Massachusetts Institute of Technology

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A Poincaré Inequality and Consistency Results for Signal Sampling on Large Graphs

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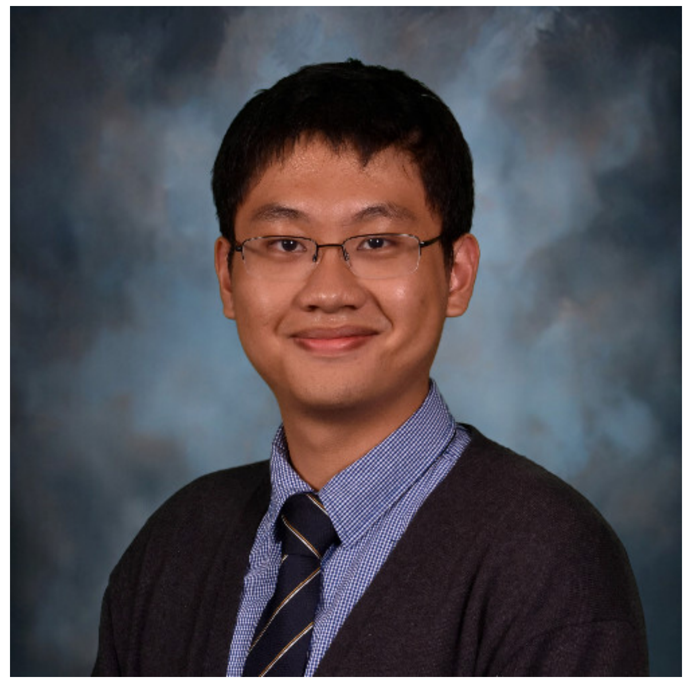


November 17th. DeepMath 2023.

Motivation

Graph algorithms scale with number of vertices

- Important data analysis algorithms scale with number of vertices n in a graph:
  - Spectral decomposition: $\Omega(n^2)$ (widely believed: $\Omega(n^{2.376...})$)
  - Graph neural networks (e.g. graph convolutional network): $\Omega(n^2)$
- In most graph-based task, complexity of the task does not scale with n
  - n represents resolution of dataset, not complexity.

Realistic graphs demonstrate intrinsic simplicity

- ‘Small world phenomenon’.
- Scale-free/power-law graphs.

