Spectral Representations of Graphons in Very Large Network Systems Control

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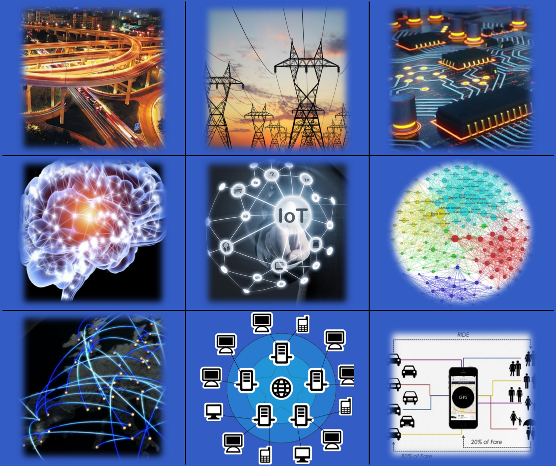
Motivation

Networks are ubiquitous, growing in size and complexity.



Online Social Networks, Brain Networks, Grid Networks, Transportation Networks, IoT ...

Background

Graphon theory: model arbitrary-size/large graphs and their limits [1]

Recent applications to dynamical systems:

- Heat equations, coupled oscillators, random walks [2]
- Dynamic games [3]
- Control of large networks of dynamical systems [4]

Other applications: static games, network centrality, signal processing... [5]

Among these, spectral properties of graphons are very significant.

Spectral analysis of large-scale dynamical systems plays a key role in low-complexity control synthesis [6]

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1 [Borgs et al., 2008, 2012; Lovász, 2012].

2 [Medvedev, 2014a,b], [Chiba and Medvedev, 2019; Kuehn and Throm, 2018], [Petit et al., 2019]

3 [Caines and Huang, 2018, 2019]

4 [Gao and Caines, 2017, 2018, 2019a,b,c; Gao, 2019]

5 [Parise and Ozdaglar, 2018; Carmona et al., 2019], [Avella-Medina et al., 2018], [Ruiz et al., 2019; Morency and Leus, 2017]

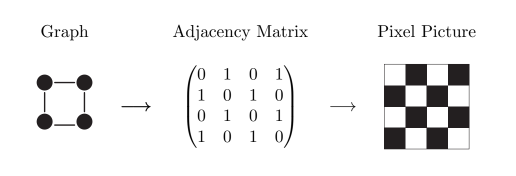
6 [Aoki, 1968; Swigart and Lall, 2014; Callier and Winkin, 1992]

Program

1. Introduction to Graphons
2. Graphon Control Systems
3. Controllability Gramian Operator
4. Spectral Approximations of Networks and Graphons
5. Controlling Epidemic Networks via Spectral Decomposition

Introduction to Graphons

Graphs, Adjacency Matrices and Pixel Pictures

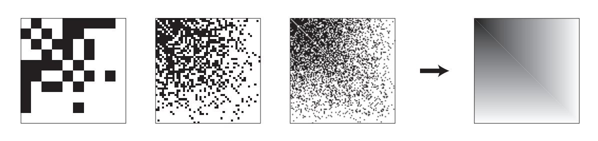


Graph, Adjacency Matrix, Pixel Picture [Lovász, 2012]

The whole pixel picture is presented in a unit square $[0,1] \times [0,1]$, so the square elements have sides of length $\frac{1}{N}$, where N is the number of nodes.

Introduction to Graphons

Graph Sequence Converging to Graphon



Graph Sequence Converging to its Limit [Lovász, 2012]

Graphons: bounded symmetric Lebesgue measurable functions

$$\mathbf{W} : [0,1]^2 \to [0,1]$$

interpreted as weighted graphs on the vertex set $[0,1]$.

Notations of Spaces

$$\tilde{\mathbf{G}}_{\mathbf{0}}^{\mathbf{sp}} := \{\mathbf{W} : [0,1]^2 \to [0,1]\}$$

$$\tilde{\mathbf{G}}_{\mathbf{1}}^{\mathbf{sp}} := \{\mathbf{W} : [0,1]^2 \to [-1,1]\}$$

$$\tilde{\mathbf{G}}_{\mathbb{R}}^{\mathbf{sp}} := \{\mathbf{W} : [0,1]^2 \to \mathbb{R}\}$$

Cut norm: $$\|\mathbf{W}\|_\square := \sup_{M,T\subset[0,1]} \left| \int_{M\times T} \mathbf{W}(x,y)dxdy \right|$$

Cut metric: $$\delta_\square(\mathbf{W},\mathbf{V}) := \inf_{\phi} \|\mathbf{W}^\phi - \mathbf{V}\|_\square, \qquad *^{1}$$

Theorem ([Lovász, 2012])

The graphon spaces $(\mathbf{G}^{\mathbf{sp}}_{\mathbf{0}}, \delta_\square)$ *and any closed bounded subset of* $(\mathbf{G}^{\mathbf{sp}}_{\mathbb{R}}, \delta_\square)$ *are compact.*

By compactness, infinite sequences of graphons will necessarily possess one or more sub-sequential limits under the cut metric.

