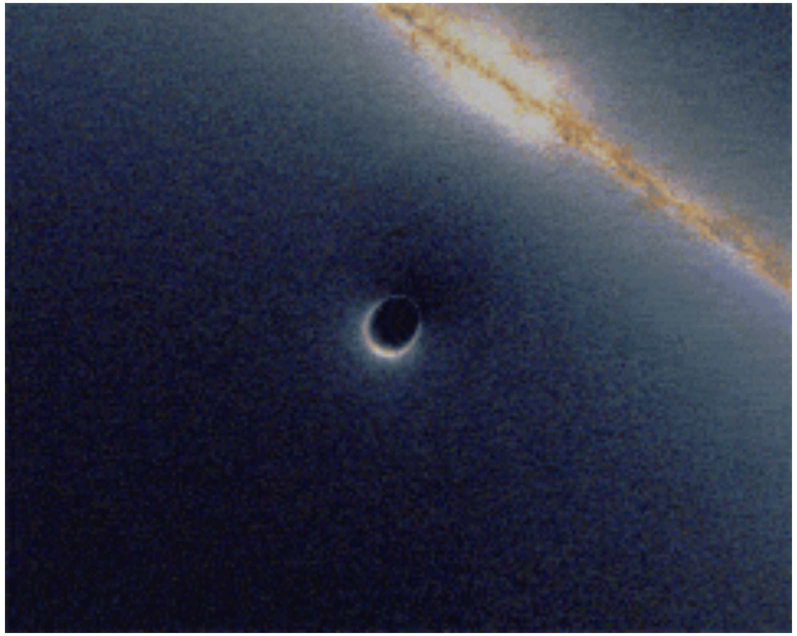
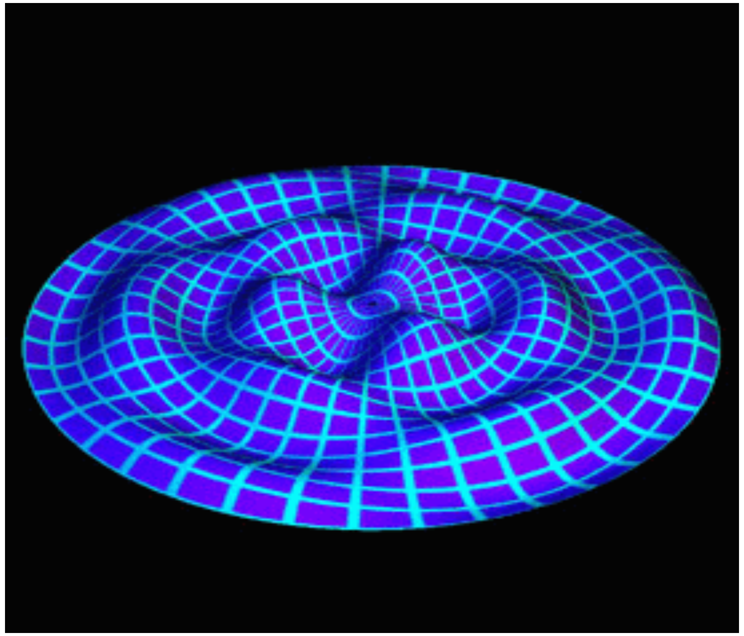
Graphs: Geometry, Operators, Spectra, and Kernels

Mike Slawinski

July 14, 2017





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Solution: Graph Kernels (measure node similarity and graph similarity)

Kernels and Vectorization

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Kernel Trick:

Example: SVM Classifier

$$z \mapsto sgn(w \cdot \varphi(z) + b) = sgn([\sum_{i=1}^{n} c_i y_i k(x_i, z)] + b) \text{ , where } w = \sum_{i=1}^{n} c_i y_i \varphi(x_i)$$

Idea is to compute similarity without actually mapping to a higher dimensional space.

Graph Kernels

Two Types:

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Type II: Measure similarity between graphs based on edge structure, labeling, etc.

Kernel Development: Graph Theoretic Analogues to Smooth Manifolds

Graph Theory	Smooth Manifolds
Functions: $f: Vert(G) \rightarrow \mathbb{R}$	Functions: $f: M \rightarrow \mathbb{R}$
Variable Node Connectivity	Variable Curvature
Laplacian L	Laplacian Δ
PDEs (Heat, Wave)	PDEs (Heat, Wave)

Curvature – Comparing f to its Average

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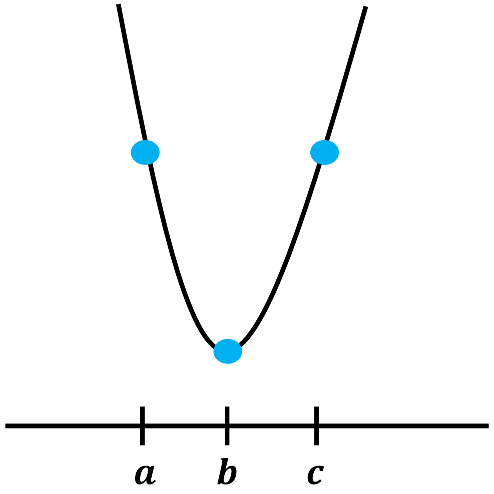

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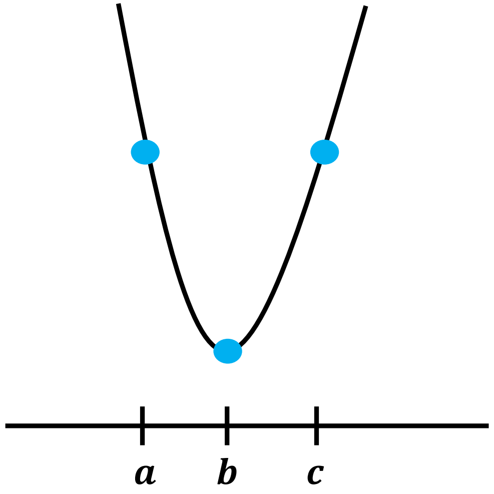

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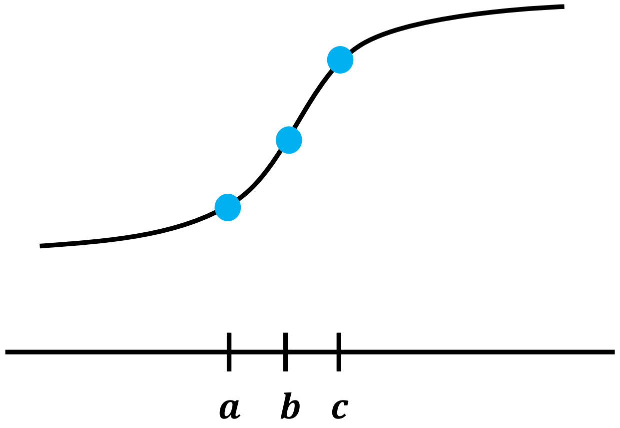
Low Curvature at b



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Key Point

$\Delta f|_{\mathrm{b}}$ measures the extent to which $f(b)$ differs from $avg_x\ f(x)$ for x in a local spherical shell centered at b

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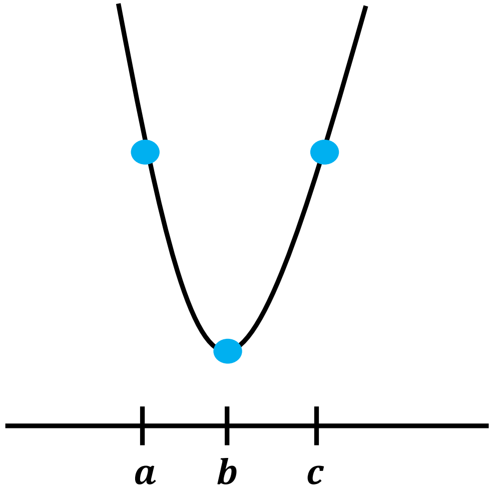

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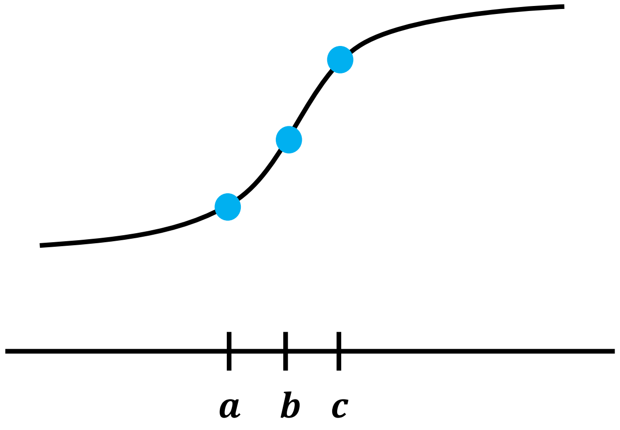

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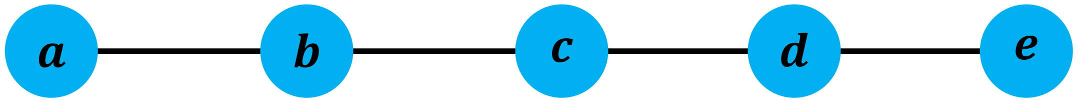

and a function $f : Vert(G) \to \mathbb{R}$ i.e., a vector $\big(f(a), f(b), f(c), f(d), f(e)\big) \in \mathbb{R}^5$

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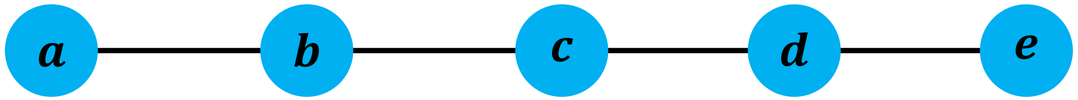
Consider the graph $G =$ 

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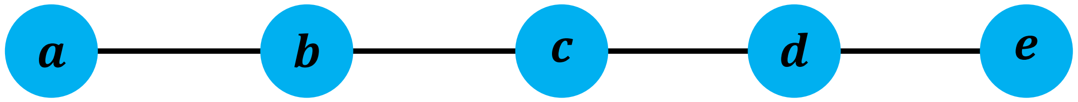

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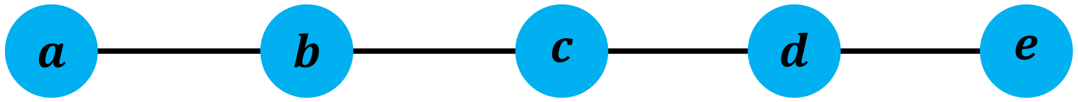

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Question 3: Is it possible to answer Question 2 in the graph case?