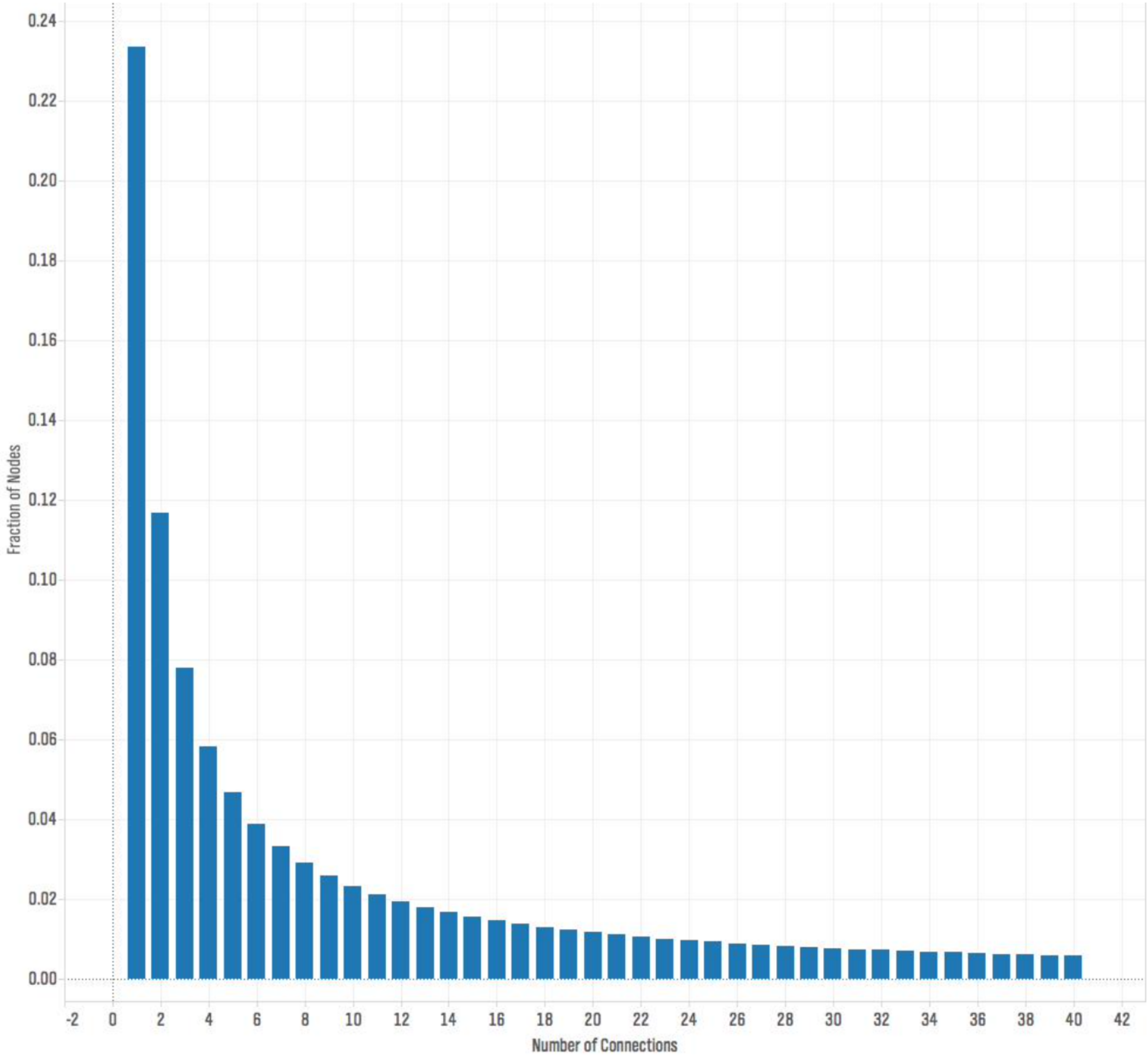


Figure by PJ Lamberson - UCLA

Reference: Kleinberg 2004, The small world phenomenon and decentralized search;
Milgram 1967, “The small world problem”;
Barabasi, Albert 1999, Emergence of scaling in random networks.

Solution: Sample small subset of nodes!

Two criteria

- Subsampling a small subset of k vertices, $k \ll n$, scales graph algorithms:

1. Find an "informative" subset.

   Strategy: optimal sampling

2. Find a "transferable" subset that is robust when the graph grows in size.

   Strategy: graph limit

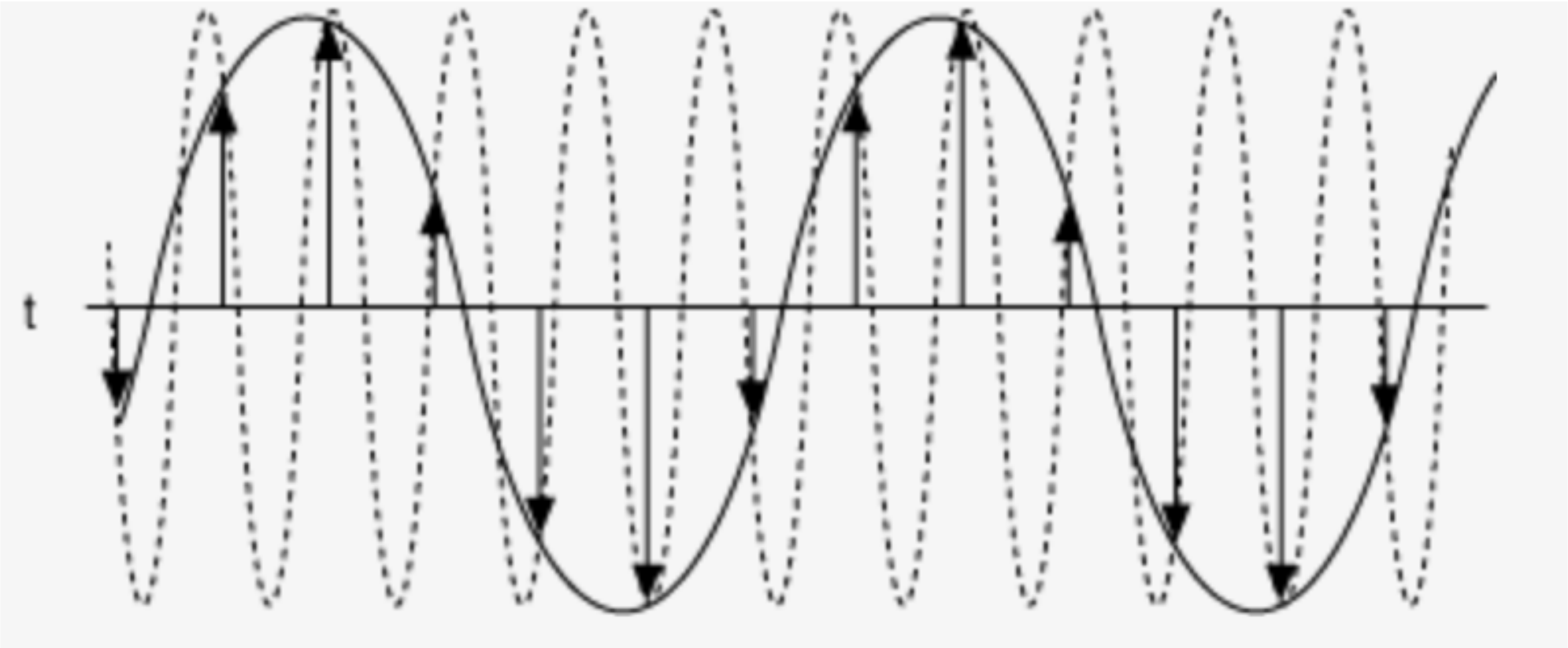
Look ahead: What can we do with such a subset?

- Faster existing algorithms:
  - Spectral decomposition (e.g. eigenvector positional encoding): $\cancel{\Omega(n^2)} \gg \Omega(k^2)$
  - Graph neural networks (e.g. graph convolutional network): $\cancel{\Omega(n^2)} \gg \Omega(k^2)$
- Theory: consistency/transferability results implies small decay in performance
- Empirical: node classification on citation network datasets

Informative subset: Sampling theory

Warm up: $L^1(\mathbb{R})$

Theorem (Shannon-Nyquist theorem): *An analog signal $f \in L^1(\mathbb{R})$ with bandwidth in $(0,2k)$ is uniquely determined by uniform discrete samples at rate k.*



Reference: Shannon, C.E., 1949. Communication in the Presence of Noise.
Figure by National Instruments

