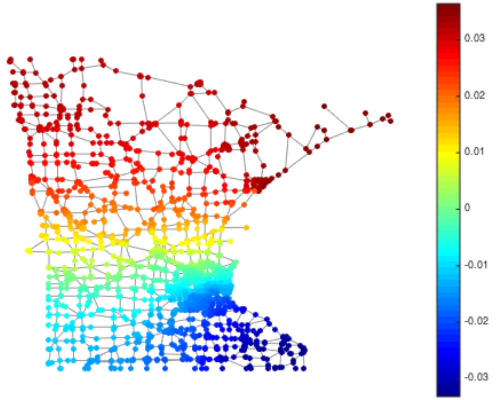
- Signal variations : no gradient but laplacian
- Laplacian eigendecomposition : a way to generalize the Fourier Transform
- Multiplicity of λ=0 : number of connected components
- Fiedler vector separates the graph in 2

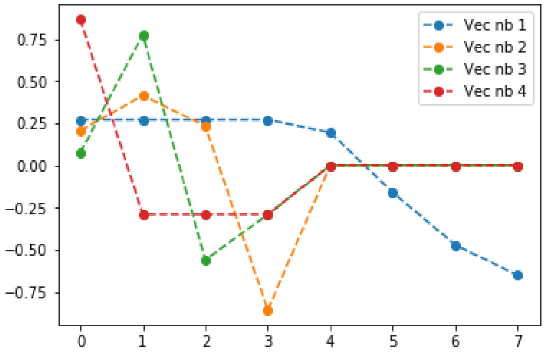


Summary of part 2

Eigenvectors :

- Not oscillating
- But as smooth as possible over the graph
- not always spread over the graph





Connections

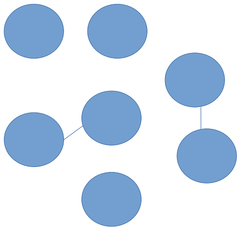
The Graph Laplacian is used in :

- Spectral Graph Theory
- Graph Signal Processing
- Graph Neural Networks and Graph Machine Learning

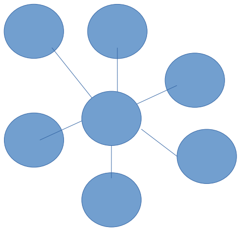
Can insights from one domain help in the other domains?

Pathologic graphs

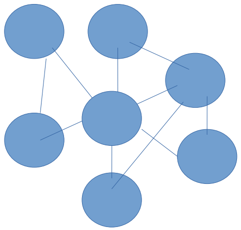
Isolated nodes
Or weakly connected



Hubs



Small world



No neighbor information

Too much neighbor information

- Bad for node classification
- “Irregular” Graph Fourier modes
- Bad for heat diffusion

You should avoid them as much as possible!

Pathologic graphs for learning
Over-smoothing and over-squashing in GNNs

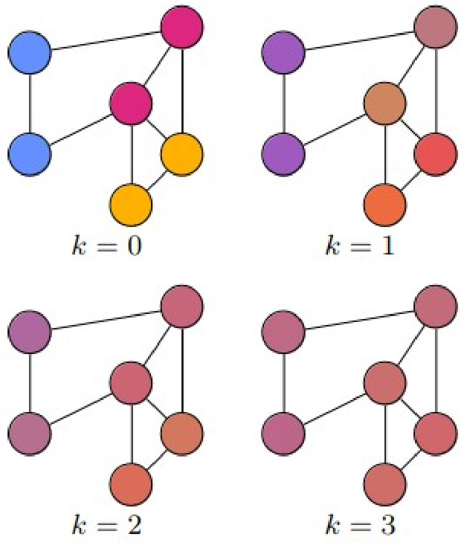


Figure 1. Over-smoothing induced by the averaging operation.

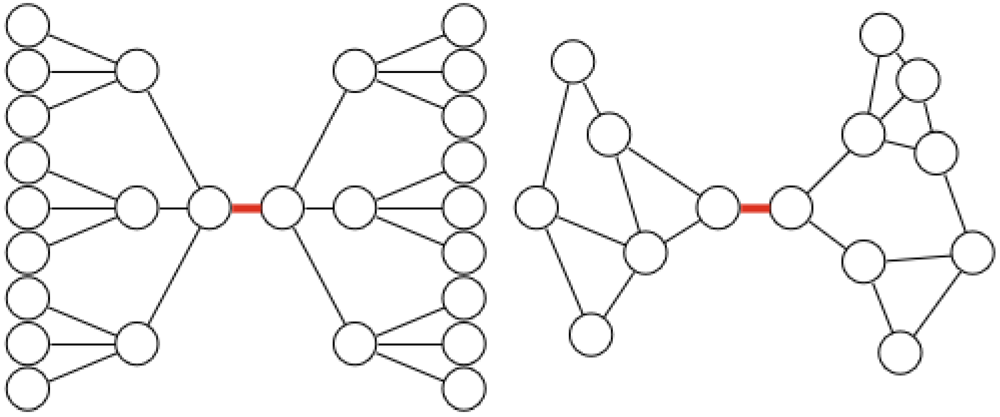


Figure 2. Bottlenecks inhibit the message passing capability of MPNNs. These bottlenecks are highlighted by bold red lines.