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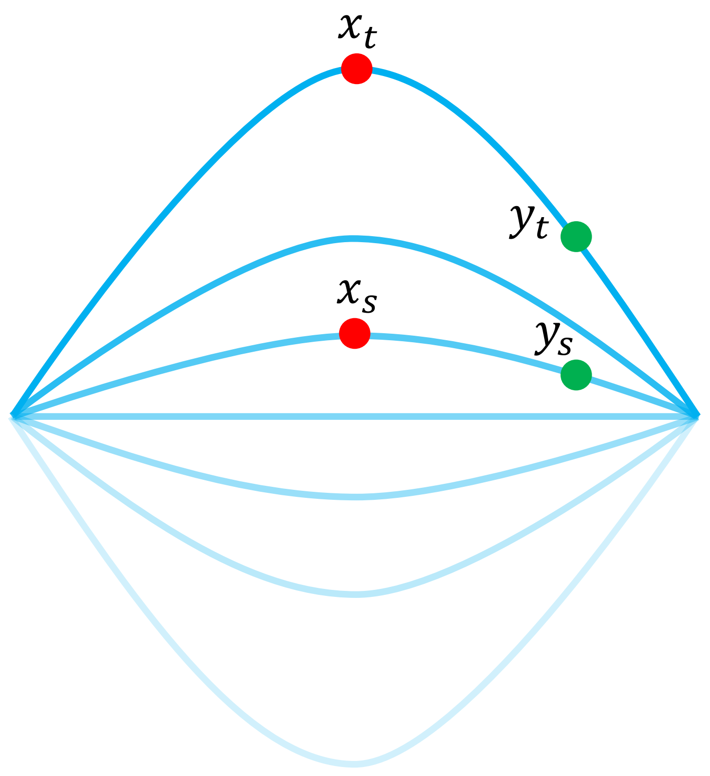

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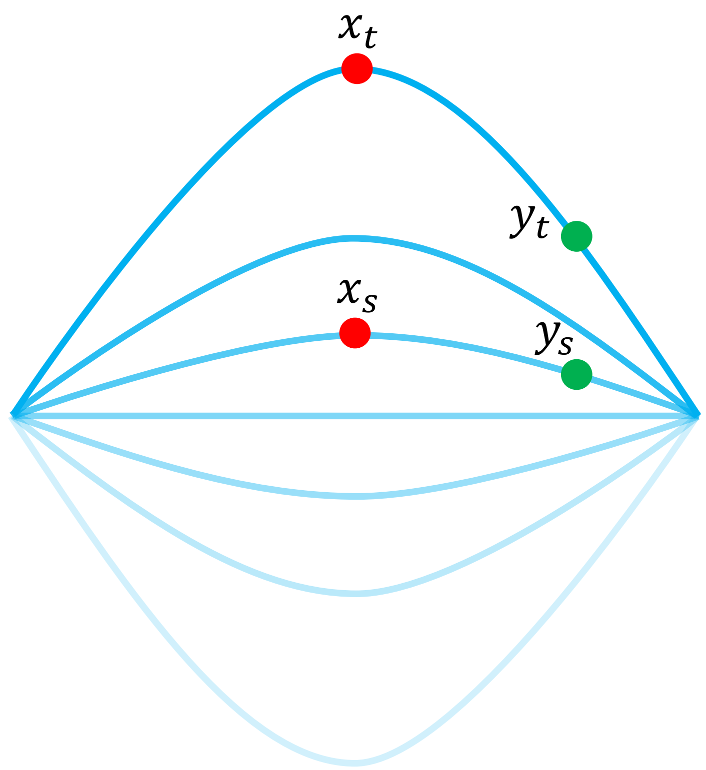

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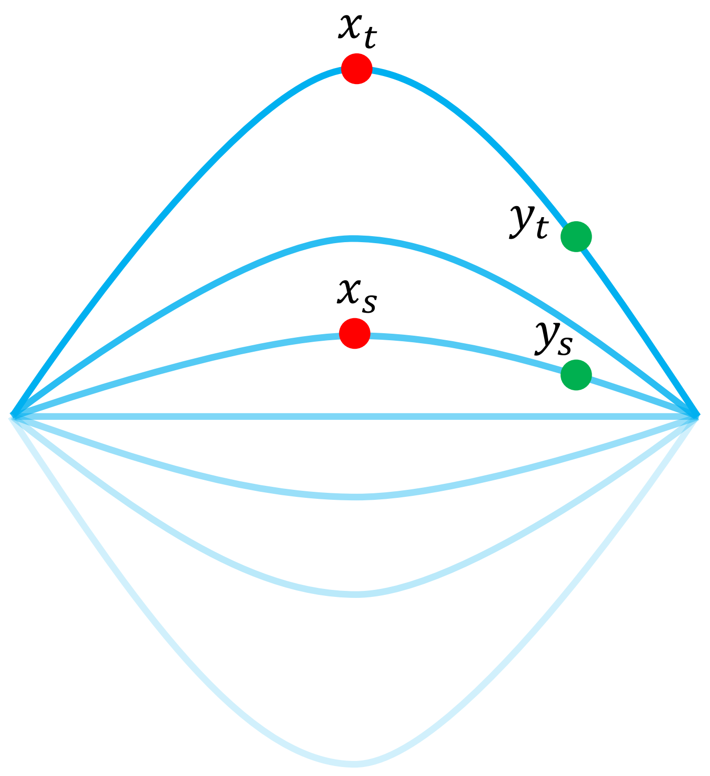

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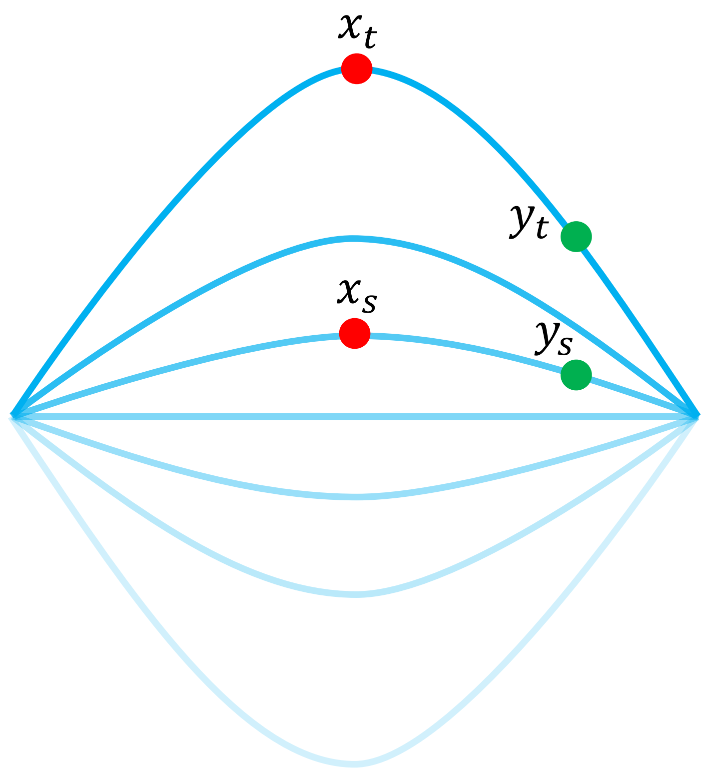

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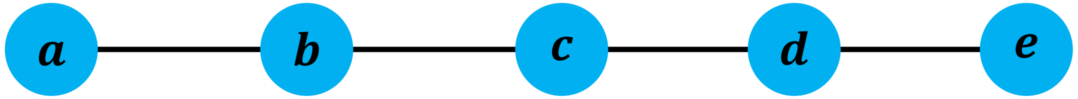
$G =$ 

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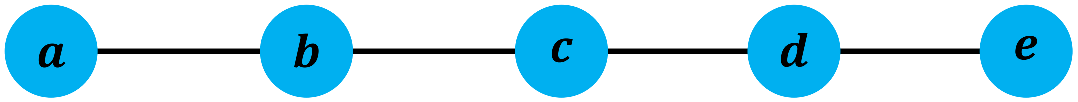
$G =$ 

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$$L = \begin{pmatrix} 1 & -1 & 0 & 0 & 0 \\ -1 & 2 & -1 & 0 & 0 \\ 0 & -1 & 2 & -1 & 0 \\ 0 & 0 & -1 & 2 & -1 \\ 0 & 0 & 0 & -1 & 1 \end{pmatrix}$$

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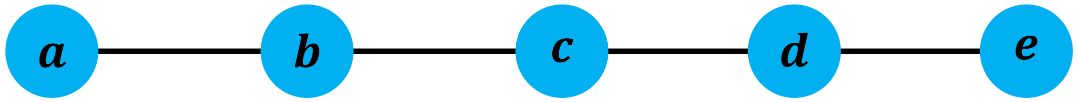
$G =$ 

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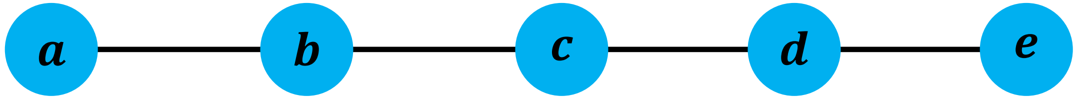

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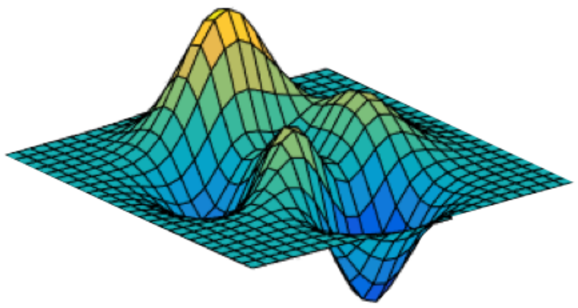
What if the structure of G varies from node to node?

Laplacian on Curved Manifolds

Consider a function $f: M \to \mathbb{R}$, on a manifold M, the structure of which varies from point to point



How should we define a notion of the Laplacian ∇_M when M has interesting structure?

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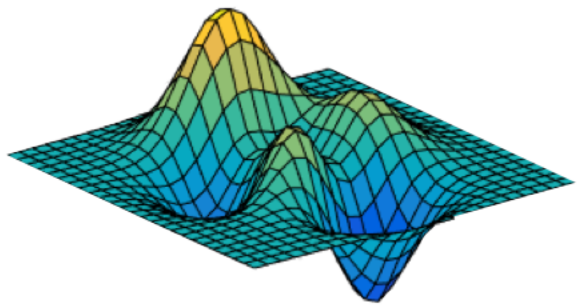
$$g_p = (g^{ij})$$



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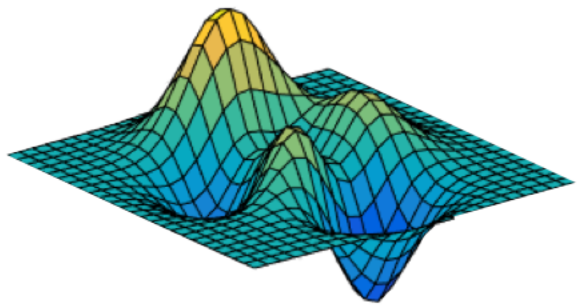

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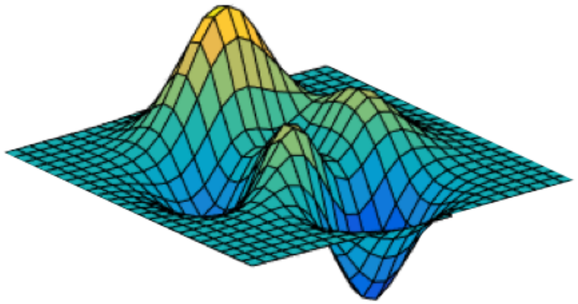

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The non constant structure of the underlying manifold, the domain of $\boldsymbol{f} : \boldsymbol{M} \to \mathbb{R}$, is reflected in the operator $\boldsymbol{\Delta_{\mathrm{M}}}$.