Informative subset: Sampling theory

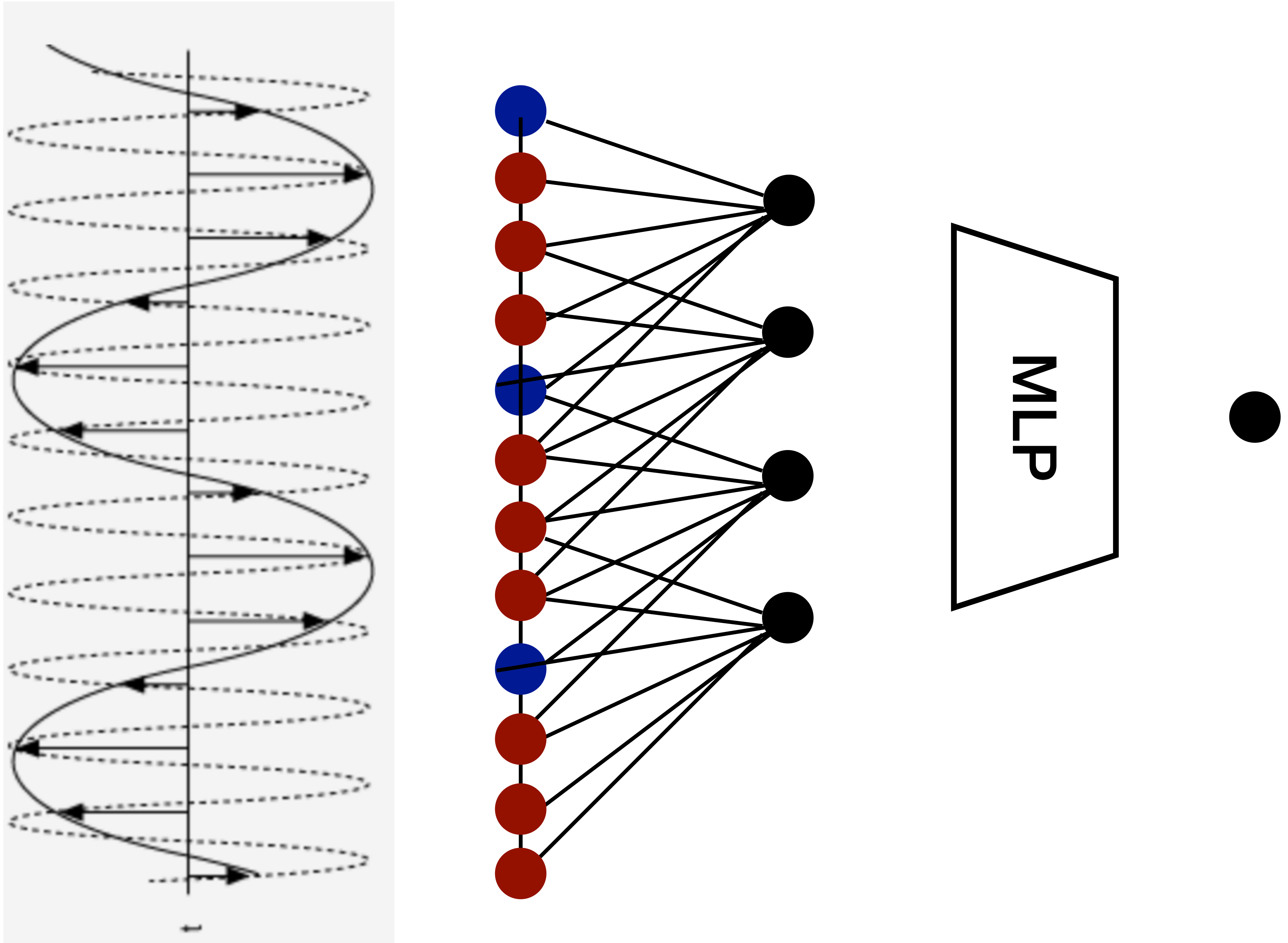
Corollary: 1D-CNN, path graph

Theorem (Shannon-Nyquist theorem): *An analog signal $f \in L^1(\mathbb{R})$ with bandwidth in $(0,2k)$ is uniquely determined by uniform discrete samples at rate k.*

Corollary (Sampling for 1D-CNN): *Given an analog 1D-image $f \in L^1([0,1])$ with bandwidth in $(0,2k)$ and n uniform pixels, only $k \ll n$ pixels is needed to uniquely determine f.*

Informative subset: Sampling theory

Corollary: 1D-CNN, path graph



blue nodes contain enough information to train the CNN

Corollary (Sampling for 1D-CNN): *Given an analog 1D-image $f \in L^1([0,1])$ with bandwidth in $(0,2k)$ and n uniform pixels, only $k \ll n$ pixels is needed to uniquely determine f.*

Informative subset: Sampling theory

Finite graph $G = (V, E)$ sampling

$f : V \to \mathbb{R}$

Theorem (Pesenson, 2008, informal): *A graph signal $f \in \ell^2(G)$ with limited bandwidth λ is uniquely determined by a uniqueness set $U \subseteq V$*