[1] $\mathbf{W}^\phi(x,y) = \mathbf{W}(\phi(x),\phi(y))$

Graphon $\mathbf{W} \in \tilde{\mathbf{G}}_{\mathbf{1}}^{\mathbf{sp}}$ as an operator: $\mathbf{W} : L^2[0,1] \to L^2[0,1]$

Operation: $$[\mathbf{W}\mathbf{v}](x) = \int_0^1 \mathbf{W}(x,\alpha)\mathbf{v}(\alpha)d\alpha \qquad \mathbf{v} \in L^2[0,1]$$

Operator Product: $$[\mathbf{U}\mathbf{W}](x,y) = \int_0^1 \mathbf{U}(x,z)\mathbf{W}(z,y)dz, \quad \mathbf{U},\mathbf{W} \in \tilde{\mathbf{G}}_{\mathbf{1}}^{\mathbf{sp}}$$

Norm relations [Gao and Caines, 2019c], [Janson, 2010; Parise and Ozdaglar, 2018]:

$$\|\mathbf{W}\|_{\mathsf{op}} \leq \|\mathbf{W}\|_2, \qquad \|\mathbf{W}\|_{\square} \leq \|\mathbf{W}\|_{\mathsf{op}} \leq \sqrt{8\|\mathbf{W}\|_{\square}}.$$

Graphon operators are Hilbert-Schmidt operators

[Rudin, 1991; J Mercer, 1909; Szegedy, 2011]

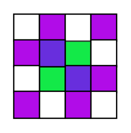
Introduction to Graphons

Two Types of Graphons: Step Function Graphons

Proposition (Spectral Rep. of Step Function Graphons)

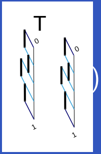
Let $A = V\Lambda_d V^{\intercal}$ where $\Lambda_d = diag(\lambda_1, ..., \lambda_d)$ and $V = (v_1, ..., v_d)$ with v_ℓ representing the normalized eigenvector of λ_ℓ. Consider the uniform partition $\{P_1, ..., P_N\}$ of $[0,1]$. Then the step function graphon $\mathbf{A}$

$$\mathbf{A}(x,y) := \sum_{i=1}^{N}\sum_{j=1}^{N} \mathbb{1}_{P_i}(x)\mathbb{1}_{P_j}(y)a_{ij}, \quad (x,y) \in [0,1]^2$$



has a spectral representation given by

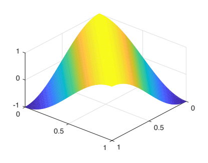
$$\mathbf{A}(x,y) = \sum_{\ell=1}^{d} \lambda_\ell [\mathbb{S}_{v_\ell} \cdot \mathbb{S}_{v_\ell}^{\intercal}](x,y), \quad (x,y) \in [0,1]^2.$$



The corresponding eigenvalues for $\mathbf{A}$ are given by $\{\frac{\lambda_\ell}{N}\}_{\ell=1}^{d}$ since $\langle \mathbb{S}_{v_\ell}, \mathbb{S}_{v_k}\rangle = 0$, if $\ell \neq k$; $\langle \mathbb{S}_{v_\ell}, \mathbb{S}_{v_k}\rangle = 1/N$, if $\ell = k$.

Introduction to Graphons

Two Types of Graphons: Sinusoidal Graphons



Sinusoidal graphon

$$\mathbf{A}(\varphi, \vartheta) := a_0 + \sum_{k=1}^{\infty} b_k \cos(2\pi k(\varphi - \vartheta)), \quad (\varphi, \vartheta) \in [0,1]^2.$$

Features

- Eigenvalues: $a_0, \{\frac{b_k}{2} : k \in \mathbb{Z}_+\}, \{\frac{b_k}{2} : k \in \mathbb{Z}_+\}$.
- Eigenfunctions form a complete orthonormal basis for $L^2[0,1]$:

$$1, \{\sqrt{2}\cos 2\pi k(\cdot) : k \in \mathbb{Z}_+\}, \{\sqrt{2}\sin 2\pi k(\cdot) : k \in \mathbb{Z}_+\}.$$