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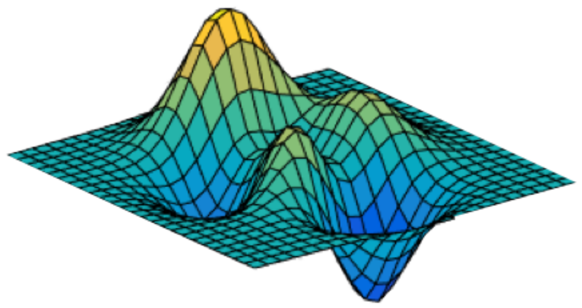
$$g_p\colon T_pM \times T_pM \to \mathbb{R}$$

$$(X(p), Y(p)) \mapsto g_p\big(X(p), Y(p)\big)$$

$$g_p = (g^{ij})$$



Laplacian:

$$\Delta_M f \coloneqq \frac{1}{\sqrt{|g|}} \partial_i(\sqrt{|g|} g^{ij} \partial_j f)$$

The non constant structure of the underlying manifold, the domain of $f\colon M \to \mathbb{R}$, is reflected in the operator Δ_{M}.

Euclidian Space Case:

$$g^{ij} = \delta_{ij}, \quad g = \begin{pmatrix} 1 & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & 1 \end{pmatrix}$$

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Laplacian on Curved Manifolds

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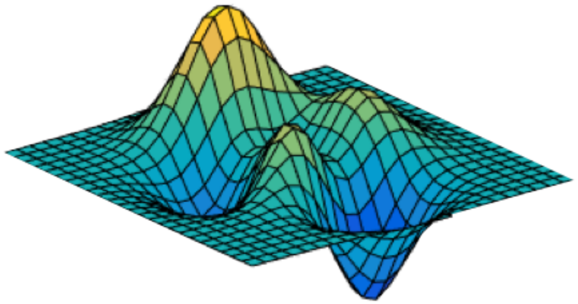

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The non constant structure of the underlying manifold, the domain of $f: M \to \mathbb{R}$, is reflected in the operator Δ_M.

The same is true in the graph case – the structure of the underlying graph, the domain of $f: G \to \mathbb{R}$, is reflected in the operator L.

Laplacian on Nonlinear Graphs

General Definition

$$L_{ij} = \begin{cases} \deg(v_i)\,, & if \;\; i = j \\ -1, & if \; v_i \sim v_j \\ 0, & otherwise \end{cases}$$

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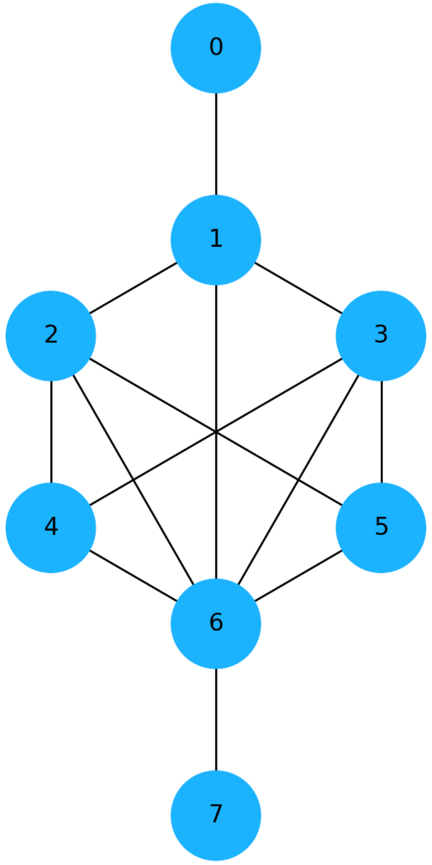

$$L$$

$$\begin{matrix} 1 & -1 & 0 & 0 & 0 & 0 & 0 & 0 \\ -1 & 4 & -1 & -1 & 0 & 0 & -1 & 0 \\ 0 & -1 & 4 & 0 & -1 & -1 & -1 & 0 \\ 0 & -1 & 0 & 4 & -1 & -1 & -1 & 0 \\ 0 & 0 & -1 & -1 & 3 & 0 & -1 & 0 \\ 0 & 0 & -1 & -1 & 0 & 3 & -1 & 0 \\ 0 & -1 & -1 & -1 & -1 & -1 & 6 & -1 \\ 0 & 0 & 0 & 0 & 0 & 0 & -1 & 1 \end{matrix}$$

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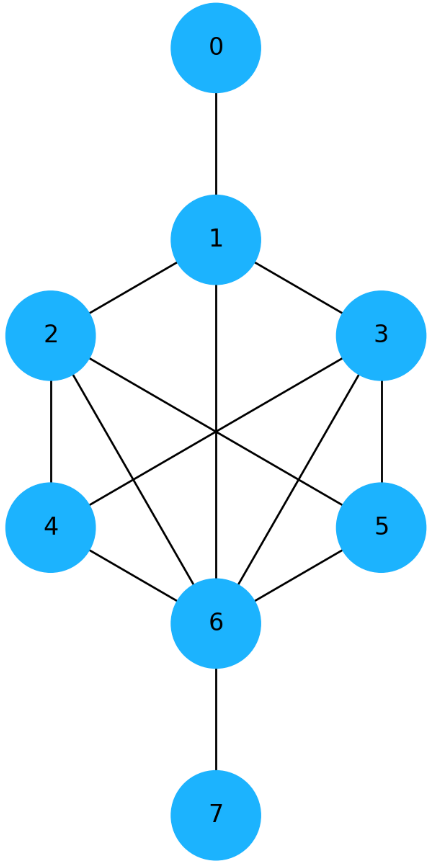

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The structure of the graph changes from node to node, and is reflected in the non-constant block diagonal structure of L.

Wave Equation on Graphs

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We can exploit the correspondence between frequency and wavelength to visualize graph spectra:

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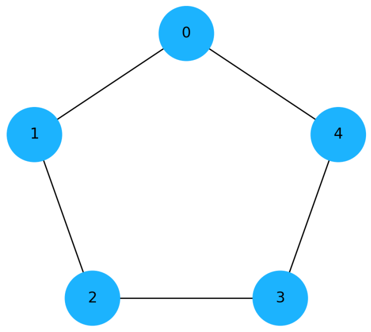

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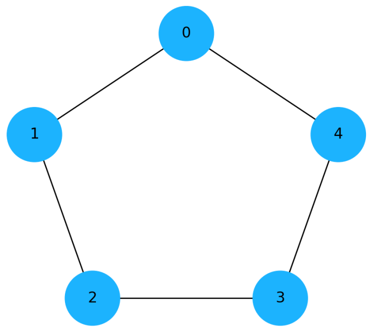

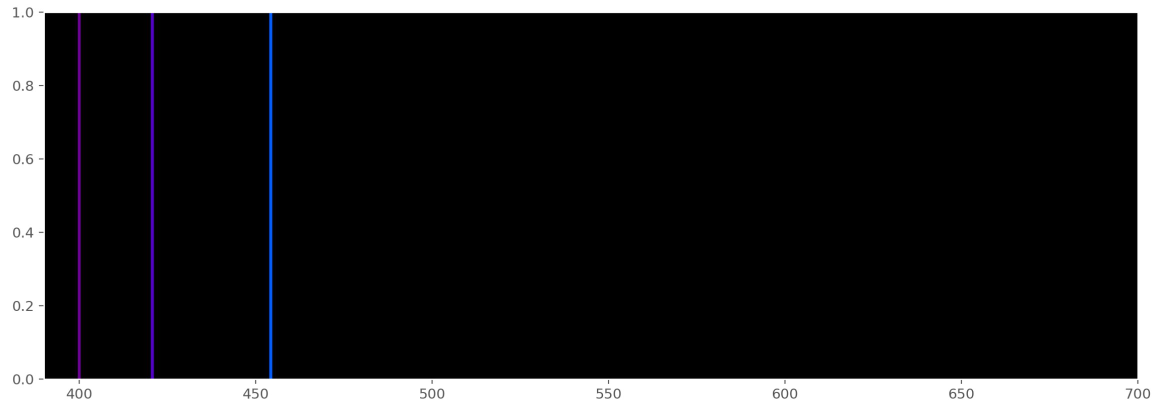

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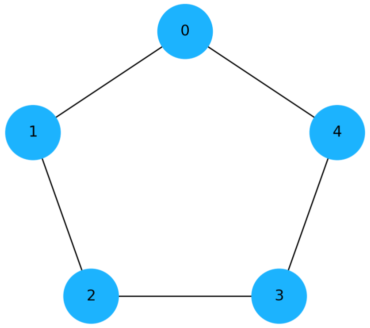

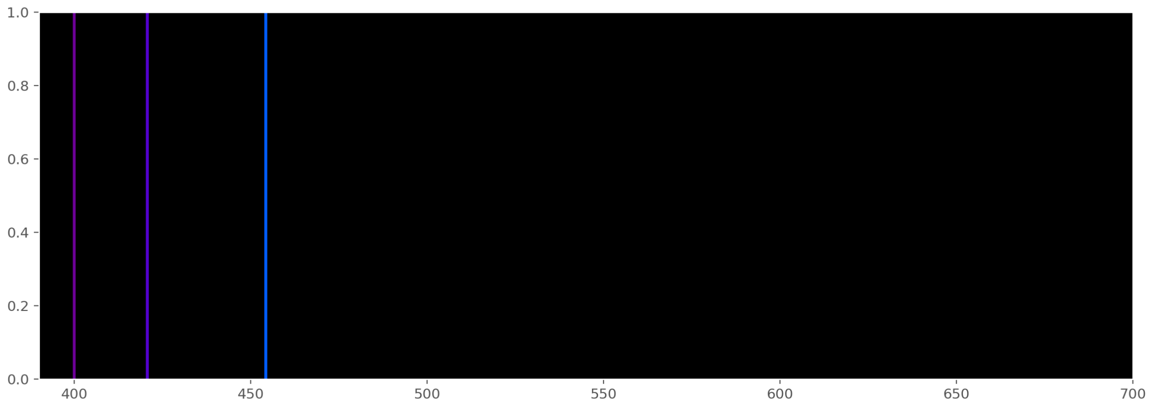

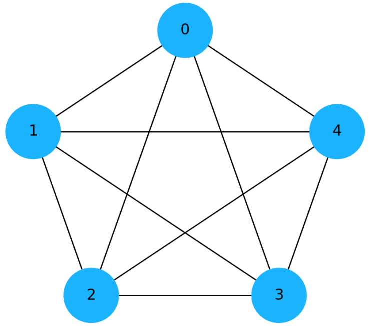

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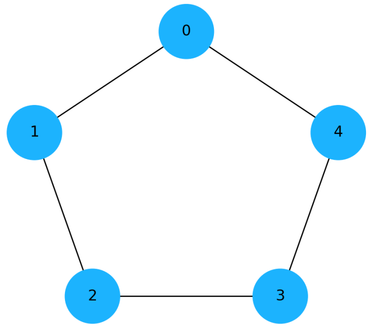