Normalized Laplacian $I - (D^\dagger)^{1/2} A (D^\dagger)^{1/2}$

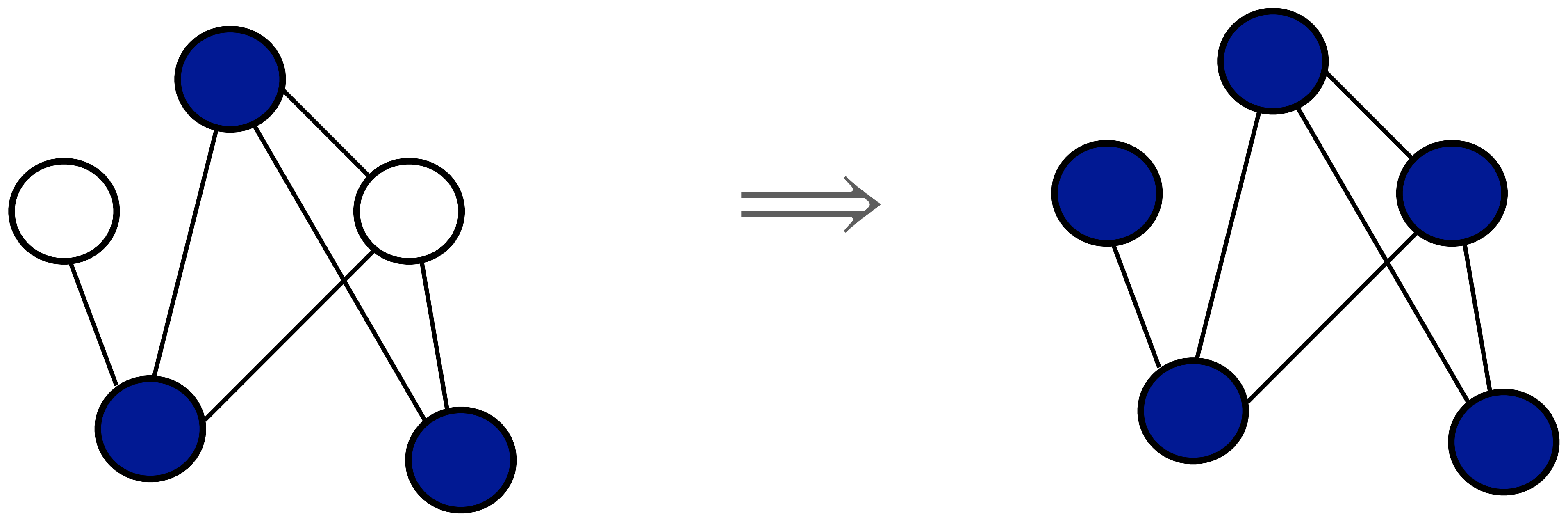
Graph Fourier transform

Eigenvalues/frequencies $\lambda_1 \leq \lambda_2 \leq \ldots \leq \lambda_n$

Bandwidth cutoff at λ

Paley-Wiener space $PW_\lambda(G)$

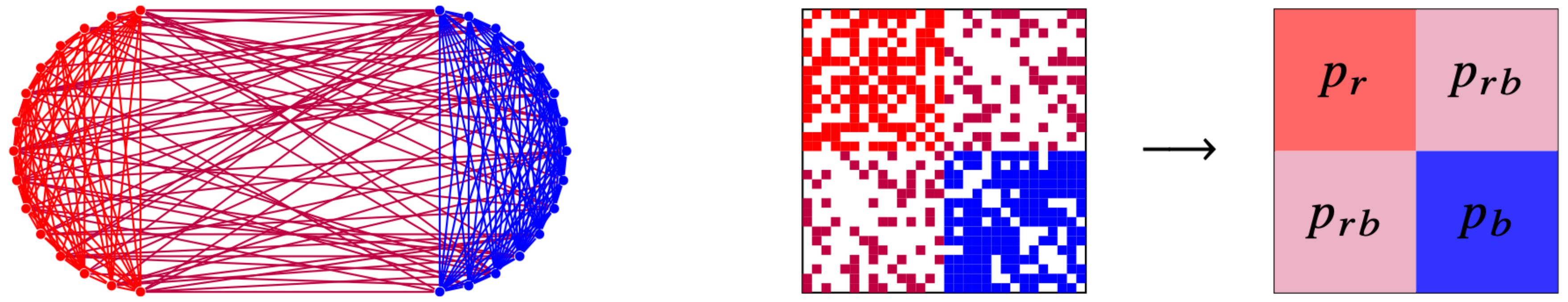
$\|f_1 - f_2\|_{\ell^2(U)} = 0 \implies \|f_1 - f_2\|_{\ell^2(G)} = 0$



Reference: Pesenson 2008. Sampling in Paley-Wiener spaces on combinatorial graphs.

Towards transferable subset: graph limit

Graphons and limit of dense graphs



- Graphons are symmetric, measurable functions $\mathbf{W} : [0,1] \times [0,1] \to \mathbb{R}$
- Interpretation:
    1. $(V = [0,1], E = \{(u, v) : \mathbf{W}(u, v) \neq 0\})$ (informal)
    2. Finite graph sampler:
        1. Given number of nodes n, sample $v_1, \ldots, v_n \overset{\text{iid}}{\sim} \text{Unif}[0,1]$
        2. For each $i < j \in [n]$, sample $(v_i, v_j) \overset{\text{iid}}{\sim} \text{Bern}(\mathbf{W}(v_i, v_j))$

Reference: Lovasz, 2012, Large network and graph limits;
Borgs, Chayes, Lovasz, Sos and Vesztergombi 2006 - 2008: Convergent sequences of dense graphs I, II: Subgraph frequencies, metric properties and testing,
Figure: Zhao, Graph Theory and Additive Combinatorics pg 134

Reference: Ruiz, Chamon, and Ribeiro, 2023. Transferability properties of graph neural networks.