- Representations of functions $\mathbf{A}^n, e^{\mathbf{A}}$ are explicit
- Symmetric and diagonally constant, and suitable to approximate infinite Toeplitz matrices [Gray et al., 2006]

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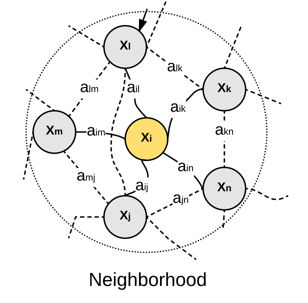
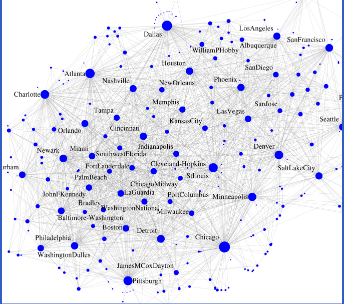
The dynamics of the i^{th} agent in the network

$$\dot{x}_t^i = \alpha_0 x_t^i + \frac{1}{N}\sum_{j=1}^{N} a_{ij} x_t^j + \beta_0 u_t^i + \frac{1}{N}\sum_{j=1}^{N} b_{ij} u_t^j, \tag{3}$$

$$t \in [0, T], \quad \alpha_0, \beta_0 \in \mathbb{R}, \quad x_t^i, u_t^i \in \mathbb{R},$$





Graphon Control Systems

Linear Network Systems Described by Graphons [Gao and Caines, 2019c]

Dynamics

$$\dot{\mathbf{x}}_{\mathbf{t}}^{[\mathbf{N}]} = (\alpha_0 \mathbb{I} + \mathbf{A}^{[\mathbf{N}]})\mathbf{x}_{\mathbf{t}}^{[\mathbf{N}]} + (\beta_0 \mathbb{I} + \mathbf{B}^{[\mathbf{N}]})\mathbf{u}_{\mathbf{t}}^{[\mathbf{N}]}, \quad t \in [0, T],$$
$$\alpha_0, \beta_0 \in \mathbb{R}, \quad \mathbf{x}_{\mathbf{t}}^{[\mathbf{N}]}, \mathbf{u}_{\mathbf{t}}^{[\mathbf{N}]} \in L^2_{pwc}[0,1], \quad \mathbf{A}^{[\mathbf{N}]}, \mathbf{B}^{[\mathbf{N}]} \in \tilde{\mathbf{G}}_{\mathbf{1}}^{\mathbf{sp}} \tag{4}$$

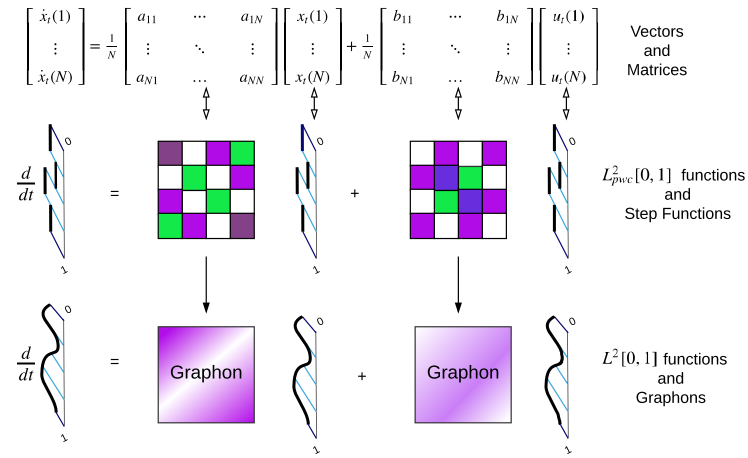
(step function) $\quad \mathbf{A}^{[\mathbf{N}]}(\vartheta, \varphi) = \sum_{i=1}^{N}\sum_{j=1}^{N} \mathbb{1}_{P_i}(\vartheta)\mathbb{1}_{P_j}(\varphi)a_{ij}, \quad (\vartheta, \varphi) \in [0,1]^2$

(pwc) $\quad \mathbf{x}_{\mathbf{t}}^{[\mathbf{N}]}(\vartheta) = \sum_{i=1}^{N} \mathbb{1}_{P_i}(\vartheta)x_t^i, \quad \forall \vartheta \in [0,1]$

$\mathbb{1}_{P_i}(\cdot)$: the indicator function. $L^2_{pwc}[0,1]$: the set of all piece-wise constant functions in $L^2[0,1]$