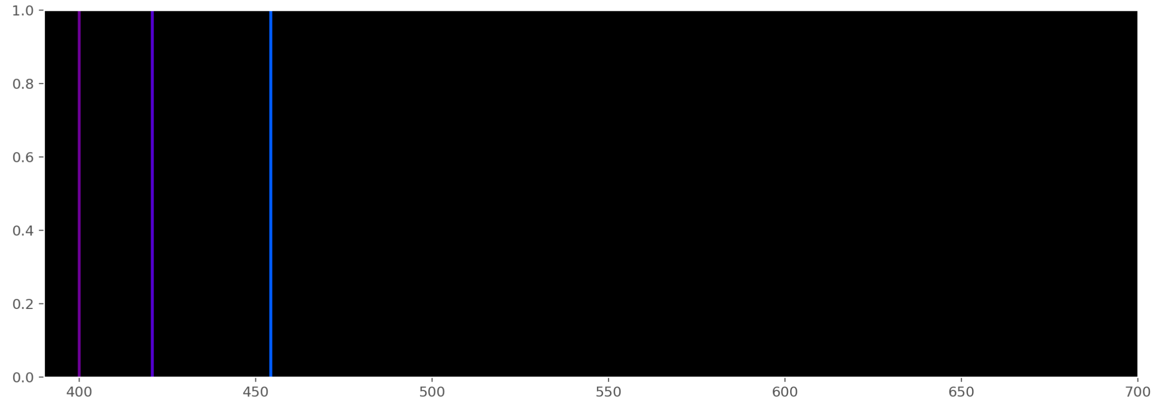

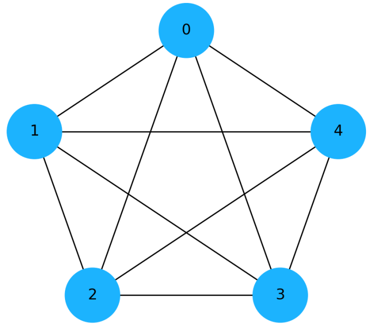

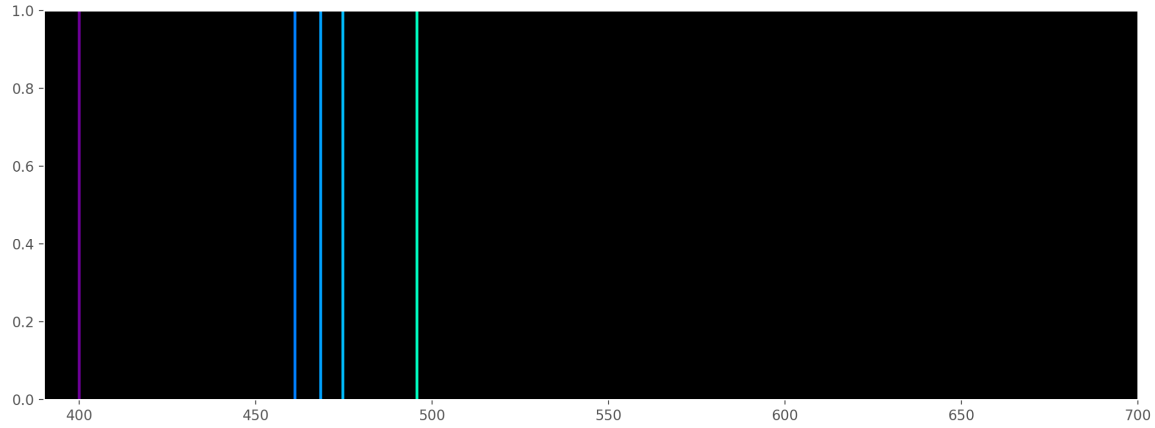

Curvature – Higher Dimensions

The Laplacian

Define $\Delta = \frac{\partial^2}{\partial x_1^2} + \frac{\partial^2}{\partial x_2^2} + \cdots + \frac{\partial^2}{\partial x_n^2}$

Application: The **Heat** Equation

$$\frac{\partial u}{\partial t} = \Delta u$$

Question 1: What do the solutions to this PDE look like?

Question 2: Is it possible to infer manifold structure from the structure of the operator?

Question 3: Is it possible to answer Question 2 in the graph case?

Heat Kernels on Graphs

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We can therefore describe $Z(t)$ for $t \in \mathbb{N}$ as

$$Z(t) = T(t)Z(0)$$

where $T(t) = (1 - \alpha L)^t$ for L the Laplacian.

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Notice K_β satisfies $\frac{d}{d\beta} K_\beta = L K_\beta$. This is precisely the heat equation on G.

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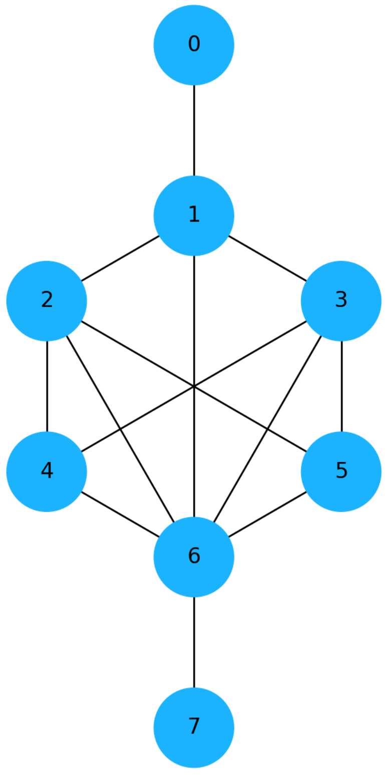

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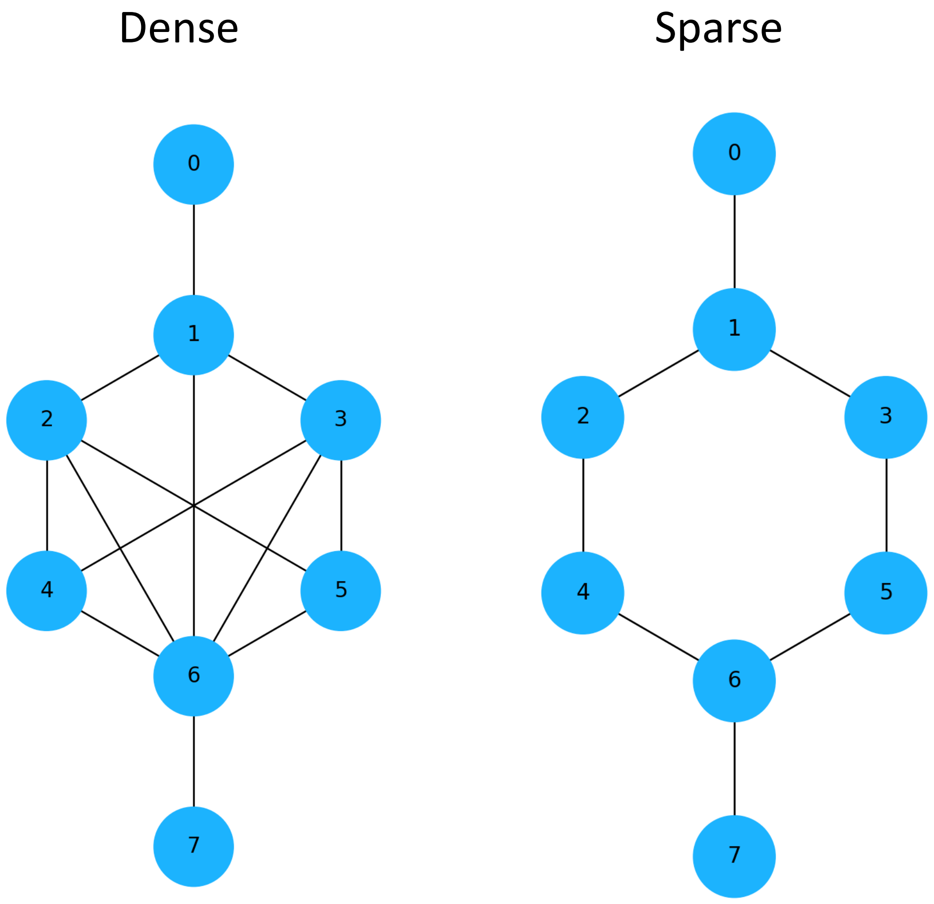

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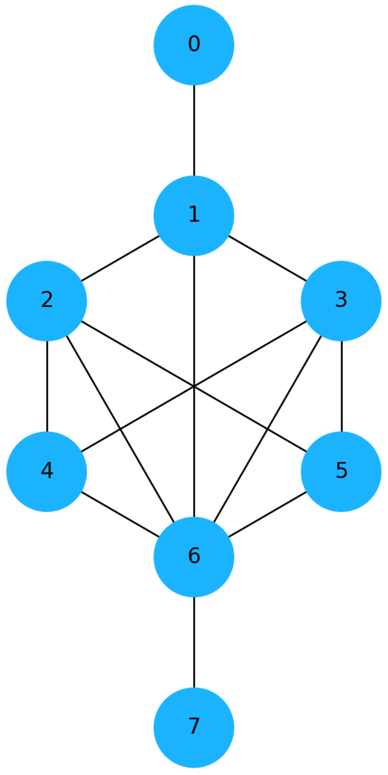
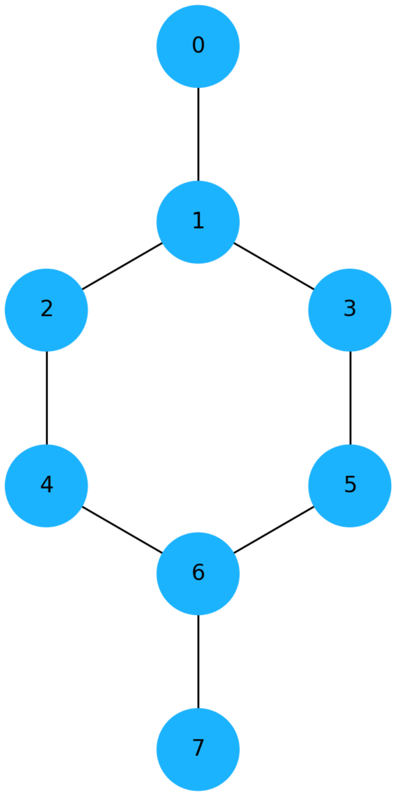