Towards transferable subset: graph limit

Transferability of graphs sampled from graphons

sampled frome same $\mathbf{W}$

- Transferability between graphs with similar structures: for some rate $c > 0$,

$$d_{?}(\mathrm{GNN}(\,\cdot\,, G_n, \theta), \mathrm{GNN}(\,\cdot\,, G_m, \theta)) \leq O(1/m^c + 1/n^c)$$

appropriate metric

input node features $\mathbb{R}^n$

input graph: n nodes

learnable parameter

Theorem (Ruiz et al. 2023; informal): *RHS = small number +* $O(1/m + 1/n)$

Transferable subset: graph limit

Putting together…

- Uniqueness set for a finite graph = informative subset
- Finite graphs sampled from the same limit graphons are structurally similar

$\implies$ Study how to sample informative subset from limit graphon and get transferability for free

Our results

Finite graph $G = (V, E)$ sampling

Informative subset: Sampling theory

$f : V \to \mathbb{R}$

Theorem (Pesenson, 2008, informal): *A graph signal $f \in \ell^2(G)$ with limited bandwidth λ is uniquely determined by a uniqueness set $U \subseteq V$*

Normalized Laplacian $I - (D^\dagger)^{1/2} A (D^\dagger)^{1/2}$

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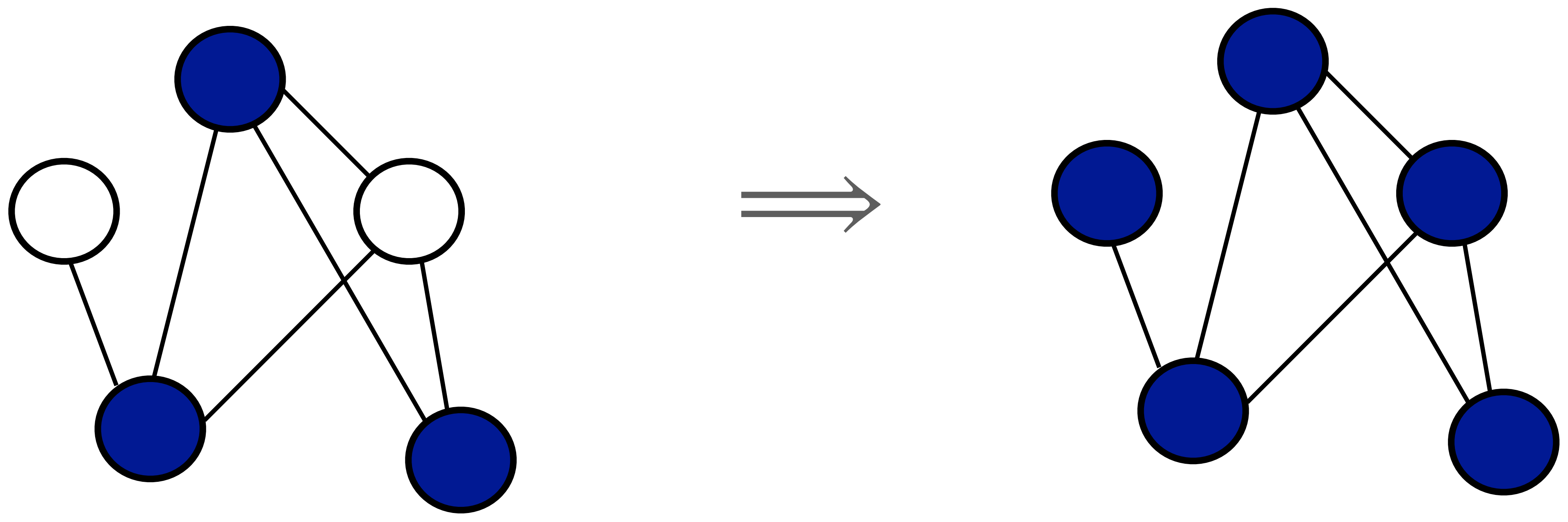


Reference: Pesenson 2008. Sampling in Paley-Wiener spaces on combinatorial graphs.

Graphon $\mathbf{W} : [0,1]^2 \to \mathbb{R}$ sampling (via Poincaré inequality)

Informative subset: Sampling theory

$f : [0,1] \to \mathbb{R}$

Theorem 2,3 (L., Ruiz, Jegelka, 2023; informal): *A graphon signal $f \in L^2([0,1])$ with limited bandwidth λ is uniquely determined by a msrbl uniqueness set s*