Nguyen, Khang, et al. "Revisiting over-smoothing and over-squashing using ollivier-ricci curvature.", PMLR, 2023.

https://proceedings.mlr.press/v202/nguyen23c.html

Heat diffusion on a graph

$$\frac{\partial f}{\partial t} = -\mathcal{L} f$$

Discrete version (without solving the eigenvalue problem):

$$\frac{f(t+\delta t) - f(t)}{\delta t} = -L f(t)$$

$$f(t+\delta t) = f(t) - \delta t \; L f(t)$$

Iterative process

$$f(n) = (1 - \delta t \; L)^n f_0$$

L *: one-hop neighbors* $\quad L^n$ *: n-hop neighbors*

Applying (1-αL) diffuse the node values, α>0

Heat diffusion on a graph

Is there a link with GNNs ?

$$f(n) = (1 - \alpha L)^n f(0)$$

With the normalized Laplacian :

$$1 - L_N = 1 - (1 - D^{-\frac{1}{2}} W D^{-\frac{1}{2}}) = D^{-\frac{1}{2}} W D^{-\frac{1}{2}}$$

Looks like what is used in GNNs !

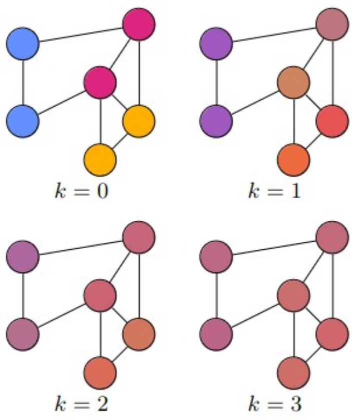


Figure 1. Over-smoothing induced by the averaging operation.

Heat diffusion on a graph

Bonus question : Can we learning heat diffusion on a graph ?

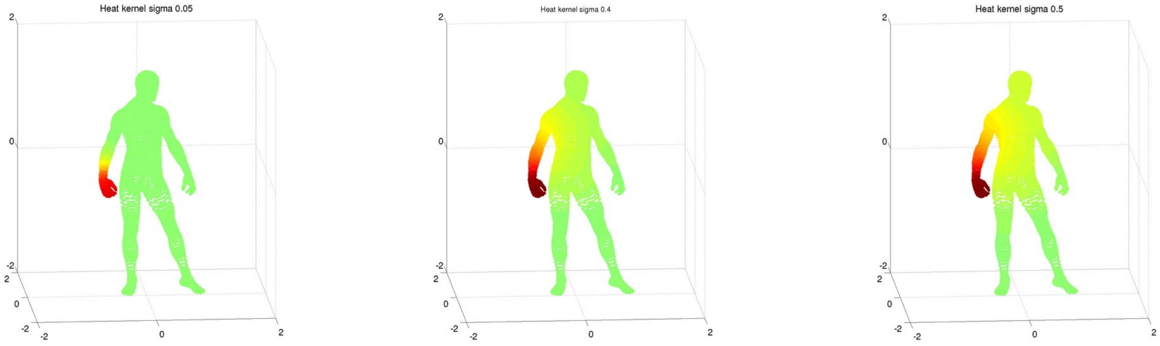
$$f(n) = (1 - \alpha L)^n f(0)$$

Some experiments on the heat diffusion from my student:
https://github.com/axdeux/heat_diff_ex

Break

- Let us compute the heat diffusion on a graph.
- Choose a graph (you may start with a path)
- Choose a initial temperature function on the graph (you may choose a peak on one node)
- Iteratively apply the Laplacian to the function

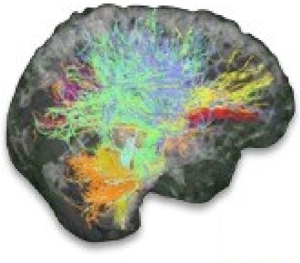
Examples of heat diffusion on graph



Works well on regular manifolds

What about a well connected graph ?

→ *Extremely fast diffusion*



Conclusion

Spectral graph theory, graph signal processing, machine learning on graphs are tightly connected.

- Diffusion, propagation, random walk
- Heat diffusion
- Fourier transform

Wave equation on a graph

For fun, one can define the wave equation on a graph (there is a Laplacian !):

$$\frac{\partial^2}{\partial t^2}u(i,t) = c^2 Lu(i,t) \qquad u(i,0) = u_0(i)$$

$$\frac{\partial^2}{\partial t^2}u(i,t) \to \frac{u(i,t-1) + u(i,t+1) - 2u(i,t)}{\delta t^2}$$

Some potiential interesting directions

- Fourier neural operators / Graph Fourier neural operators
  https://zongyi-li.github.io/neural-operator/

- Solving partial differential equations using graph neural networks
  Graphcast from Deepmind predicts the weather forecast.
  https://www.science.org/stoken/author-tokens/ST-1550/full