Sparse



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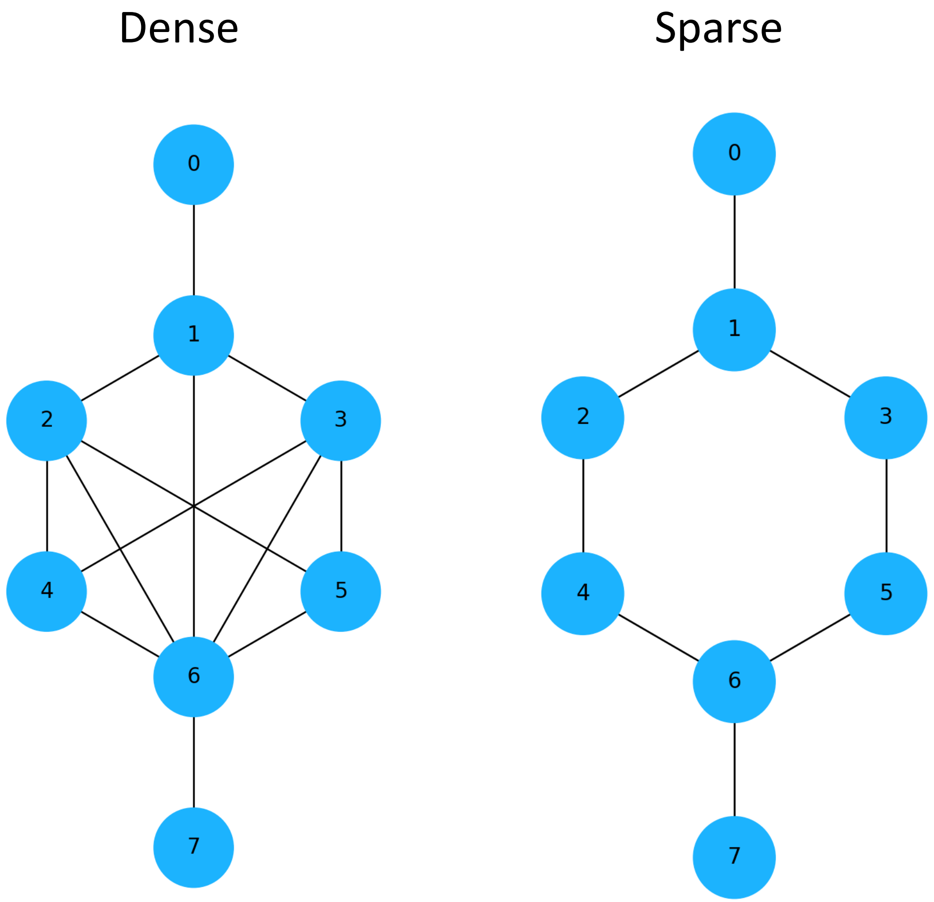

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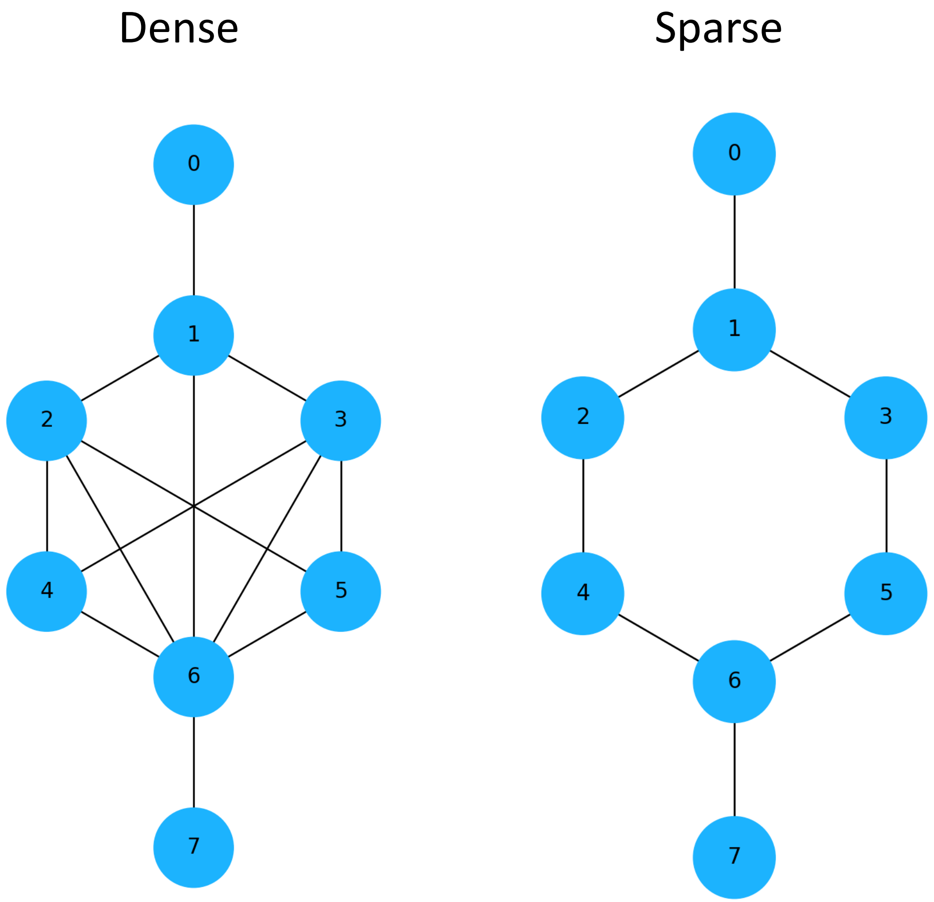
Step 3: Compute node similarity based on node to node heat transfer between times 0 and ∞



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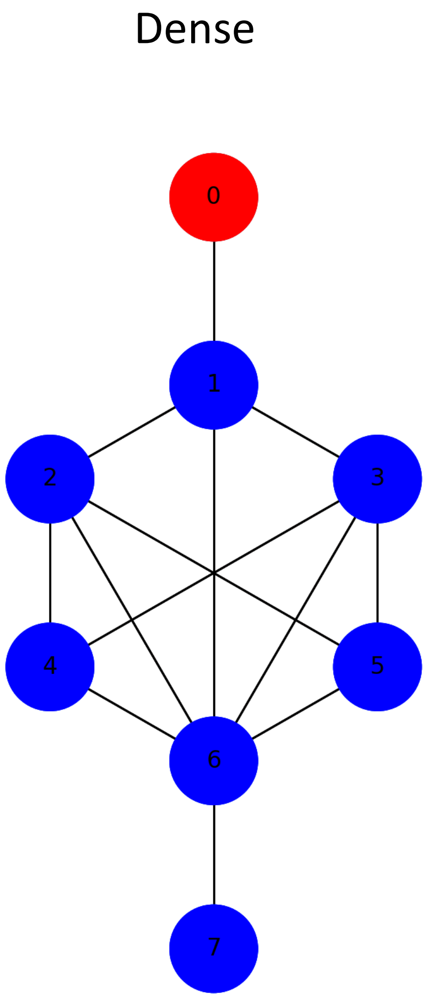