Normalized graphon Laplacian

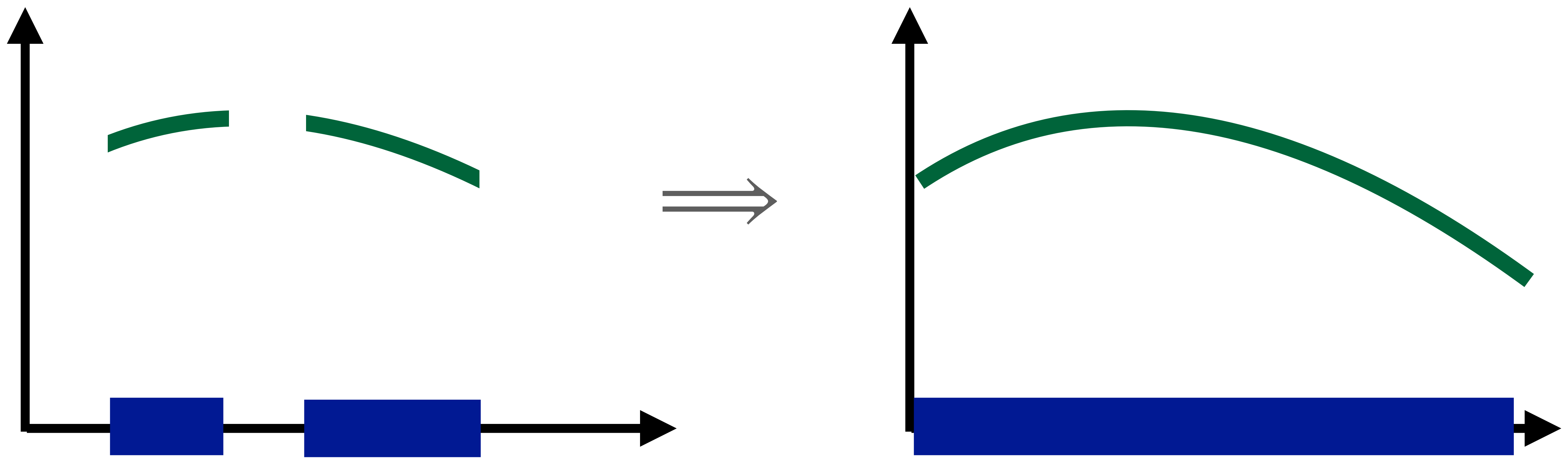
↓ Graphon Fourier transform

Eigenvalues/frequencies $\lambda_1 \leq \lambda_2 \leq \ldots \leq \lambda_{-1}$

↓ Bandwidth cutoff at λ

graphon Paley-Wiener space $PW_\lambda(\mathbf{W})$

$$\|f_1 - f_2\|_{L^2(U)} = 0 \implies \|f_1 - f_2\|_{L^2([0,1])} = 0$$



Towards a sampling algorithm

Input: large graph G_N. Output: small uniqueness set for all $G_n, n \geq N$

1. Obtain an approximation of the limit graphon with G_N.

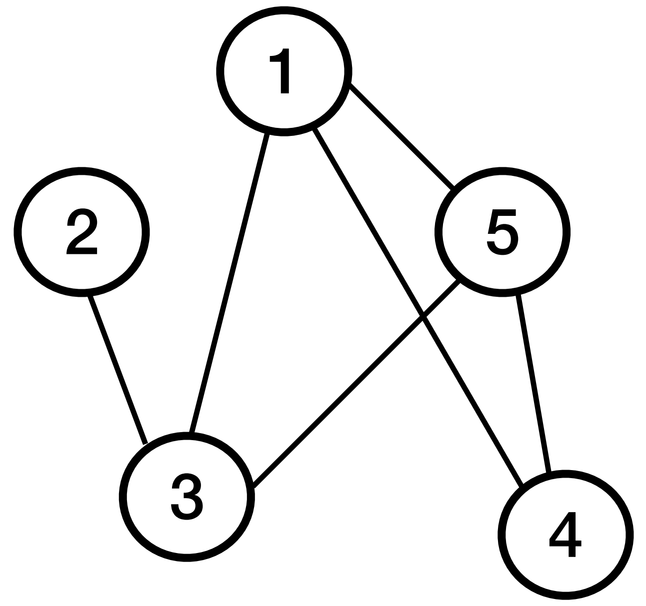
2. Approximate uniqueness set $U \subseteq [0,1]$ by G_N uniqueness set $U_N \subseteq [N]$.

3. Map $U_N \subseteq [N]$ to nodes $U_n \subseteq [n]$ of finite graph $G_n, n \geq N$.

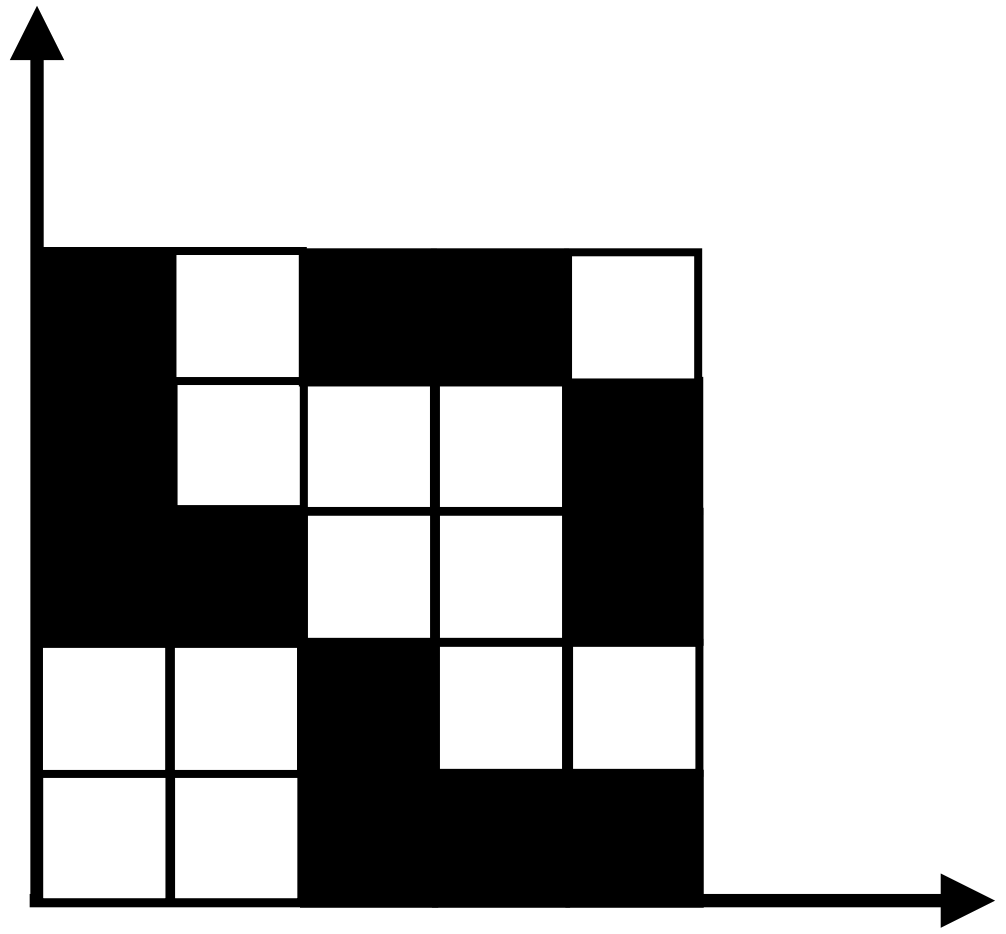
1. Obtain an approximation of limit graphon