Graphon Control Systems

Linear Network Systems Described by Graphons



Graphon Control Systems

Graphon linear control system $(\mathbb{A};\mathbb{B})$:

$$\dot{\mathbf{x}}_{\mathbf{t}} = \mathbb{A}\mathbf{x}_t + \mathbb{B}\mathbf{u}_t, \quad t \in [0,T], \tag{5}$$

$\mathbb{A} = (\alpha_0\mathbb{I} + \mathbf{A})$, $\mathbb{B} = (\beta_0\mathbb{I} + \mathbf{B})$ with $\mathbf{A}, \mathbf{B} \in \tilde{\mathbf{G}}_{\mathbf{1}}^{\mathbf{sp}}$ and $\alpha_0, \beta_0 \in \mathbb{R}$

$\mathbf{x}_t \in L^2[0,1]$: system state. $\mathbf{u}_t \in L^2[0,1]$: control input.

Proposition ([Bensoussan et al., 2007])

The system $(\mathbb{A};\mathbb{B})$ *in* (5) *has a unique mild solution* $\mathbf{x} \in C([0,T]; L^2[0,1])$ *for any* $\mathbf{x_0} \in L^2[0,1]$ *and any* $\mathbf{u} \in L^2([0,T]; L^2[0,1])$.

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Controllability Gramian Operator

$\mathbb{A} = (\alpha_0 \mathbb{I} + \mathbf{A})$, $\mathbb{B} = (\beta_0 \mathbb{I} + \mathbf{B})$

Definition

A graphon dynamical system $(\mathbb{A}; \mathbb{B})$ in (5) is *exactly controllable* in $L^2[0,1]$ over the time horizon $[0,T]$ if the system state can be driven to the origin at time T from any initial state $\mathbf{x}_0 \in L^2[0,1]$.

1. No exact controllability for $(\mathbb{A}; \mathbb{B})$ with a compact operator $\mathbb{B}$ over a finite horizon [Triggiani, 1975].
2. If $\mathbb{B}$ lies in the graphon unitary operator algebra [Gao and Caines, 2019c], then $(\mathbb{A}; \mathbb{B})$ in (5) over $[0,T]$ is exact controllable iff $\beta_0 \neq 0$.

Controllability Gramian operator: $\mathbb{W}_T := \int_0^T e^{\mathbb{A}\tau} \mathbb{B}\mathbb{B}^\intercal e^{\mathbb{A}^\intercal \tau} d\tau.$

- Minimum control energy: $J(\mathbf{x}_0) = \langle e^{\mathbb{A}T}\mathbf{x}_0, \mathbb{W}_T^{-1} e^{\mathbb{A}T}\mathbf{x}_0 \rangle$

Controllability Gramian Operator

$\mathbb{A} = (\alpha_0 \mathbb{I} + \mathbf{A})$, $\mathbb{B} = (\beta_0 \mathbb{I} + \mathbf{B})$

Proposition (Explicit Rep. of Controllability Gramian)

Let $\mathbf{A} \in \tilde{\mathbf{G}}_{\mathbf{1}}^{\mathbf{sp}}$ *and* $\mathbf{B} = \sum_{k=1}^{d} \beta_k \mathbf{A}^k$. *Denote* $\eta_\ell = \sum_{k=0}^{d} \beta_k \lambda_\ell^k$. *Then the controllability Gramian operator for the system* $(\mathbb{A}, \mathbb{B})$ *in (5) is given by*

$$\mathbb{W}_T = \int_0^T e^{\alpha_0 t} dt \beta_0^2 \mathbb{I} + \sum_{\ell \in I_\lambda} \left((\eta_\ell)^2 \int_0^T e^{2(\alpha_0 + \lambda_\ell) t} dt - \int_0^T e^{\alpha_0 t} dt \beta_0^2 \right) \mathbf{f}_\ell \mathbf{f}_\ell^\mathsf{T}; \tag{6}$$

furthermore, if $\beta_0 \neq 0$, *then the inverse of the controllability Gramian operator for* $(\mathbb{A}; \mathbb{B})$ *in (5) is explicitly given by*

$$\mathbb{W}_T^{-1} = \frac{1}{\int_0^T e^{\alpha_0 t} dt \beta_0^2} \mathbb{I} - \frac{1}{\int_0^T e^{\alpha_0 t} dt \beta_0^2} \sum_{\ell \in I_\lambda} \frac{(\eta_\ell)^2 \int_0^T e^{2\lambda_\ell t} dt - T\beta_0^2}{(\eta_\ell)^2 \int_0^T e^{2\lambda_\ell t} dt} \mathbf{f}_\ell \mathbf{f}_\ell^\mathsf{T}. \tag{7}$$

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Spectral Approximations of Networks

Eigenvalues a graphon $\mathbf{A}_n$ form two sequences converging to 0 [Borgs et al., 2012]:

$$\mu_1(\mathbf{A}_n) \geq \mu_2(\mathbf{A}_n) \geq ... \geq 0 \quad \text{and} \quad \mu'_1(\mathbf{A}_n) \leq \mu'_2(\mathbf{A}_n) \leq ... \leq 0$$

Theorem ([Borgs et al., 2012])

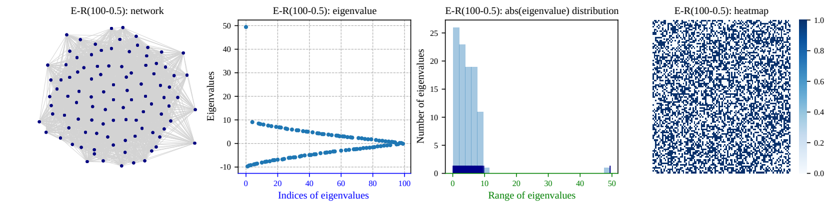
Let $\{\mathbf{A}_i\}_{i=1}^{\infty}$ be a sequence of uniformly bounded graphons, converging in the cut metric to a graphon $\mathbf{A}$. Then for every $i \geq 1$,

$$\mu_i(\mathbf{A}_n) \to \mu_i(\mathbf{A}) \quad \textit{and} \quad \mu'_i(\mathbf{A}_n) \to \mu'_i(\mathbf{A}) \qquad \textit{as } n \to \infty.$$

Implication: If a sequence of graphons converges in the cut metric to a graphon limit with a few non-zero eigenvalues, then elements of the sequence admit low-dimensional spectral approximations.

Spectral Approximations of Networks

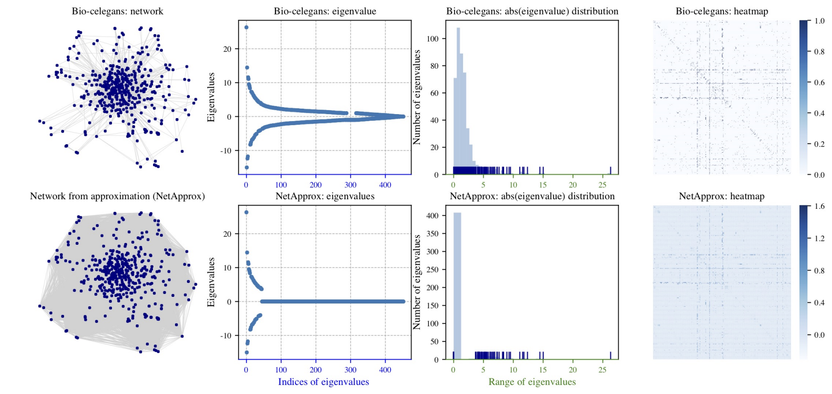
Random graphs generated by the Erdös-Rényi model
Parameters: $p = 0.5$, $n = 100$



The eigenvalue distribution of a graph with 100 nodes in a convergent sequence of random graphs to the graphon limit $W(x, y) = 0.5$.

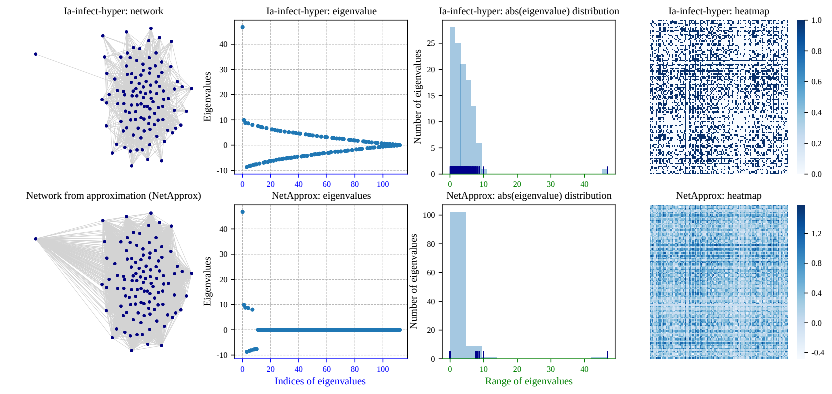
Reasonable low-rank approximations exist for general random graphs generated by dense low-rank models [Chung and Radcliffe, 2011], e.g., stochastic block models (SBM).

Spectral Approximations of Networks



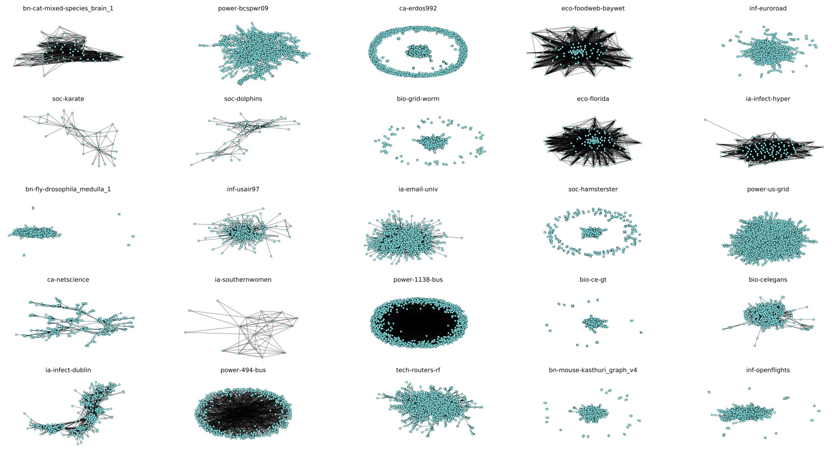
ND1: C-elegans metabolic network where edges represent metabolic reactions between substrates [Jeong et al., 2000].

Spectral Approximations of Networks



ND2: Infectious contact network [SocioPatterns, 2009].

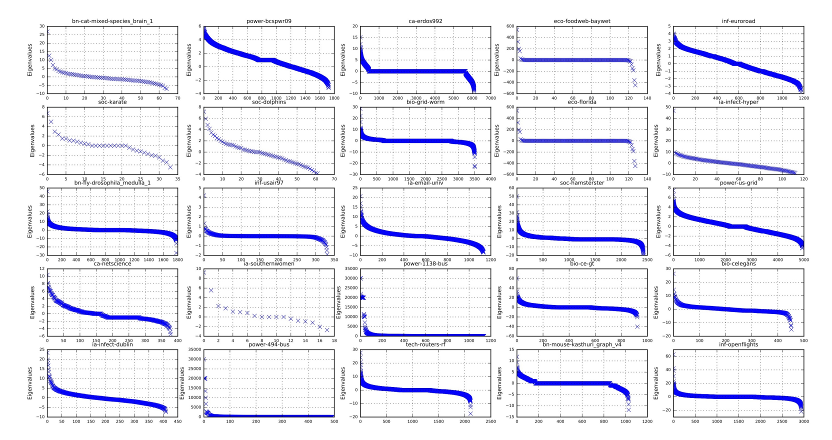
Spectral Approximations of Networks



*Original network data is collected from [Rossi and Ahmed, 2015]

http://networkrepository.com

Spectral Approximations of Networks



Eigenvalues in decreasing order

Spectral Approximation of Graphons

Approximation of a graphon $\mathbf{A}$: $\mathbf{A}_m(x,y) = \sum_{\ell=1}^{m} \lambda_\ell \mathbf{f}_\ell(x)\mathbf{f}_\ell(y)$.

Approximation error:

$$\|\mathbf{A} - \mathbf{A}_m\|_2 = \sqrt{\|\mathbf{A}\|_2^2 - \sum_{\ell=1}^{m} \lambda_\ell^2}. \tag{8}$$

Denote the spectral sum with Fourier approximated eigenfunctions as

$$\mathbf{A}_{pm}(\vartheta,\psi) = \sum_{\ell=1}^{m} \lambda_\ell p_\ell(e^{2\pi i\vartheta}) p_\ell(e^{2\pi i\psi}) \tag{9}$$

Proposition ([Gao, 2019])

If there exists $c > 0$ such that $\|\mathbf{A}\|_2 \le c$ and $\|\mathbf{A}_{pm}\|_2 \le c$, then

$$\|\mathbf{A}^n - (\mathbf{A}_{pm})^n\|_2 \le nc^n \|\mathbf{A} - \mathbf{A}_{pm}\|_2, \tag{10}$$

$$\|e^{\mathbf{A}} - e^{\mathbf{A}_{pm}}\|_{\mathsf{op}} \le ce^c \|\mathbf{A} - \mathbf{A}_{pm}\|_2. \tag{11}$$

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Meta-population model [Nowzari et al., 2016]:

$$\dot{p}_t^i = -\alpha p_t^i + \eta \sum_{j=1}^{N} a_{ij} p_t^j (1 - p_t^i), \quad t \in [0, T], \tag{12}$$

$p_t^i \in [0,1]$: infected fraction in the i^{th} subpopulation
α: recovering rate
η: infection strength
N: number of subpopulations (i.e. communities, cities)

Notice $(1 - p_t^i) \leq 1$ is close to 1 when p_t^i is close to zero. Under normal conditions $p_t^i \in [0,1]$ should be small.

Controlling Epidemic Networks via Spectral Decomposition

Linearized model:

$$\dot{p}_t^i = -\alpha_0 p_t^i + \eta \frac{1}{N} \sum_{j=1}^{N} \bar{a}_{ij} p_t^j + \beta_0 u_t^i, \quad t \in [0, T] \tag{13}$$

u_t^i : control action at node i (via vaccinations or medications)

Quadratic cost:

$$J(u) = \frac{1}{N} \sum_{i=1}^{N} \int_0^T \Big[\big(q_t (p_t^i)^2 + (u_t^i)^2 + (u_t^i - \frac{1}{N} \sum_{j=1}^{N} \bar{a}_{ij} u_t^j)^2 \big) dt + q_T (p_T^i)^2 \Big]$$

where $q_t, q_T \geq 0$.

Eigendecomposition: $\bar{A} = \sum_{\ell=1}^{L} \mu_\ell v_\ell v_\ell^\intercal$ (Symmetric matrix)

v_ℓ : normalized eigenvector; $L \leq N$: # of non-zero eigenvalues.

Optimal solution at community i:

$$u_t^i = \frac{\beta_0}{2}\breve{\Pi}_t p_t^i + \sum_{\ell=1}^{L}\Big(\frac{\beta_0 \Pi_t^\ell}{(\frac{\mu_\ell}{N})^2 - 2\frac{\mu_\ell}{N} + 2} - \frac{\beta_0 \breve{\Pi}_t}{2}\Big) p_t^\intercal v_\ell v_\ell(i),$$

$$\begin{aligned} -\dot{\breve{\Pi}}_t &= -2\alpha_0 \breve{\Pi}_t - \frac{\beta_0^2 (\breve{\Pi}_t)^2}{2} + q_t, \\ -\dot{\Pi}_t^\ell &= -2(\alpha_0 - \frac{\eta \mu_\ell}{N})\Pi_t^\ell - \frac{\beta_0^2 (\Pi_t^\ell)^2}{(\frac{\mu_\ell}{N})^2 - 2\frac{\mu_\ell}{N} + 2} + q_t, \end{aligned} \tag{14}$$

with $\breve{\Pi}_T = \Pi_T^\ell = q_T$, and $p_t = [p_t^1, \ldots, p_t^N]^\intercal$. See e.g. [Gao and Mahajan, 2019]

Controlling Epidemic Networks via Spectral Decomposition

Limit Graphon Control Problem ($\mathbf{p}_t, \mathbf{u}_t \in L^2[0,1]$, $\bar{\mathbf{A}} = \sum_{\ell=1}^{\infty} \lambda_\ell \mathbf{f}_\ell \mathbf{f}_\ell^\mathsf{T}$)

If the graphon limit $\bar{\mathbf{A}}$ for $\{\bar{\mathbf{A}}_n\}$ exists, then for $\gamma \in [\underline{\gamma}, \overline{\gamma}] \subset [0,1]$,

$$\begin{aligned} \dot{\mathbf{p}}_t(\gamma) &= -\alpha_0 \mathbf{p}_t(\gamma) + \eta \int_0^1 \bar{\mathbf{A}}(\gamma,\rho)\mathbf{p}_t(\rho)d\rho + \beta_0 \mathbf{u}_t(\gamma), \\ J(\mathbf{u}) &= \int_0^T (q_t\|\mathbf{p}_t\|_2^2 + \|\mathbf{u}_t\|_2^2 + \|(\mathbb{I} - \bar{\mathbf{A}})\mathbf{u}_t\|_2^2)dt + q_T\|\mathbf{p}_T\|_2^2 \end{aligned} \tag{15}$$

Optimal solution at location γ:

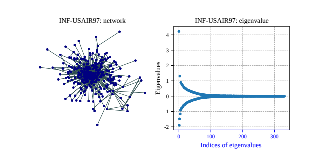
$$\mathbf{u}_t(\gamma) = \frac{\beta_0}{2}\breve{\Pi}_t \mathbf{p}_t(\gamma) + \sum_{\ell=1}^{\infty} \Big(\frac{\beta_0 \Pi_t^\ell}{2 - 2\lambda_\ell + \lambda_\ell^2} - \frac{\beta_0}{2}\breve{\Pi}_t\Big)\langle \mathbf{p}_t, \mathbf{f}_\ell\rangle \mathbf{f}_\ell(\gamma) \tag{16}$$

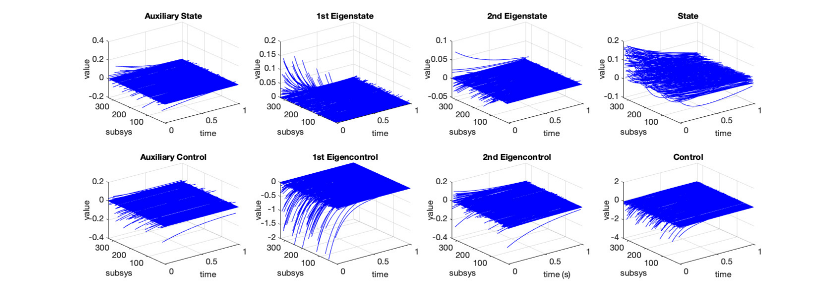
$$\begin{aligned} -\dot{\breve{\Pi}}_t &= -2\alpha_0\breve{\Pi}_t - \frac{\beta_0^2(\breve{\Pi}_t)^2}{2} + q_t, \qquad \breve{\Pi}_T = q_T \\ -\dot{\Pi}_t^\ell &= -2(\alpha_0 - \eta\lambda_\ell)\Pi_t^\ell - \frac{\beta_0^2(\Pi_t^\ell)^2}{(\lambda_\ell)^2 - 2\lambda_\ell + 2} + q_t, \qquad \Pi_T^\ell = q_T \end{aligned} \tag{17}$$

See e.g. [Gao and Caines, 2019b].

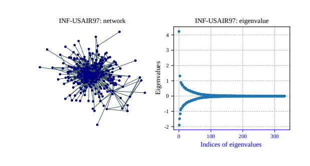
Controlling Epidemic Networks via Spectral Decomposition

Parameters:
$\alpha_0 = -0.5, \beta_0 = 1, \eta = 1.5,$
$q_t = 2, q_T = 4, T = 1$ time unit.





The simulation of the controlled disease process with couplings represented by the contact network corresponding to USAir97 [Pajek].



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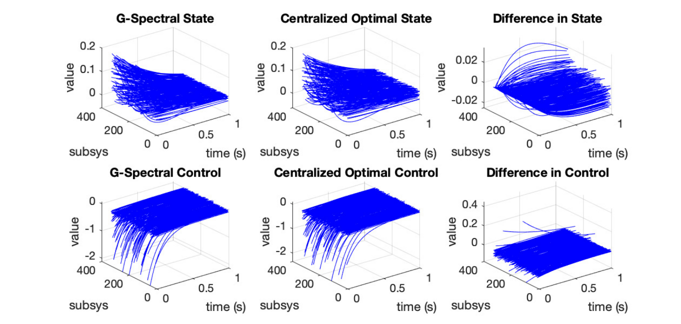
$\alpha_0 = -0.5, \beta_0 = 1, \eta = 1.5,$

$q_t = 2, q_T = 4, T = 1$ time unit.



Approximate control based on the spectral approximation with the most significant eigendirection for the contact network USAir97 [Pajek].

Conclusion

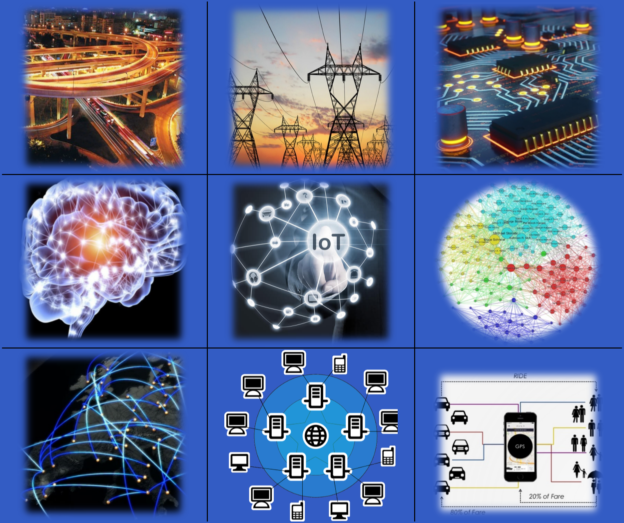
Summary

- Spectral representations of two types of graphons
- Explicit representation of controllability Gramian based on spectral decompositions
- Low-dimensional spectral approximations of networks/graphons
- Initial Exploratory investigation of the utility of the spectral analysis in graphon systems to control epidemic process.

Future work

- Positivity constrains on states and control
- Selection of threshold for spectral approximation
- Graphon as non-parametric models for control design
- Relationship between structures and spectral properties
- ...

Thank you!



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