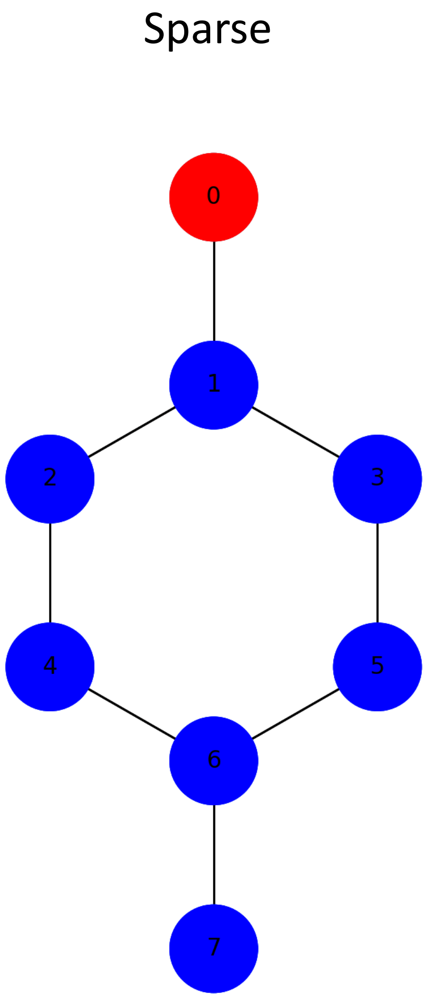

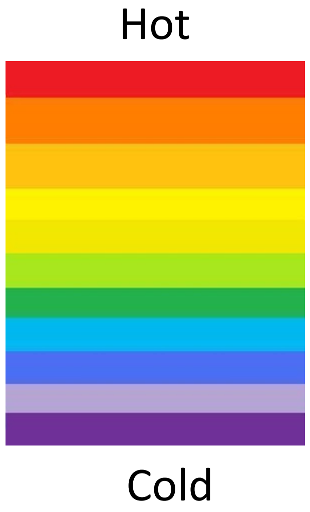

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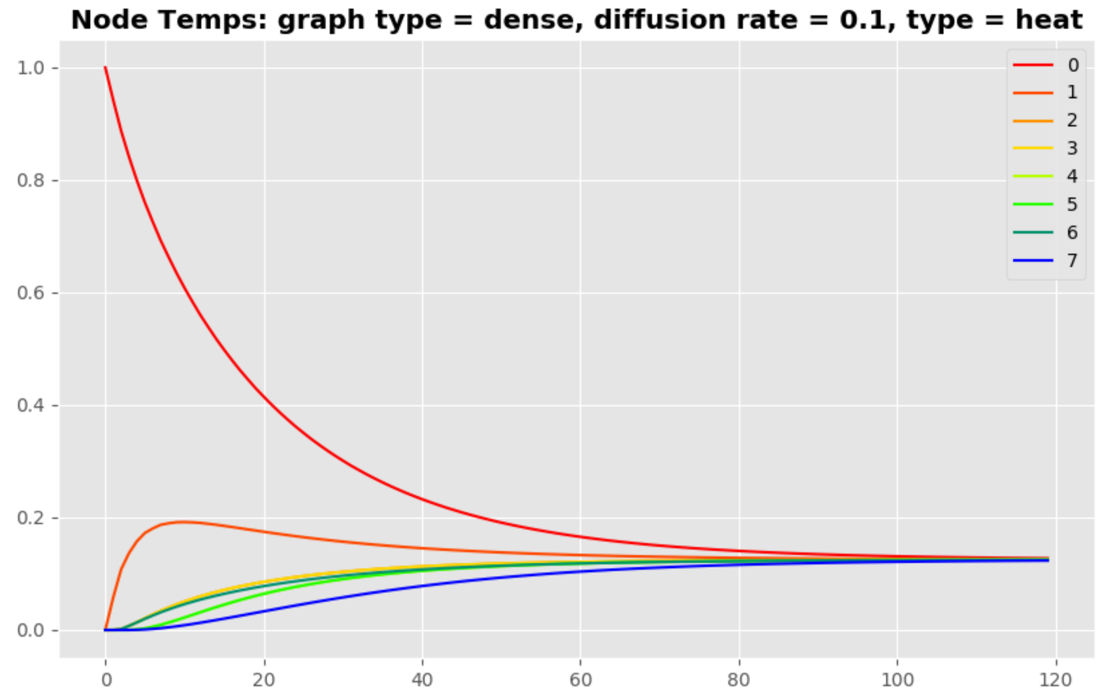
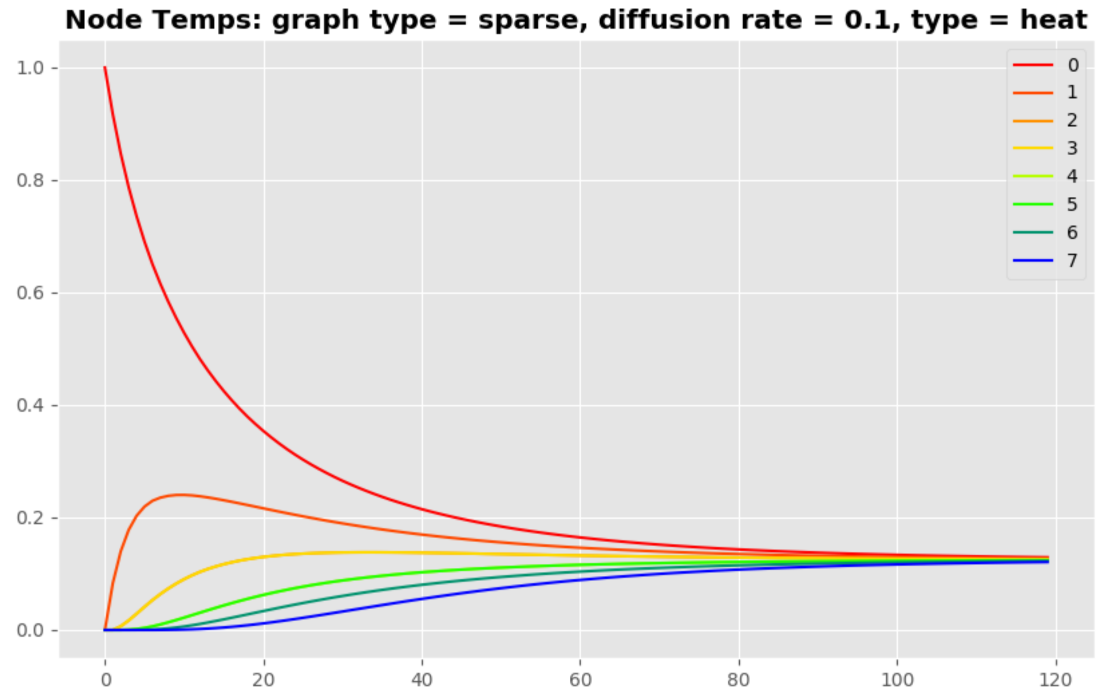
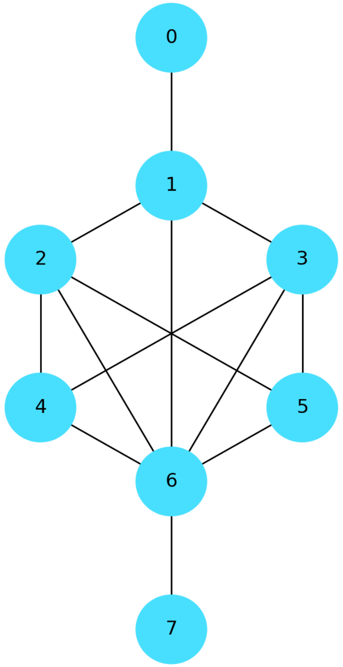


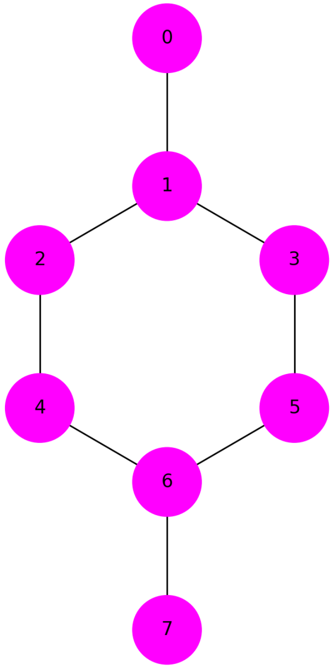
Sparse

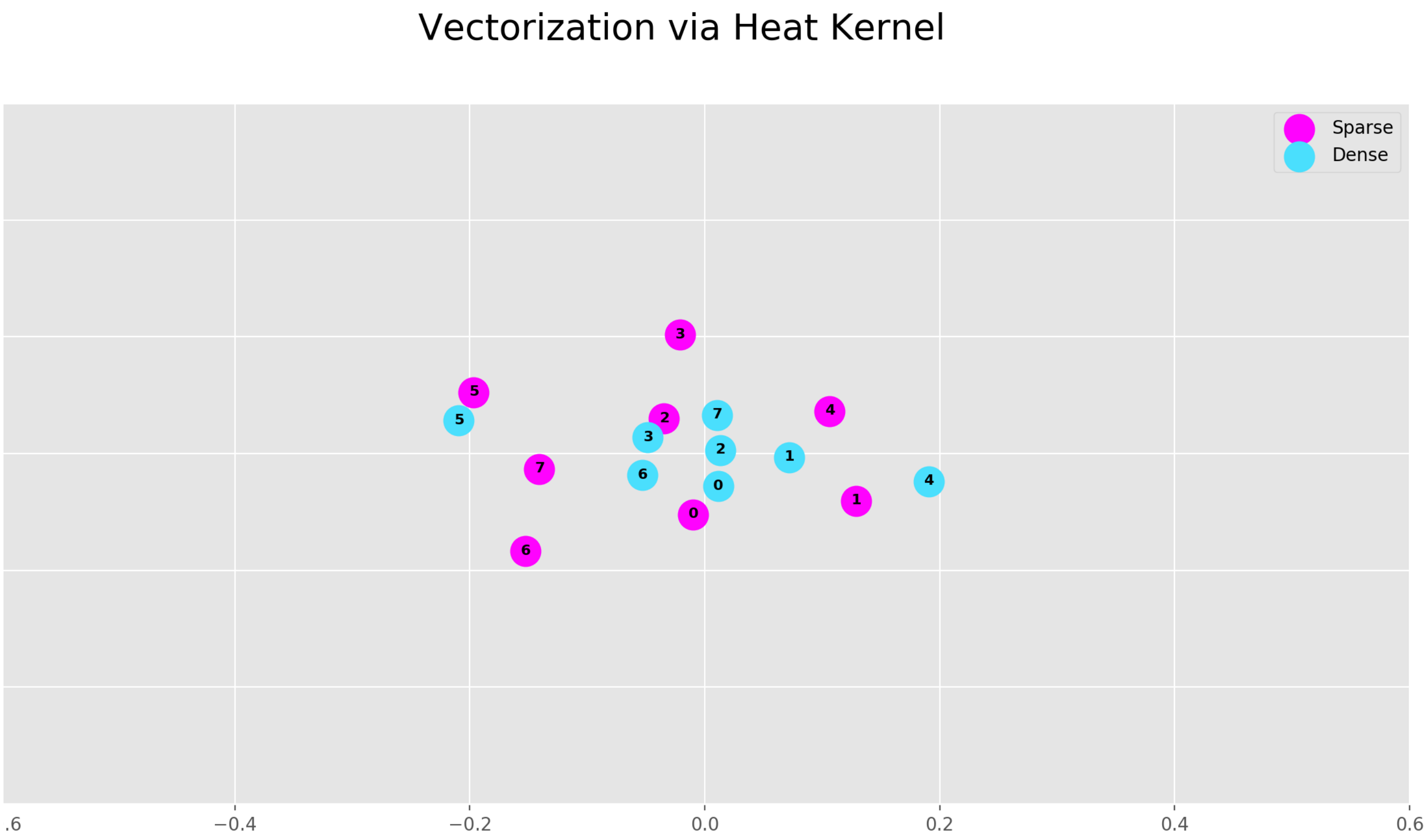


Heat Kernels - Vectorization

Vectorize each graph via Cholesky factorization of $K_\beta = F^T F$. Vectors correspond to columns of F.







Transfer Kernels

Once we have intuition, we can build our own kernels via perturbations of known kernels.

Alter process by considering a directed graph version of the above example, and only allow heat transfer along directed edges.

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Original heat kernel process: Undirected graph G with $V \coloneqq Vert(G)$.

$$Z(t) = \left(Z_1(t), Z_2(t), \dots, Z_{|V|}(t)\right)^T, \text{ where}$$

$$Z_i(t+1) = Z_i(t) + \alpha \sum_{j \in V : j \sim i} \left(Z_j(t) - Z_i(t)\right)$$

$$Z(t) = T(t)Z(0)$$

where $T(t) = (1 - \alpha L)^t$ for L the Laplacian.

Note that $L = D - A$,

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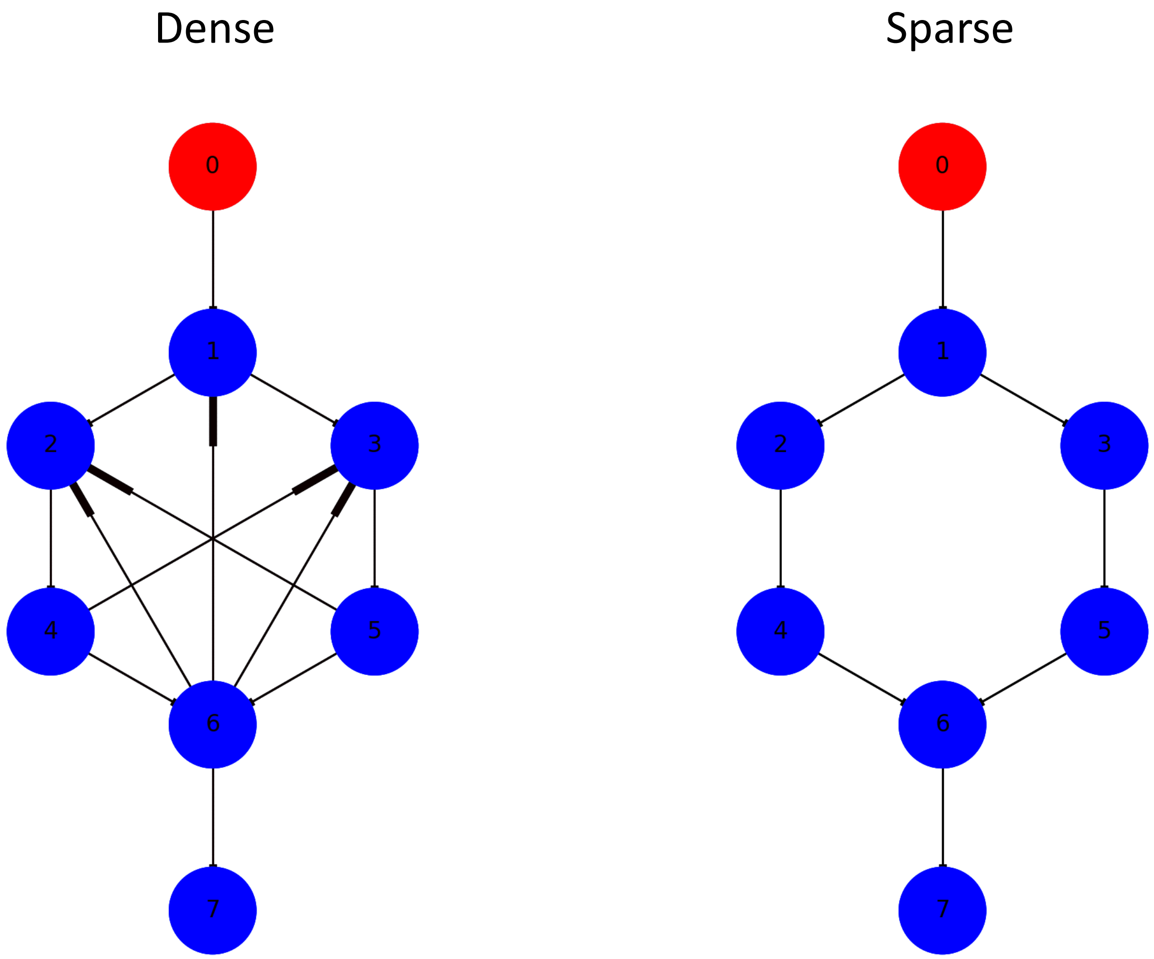
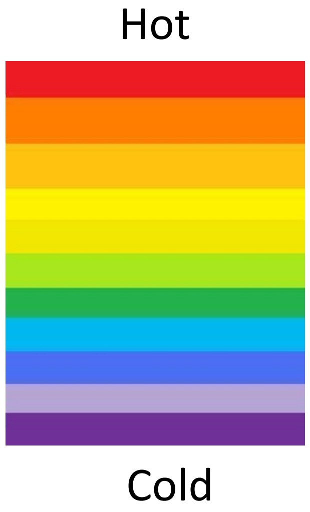
Note that $L_O = D_{out} - A$,

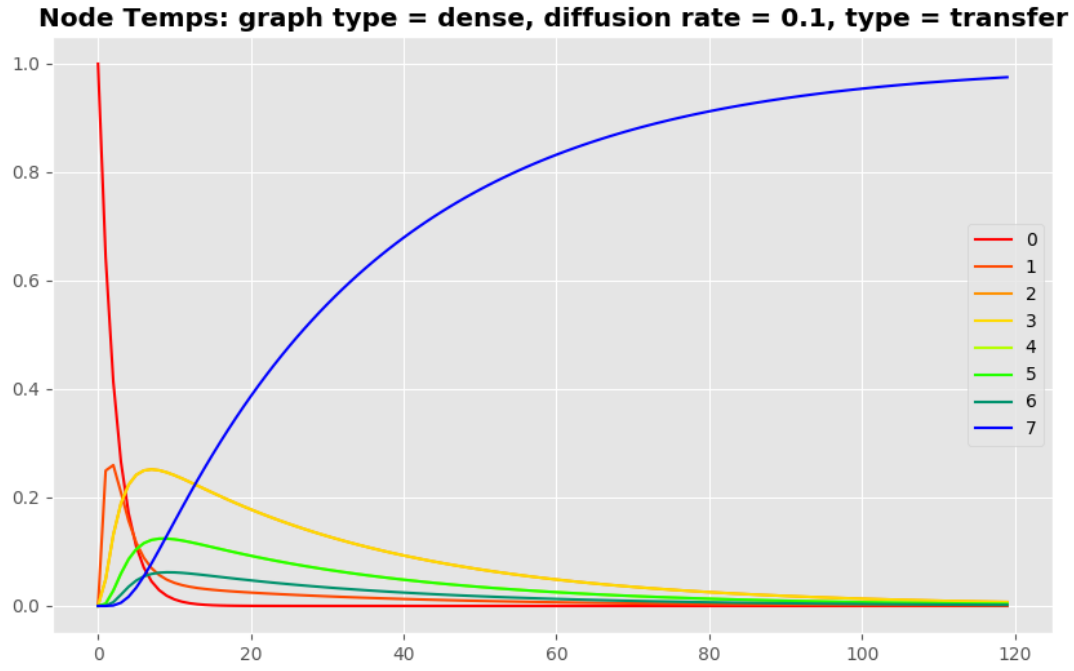
Transfer (Dense vs Sparse)



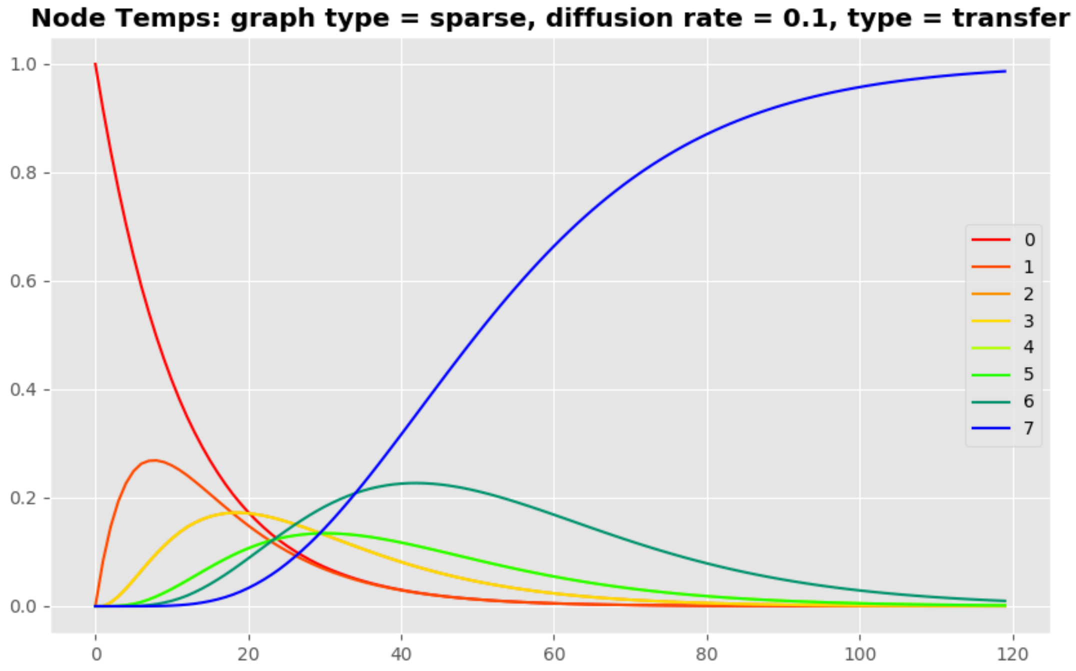


Transfer (Dense and Sparse)

Dense



Sparse



Heat Kernels - Applications

Assume we have a kernel K defined on some set Ω, that is, we have a map $K: \Omega \times \Omega \to \mathbb{R}$

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Answer: Construct the tensor product $K^n \coloneqq \bigotimes_{i=1}^n K$ defined by $K^n(x, x') = \prod_{i=1}^n K(x_i, x_i')$

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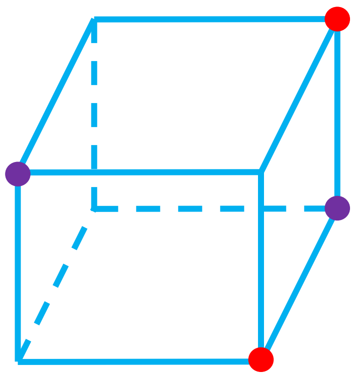
Example: Construct kernel on binary strings via the construction of a graph kernel on the hypercube



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Idea is to measure similarity between points $(0,0,1)$ and $(1,1,0)$, and between points $(1,0,0)$ and $(1,1,1)$, while taking into account the graph structure.

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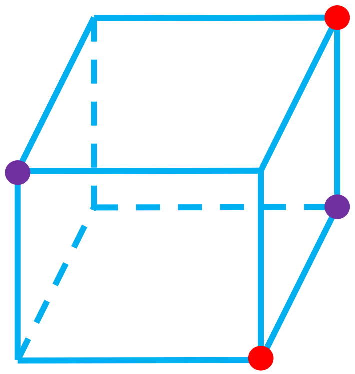

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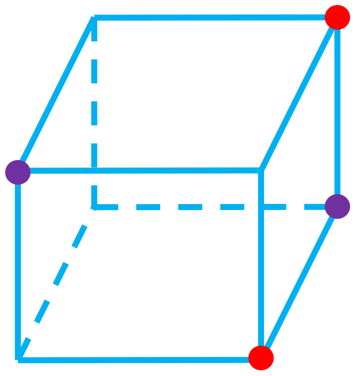

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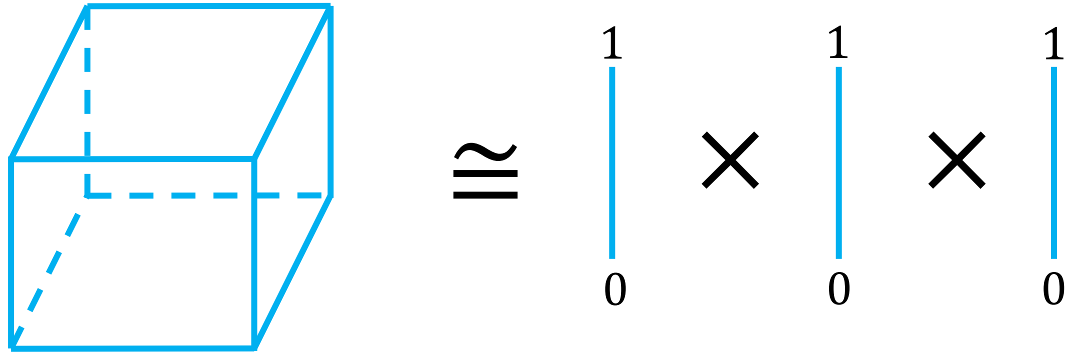
The hypercube can be constructed by successive cross products of simpler graphs.

$L_{ij} = -1 + \delta_{ij} n$ for an unweighted complete graph.



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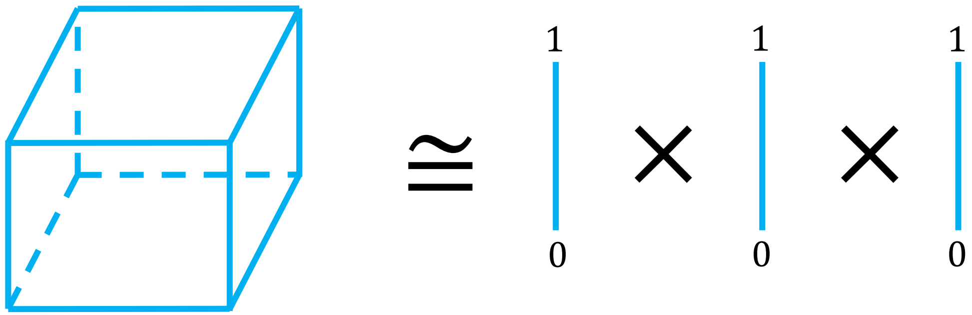

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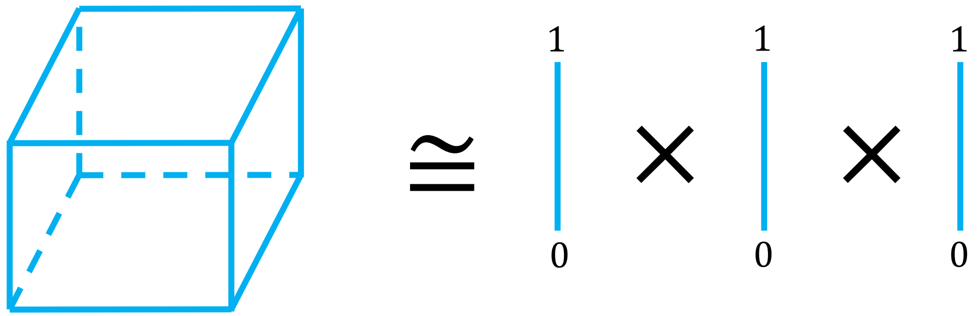

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Solving $\frac{d}{d\beta}K_\beta = LK_\beta$ on the complete graph with n vertices yields

$$K(i,j) = \begin{cases} \dfrac{1 + (n-1)e^{-n\beta}}{n}, & for\ i = j \\ \dfrac{1 - e^{-n\beta}}{n}, & for\ i \neq j \end{cases}$$

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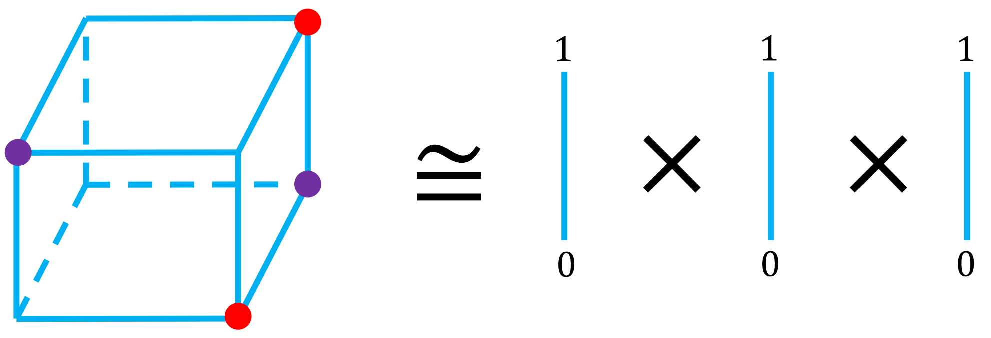

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and applying $K^n(x, x') = \prod_{i=1}^{n} K(x_i, x_i')$ gives the kernel $K(x, x') \propto \left(\dfrac{1 - e^{-2\beta}}{1 + e^{-2\beta}} \right)^{d(x,x')}$

$$= (\tanh \beta)^{d(x,x')}$$

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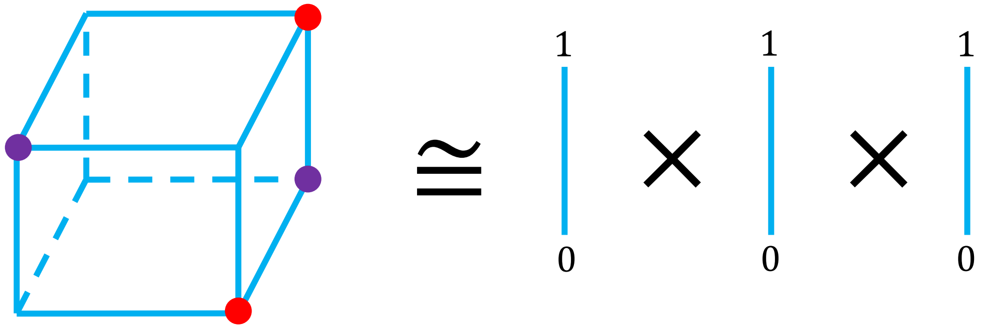

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$$K(\bullet, \bullet) = \tanh(0.1)^3 = 0.00099$$

$$K(\bullet, \bullet) = \tanh(0.1)^2 = 0.00993$$

Thank you!

The End

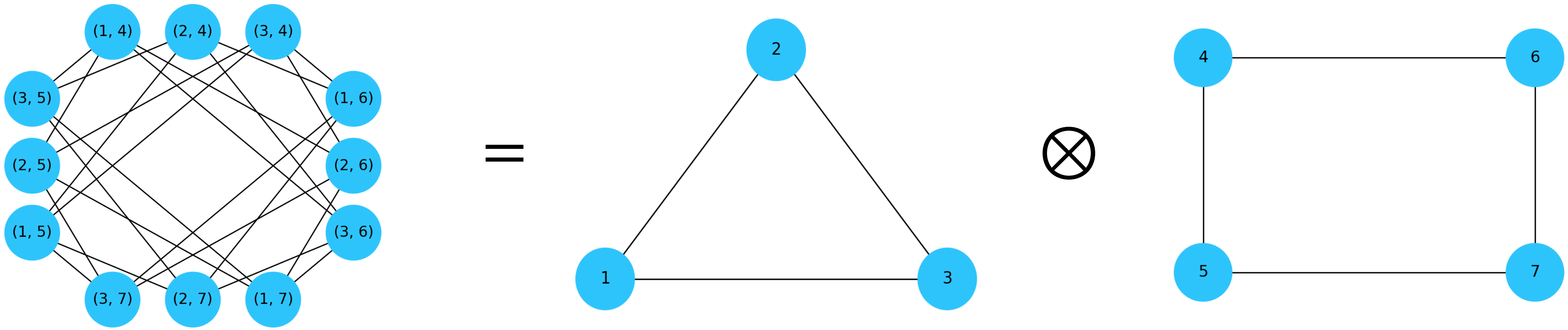
Inter Graph Diffusion Kernels

Tensor Product of Graphs

$$G_\times \coloneqq G \otimes G'$$

$$V_\times = \{(v_i, v_r'): v_i \in V, v_r' \in V'\}$$

$$E_\times = \left\{\left((v_i, v_r'), (v_j, v_s')\right): \left(v_i, v_j\right) \in E \wedge (v_r', v_s') \in E'\right\}$$



Inter Graph Diffusion Kernels

- Construction of Kernel between edge-labeled graphs

Inter Graph Diffusion Kernels

- Dotnet function to function graphs – example of kernel between these graphs
- Plot TSNE vectorization using edge-labeled kernel

Inter Graph Diffusion Kernels

- Functions defined on the set of vertices

Inter Graph Diffusion Kernels

- Lebesgue integral of functions on vertex set

Inter Graph Diffusion Kernels

- Use this vectorization and TNSE or LargeViz to plot a bunch of dotnet function to function graphs
- Good vs Bad red and blue scatter plot

Inter Graph Diffusion Kernels

Kronecker Product: Let M and N be matrices. Then

$$A \otimes B = \begin{bmatrix} a_{11}B & \cdots & a_{1n}B \\ \vdots & \ddots & \vdots \\ a_{m1}B & \cdots & a_{mn}B \end{bmatrix}$$

$$\begin{bmatrix} 1 & 2 \\ 3 & 4 \end{bmatrix} \otimes \begin{bmatrix} 0 & 5 \\ 6 & 7 \end{bmatrix} = \begin{bmatrix} 1 \cdot \begin{bmatrix} 0 & 5 \\ 6 & 7 \end{bmatrix} & 2 \cdot \begin{bmatrix} 0 & 5 \\ 6 & 7 \end{bmatrix} \\ 3 \cdot \begin{bmatrix} 0 & 5 \\ 6 & 7 \end{bmatrix} & 4 \cdot \begin{bmatrix} 0 & 5 \\ 6 & 7 \end{bmatrix} \end{bmatrix} = \begin{bmatrix} 0 & 5 & 0 & 10 \\ 6 & 7 & 12 & 14 \\ 0 & 15 & 0 & 20 \\ 18 & 21 & 24 & 28 \end{bmatrix}$$

Inter Graph Diffusion Kernels

- Describe how a heat kernel can serve to measure similarity
- Derivation of Heat Kernels
- String Kernel
- Vectorization

$$A \otimes B$$

$$\Phi(X) A \otimes B \; \Phi(X')$$

$$k(G, G') \coloneqq \sum_{k=0}^{\infty} \mu(k) q_{\times}^{T} W_{\times}^{k} p_{\times}$$

Inter Graph Diffusion Kernels

- Picture with graph of results
- Application to clusters within graph

$$k(G, G') \coloneqq \sum_{k=0}^{\infty} q_\times^T (P_\times D_\times P_\times^{-1})^k p_\times$$

$$q_\times^T P_\times \left(\sum_{k=0}^{\infty} \mu(k) D_\times^k) \right) P_\times^{-1} p_\times$$

$$k(G, G') \coloneqq q_\times^T P_\times e^{\lambda D_\times} P_\times^{-1} p_\times$$

$$k(G, G') \coloneqq q_\times^T P_\times (\mathrm{I} - \lambda D_\times)^{-1} P_\times^{-1} p_\times$$

References

- Chung, F.
- More…