Graphon is the closure of graphs (under cut norm)

- Embed G_N vertices into $[0,1]$ - induced graphon



$\Longrightarrow$



Theorem (Lovász and Szegedy 2007): *Graphon space is compact. Finite graphs are dense.*

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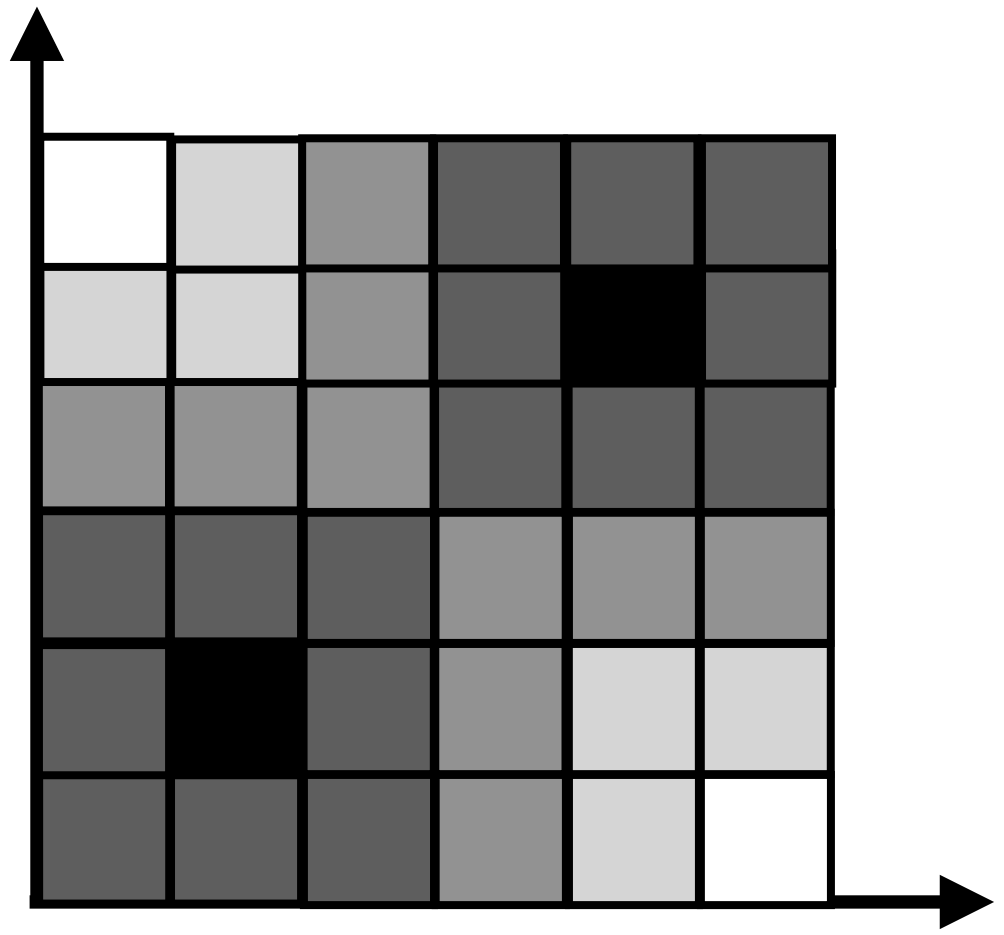
2. Approximate uniqueness set of graphons

Graphon $\mathbf{W} \equiv$ mixture model of random graphs $\mathbf{K} = \left(\Omega, \sum_i \mathbb{P}_i, \mathbf{k}\right)$

Proposition 2 (L., Ruiz, Jegelka, 2023; informal): *A graphon random model is equivalent to mixture models of random graphs. Well-fittedness measured by a difficulty function $\varphi(\mathbf{W}; \mathbf{k}, \mathbb{P}_i)$ (Schiebinger et al. 2015)*



$$\equiv d\mathbb{P} = \frac{p_{\mathcal{N}(0.25,\sigma^2)} + p_{\mathcal{N}(0.,75,\sigma^2)}}{2}$$

2. Approximate uniqueness set of graphons

Gaussian elimination find uniqueness set with high probability

Theorem (L., Ruiz, Jegelka, 2023; informal) - Corollary of Theorem 2 (Schiebinger et. al, 2015): *If $\varphi \ll 1$, GE <u>with pivoting</u> find uniqueness set with high probability.*

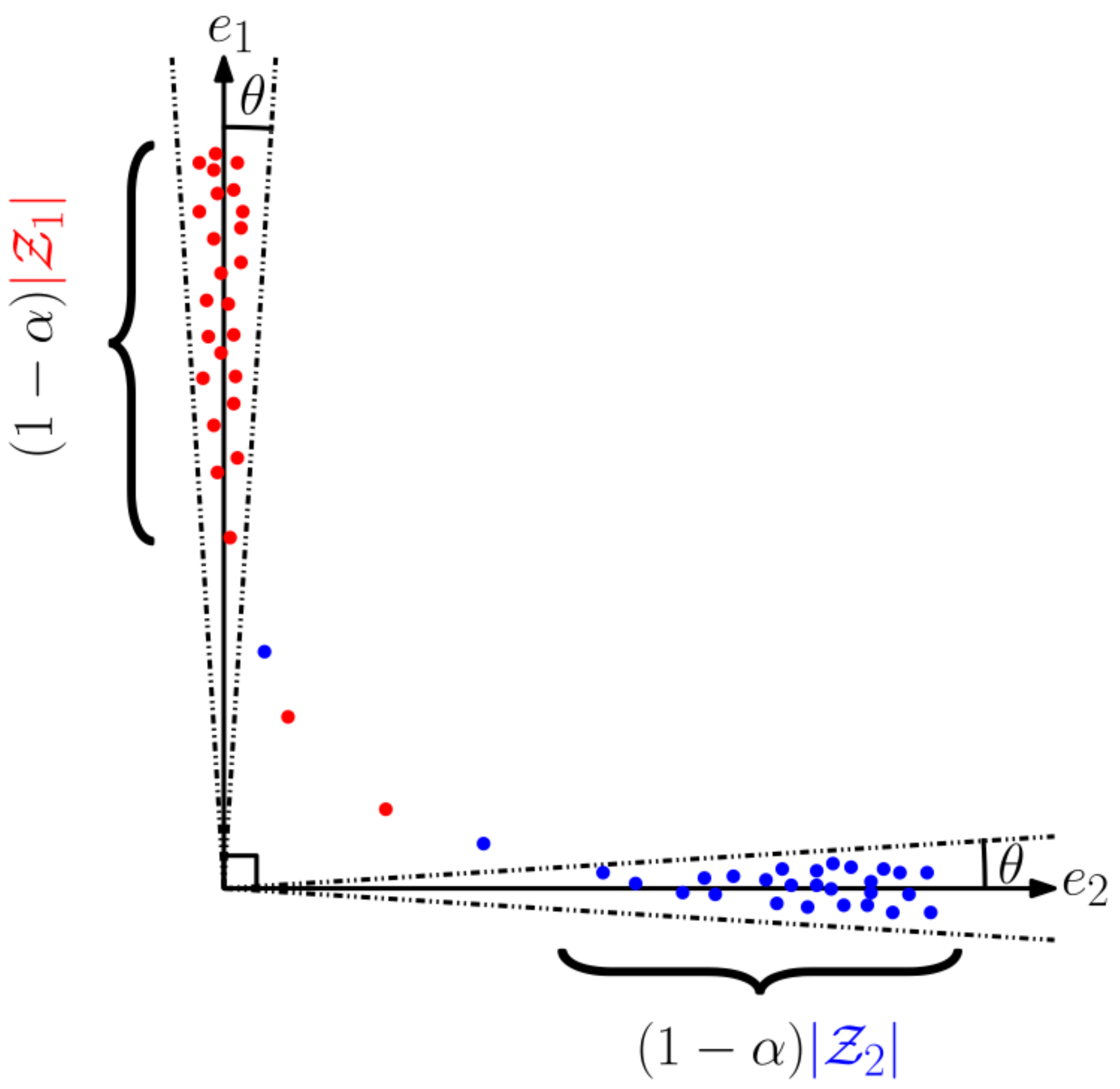


Figure from Schiebinger et al.
Reference: Schiebinger, Wainwright, Yu 2015. The geometry of kernelized spectral clustering

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3. Map graphon uniqueness set to nodes in graph

Consistency result

Proposition 6 (L., Ruiz, Jegelka, 2023; informal): *If $\varphi \ll 1$, for a sequence of graphs $G_N \to \mathbf{W}$, there exists a number of node N such that for all $n > N$, uniqueness set of G_N is also a uniqueness set of G_n.*

Empirical results

Experiments

Transferability

Table 2: Classification accuracy on the MalNet-Tiny dataset, (i) w/o positional encodings (PEs), (ii) w/ PEs computed on the full graph, (iii) w/ PEs computed on a graphon-sampled subgraph (removing or not isolated nodes), and (iv) w/ PEs computed on a subgraph with randomly sampled nodes (removing or not isolated nodes).

	no PEs	full graph PEs	graphon sampled PEs		randomly sampled PEs	
			w/ isolated	w/o	w/ isolated	w/o
mean	0.26±0.03	0.43±0.07	**0.29±0.06**	**0.33±0.06**	0.28±0.07	0.27±0.07
max	0.30	0.51	**0.40**	**0.42**	0.35	0.37

Conclusion

- Subsampling a small subset of k vertices, $k \ll n$, scales graph algorithms:
  - Find an `informative' subset: sampling theory
  - Find a `transferable' subset: graph limit
- We derived a consistent algorithm that approximately samples from the limiting graphon uniqueness set, under theoretical guarantees.
- We tested our approach in real-world datasets, showing improvement over uniformly random sampling.

Thank you!

Q&A

Massachusetts Institute of Technology

- Major thanks to my collaborators Luana Ruiz and Stefanie Jegelka
- Contact: thienle@mit.edu
- Full paper: