

Interpretable Machine Learning for Predicting the Synchronization of Coupled Oscillators

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Background

- **Problem of Interest:** The long-term global synchronization of coupled oscillators on graphs.
- **Difficulty:** In spite of several sufficient conditions for model parameters (e.g., large coupling strength) or initial configuration (e.g., phase concentration being an open semicircle) are known, it often seems intractable to obtain analytical or asymptotic solutions to prediction problems in general.

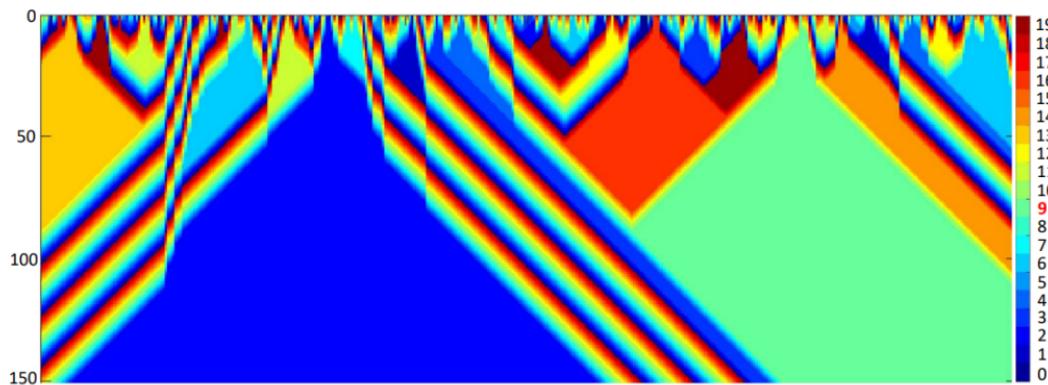


Figure: Example of Partial Synchronization of a System of Coupled Oscillators. (Simulation of 20-color FCA on a path of 400 nodes for 150×20)

Prior Work & Our Approach

- **Prior Work:** *Learning to Predict Synchronization (L2PSync)* views the synchronization prediction problem as a **binary classification task**. This framework shows fundamental classification algorithms trained on large enough datasets of initial dynamics can successfully predict whether a system on highly heterogeneous sets of unknown graphs will eventually synchronize with surprisingly high accuracy.

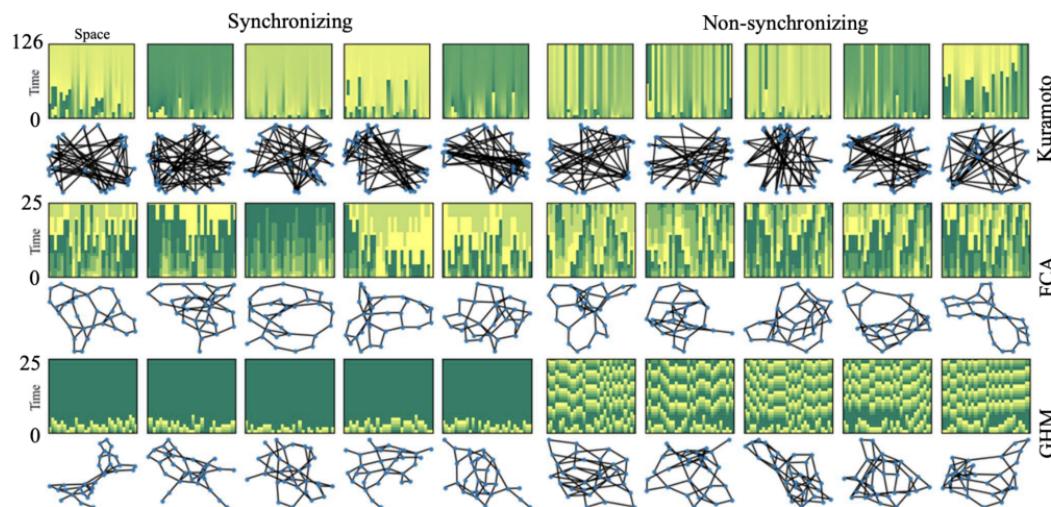


Figure: Sample points in the 30-node training data set for synchronization predict

Prior Work & Our Approach

- **Our Work: Interpretable L2PSync.** Given any connected graph $G = (V, E)$, coupling ϕ , and fixed parameters $n \in \mathbb{N}, T \gg r > 0$. Develop a machine learning method that can predict the following indicator function $\mathbf{1}(X_T \text{ is synchronized})$, while also output **discriminating features** that are used for classification, based on the initial trajectory $(X_t)_{0 \leq t \leq r}$ that are determined by graph topology and the coupling ϕ and optionally also with statistics of graph G .

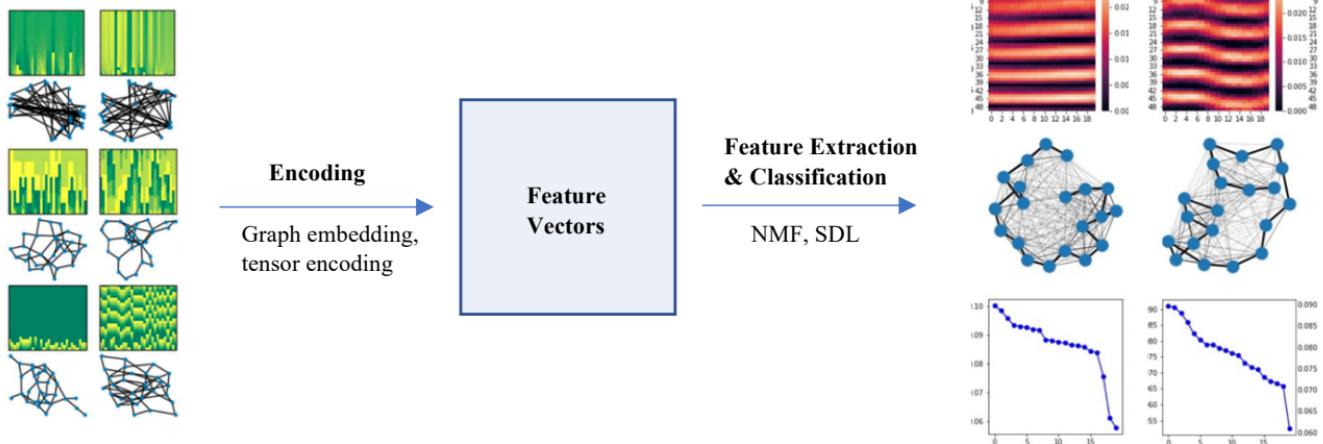


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Models of Coupled Oscillators

- Main barrier: Most traditional oscillator models assume that each oscillator is **continuous-time** and **continuous-state** —→ the dynamics quickly become intractable on heterogeneous underlying graphs.
- Solution: **Discretize** the time and state of the model by using *Cellular Automata* instead of the usual continuous model.
- Three commonly studied models of Coupled Oscillators:
 - (1) Kuramoto Model (KM)
 - (2) Firefly Cellular Automata (FCA)
 - (3) Greenberg-Hastings Model (GHM)

Kuramoto Model

- One of the most well-studied continuous-state oscillator models over the years.
- The evolution of the phase dynamics of the initial phase configuration $X_0 : V \rightarrow \Omega = \mathbb{R}/2\pi\mathbb{Z}$ is determined by the following system of ordinary differential equations.

$$\frac{d}{dt}X_t(v) = \omega_v + K \sum_{u \in \mathcal{N}(v)} \sin(X_t(u) - X_t(v)) \quad \forall v \in V \quad (1)$$

where $\mathcal{N}(v)$ represents the set of nodes neighboring v in G , ω_v denotes the intrinsic frequency of v , and K denotes the *coupling strength* of the model.

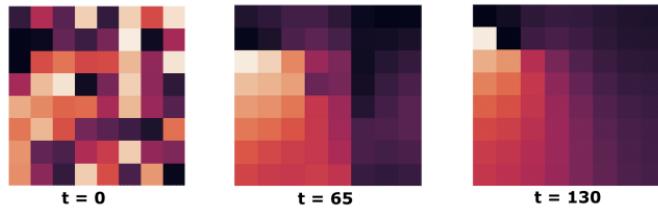


Figure: Simulation of the Kuramoto Model on an 8×8 2D-Grid graph (8-by-8 2D Lattice)

Firefly Cellular Automata (FCA)

The map X maps the set of vertices to a corresponding state, written as $X : V \rightarrow Z/\kappa Z$. At any specific time t , the node v takes the state/coloring of $X_t(v)$. Define the neighbors of blinking states as a set $\mathcal{N}(b)$, the blinking state as $b(\kappa) = \lfloor \frac{\kappa-1}{2} \rfloor$, then the transition rule of FCA writes:

$$(FCA) \quad X_{t+1}(v) = \begin{cases} X_t(v) & X_t(v) > b(\kappa), \text{ and } X_t(u) = b(\kappa) \text{ for some } u \in N(v), \\ X_t(v) + 1 & \text{otherwise} \end{cases} \quad (2)$$

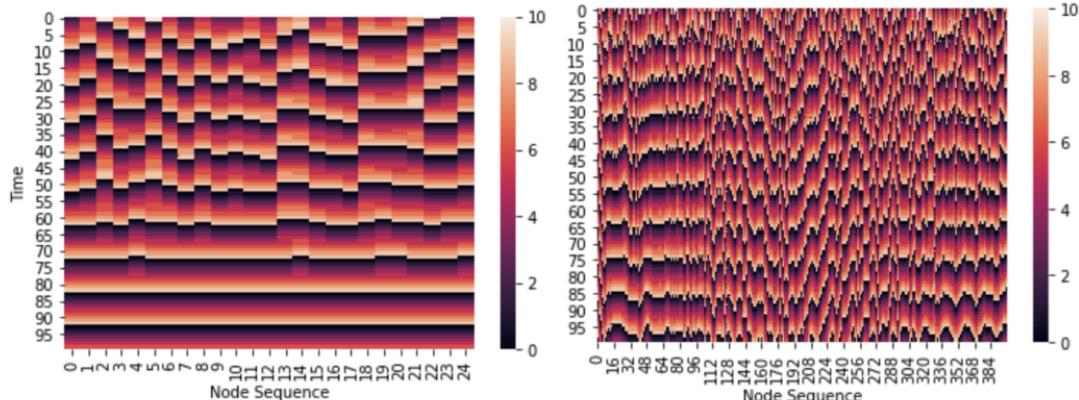


Figure: Illustrative example of FCA($\kappa = 10$). Left: A synchronizing example of FCA model on 5×5 2d grid. Right: A non-synchronizing example of FCA model on 20×20 2d grid.

Greenberg-Hastings Model (GHM) Transition Rule

GHM: Emulates an excitable media where the neighbors affect each other in a diffusive local transportation fashion. e.g. forest fire

GHM Transition Rule: The time evolution follows the following rules where $N(v)$ gives the neighbor set of node v .

$$X_{t+1}(v) = \begin{cases} 0 & \text{if } X_t(v) = 0 \quad \& \quad X_t(u) \neq 1 \forall u \in N(v) \\ 1 & \text{if } X_t(v) = 0 \quad \& \quad \exists u \in N(v) \text{ s.t. } X_t(u) = 1 \\ (X_t(v) + 1) \bmod (\kappa) & \text{otherwise} \end{cases} \quad (3)$$

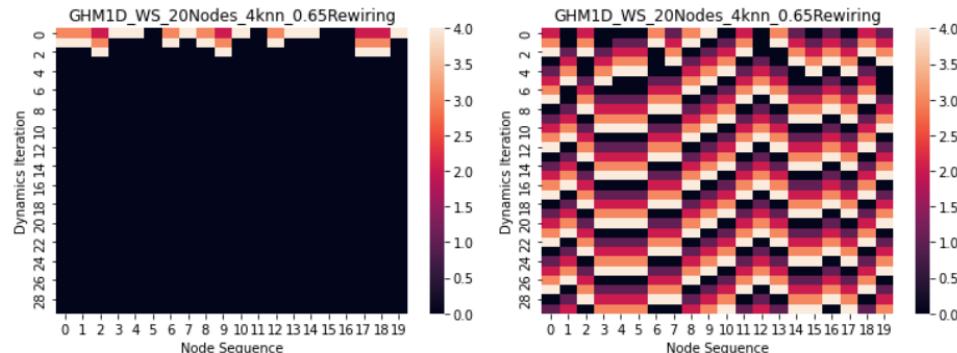


Figure: Simulation of the GHM synchronizing and non-synchronizing cases on 20-node Watts Strogatz graphs of 4 nearest neighbors with 0.65 rewiring probability.

Feature encoding methods

- ▶ (Subgraph sampling):

Use random Hamiltonian path sampling to get structured subgraphs

- ▶ (Encoding graph structure):

Vectorizing adjacency matrix

Spectral embedding

Graph embedding algorithms (e.g., node2vec, graph2vec)

- ▶ (Encoding graph structure & dynamics):

Colored adjacency matrix encoding

Tensor encoding of dynamics on graphs

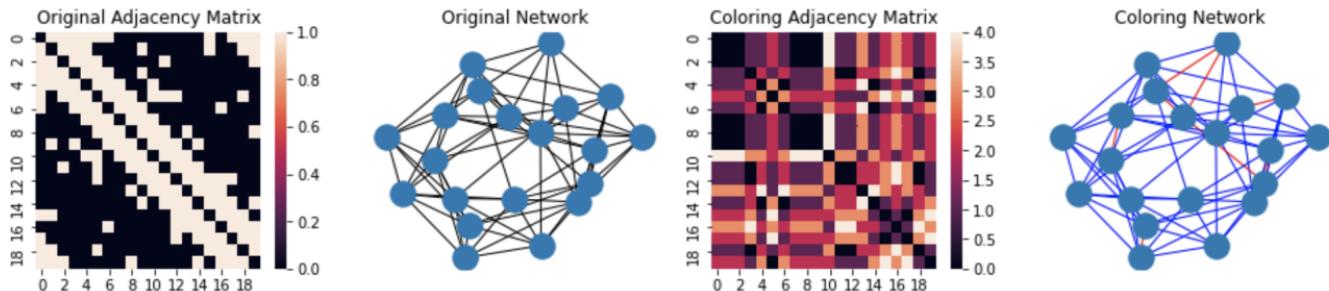


Figure: Left: Original adjacency matrix and network plot on a randomly generated 20-node NWS network. Right: Colored adjacency matrix and colored network plot on the same NWS network. Red edges indicate there is no color difference between two vertices, while blue edges indicate there is color different between two vertices.

Feature extraction by dictionary learning

- Dictionary Learning is a machine learning technique that is used to learn interpretable latent structures of complex data sets in order to realize what features of the data the model considers to be the most relevant ones for its task. It consists of two main tasks:
 - Sampling a large number of structured subsets (usually square patches) of a data set.
 - Applying *non-negative matrix factorization* as described below, to find a set of basis elements that form our *dictionary*.

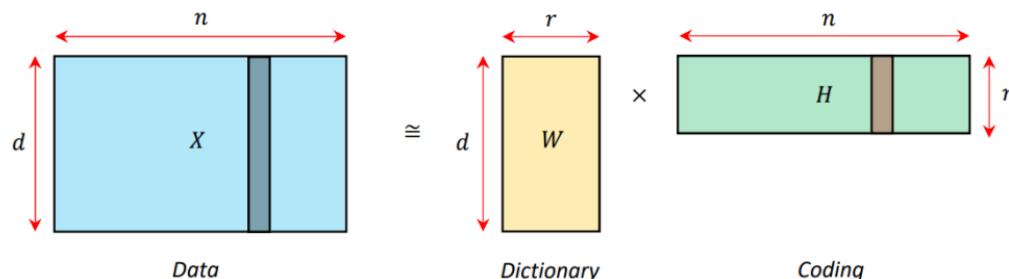


Figure: Illustration of matrix factorization.

$$\inf_{\mathbf{W} \in \mathbb{R}_{\geq 0}^{d \times r}, \mathbf{H} \in \mathbb{R}_{\geq 0}^{r \times n}} \|\mathbf{X} - \mathbf{WH}\|_F^2$$

Supervised Dictionary Learning

- Supervised dictionary learning (SDL) provides systematic approaches to balance some degree of trade-off between dictionary learning and classification, the objective of SDL can naturally be formulated as a multi-objective optimization problem as below:

$$\min_{\mathbf{W}, \mathbf{H}, \boldsymbol{\beta}} L(\mathbf{W}, \mathbf{H}, \boldsymbol{\beta}) := \underbrace{\left(\sum_{i=1}^n \ell(y_i, \mathbf{g}(\mathbf{a}(\mathbf{x}_i, \mathbf{W}, \mathbf{h}_i, \boldsymbol{\beta}))) \right)}_{\text{classification loss}} + \xi \underbrace{\|\mathbf{X}_{\text{data}} - \mathbf{WH}\|_F^2}_{\text{dictionary learning loss}}$$

subject to: Constraints on $\mathbf{W} \in \mathbb{R}^{p \times r}$, $\mathbf{H} \in \mathbb{R}^{r \times n}$, and $\boldsymbol{\beta} \in \mathbb{R}^{r \times \kappa}$

where $\mathbf{X}_{\text{data}} = [\mathbf{x}_1, \dots, \mathbf{x}_n] \in \mathbb{R}^{p \times n}$, $\mathbf{H} = [\mathbf{h}_1, \dots, \mathbf{h}_n] \in \mathbb{R}^{r \times n}$, and $\ell(\cdot)$ is a classification loss and is usually taken as the negative log likelihood

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Effect of Sub-Graph Size – Experimental Setup

- Three global networks: UCLA, Caltech, and NWS - Facebook100 dataset Fall 2005

Table: Graph Statistics of the Networks used for sampling subgraphs

Networks	UCLA	Caltech	NWS
Number of Nodes	20467	769	20000
Number of Edges	747613	16656	16702185
Edge Density	0.0036	0.0564	0.0835
Average Clustering Coefficient	0.2149	0.4092	0.3092

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- Generated k-paths from each networks for $10 \leq k \leq 40$, sampled 100 sub-graphs for each path, and ran the Kuramoto dynamics on each, to compute the ratio of graphs on which the Kuramoto dynamics synchronize.

Effect of Sub-Graph Size – Experimental Setup

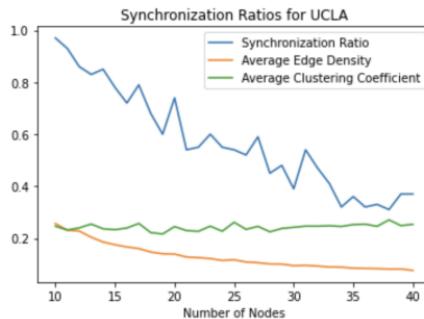
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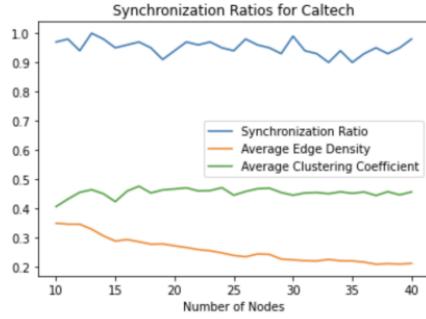
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- Generated k-paths from each networks for $10 \leq k \leq 40$, sampled 100 sub-graphs for each path, and ran the Kuramoto dynamics on each, to compute the ratio of graphs on which the Kuramoto dynamics synchronize.
- Also noted the average Clustering Coefficient and Edge Density for each iteration to learn correlations.

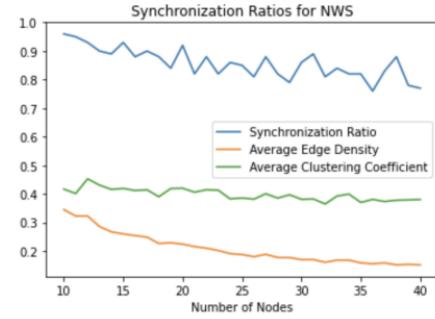
Effect of Sub-Graph Size – Results



(a) UCLA Synchronization Ratio



(b) Caltech Synchronization Ratio

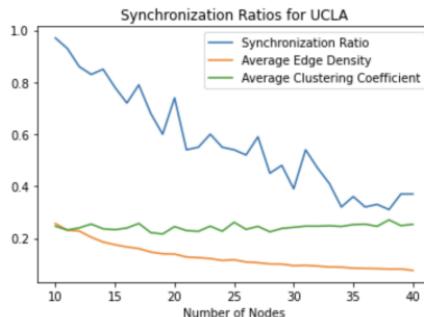


(c) NWS Synchronization Ratio

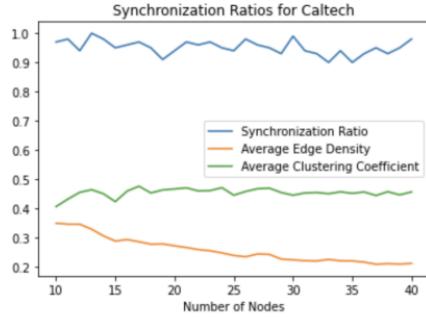
Figure: Plots showing the *Average Synchronization Ratio* for the 100 subgraphs sampled from UCLA, Caltech and NWS networks with the number of nodes ranging from 10 to 40. Also superimposed on the plot is the *Average Edge Density* and the *Average Clustering Coefficient* for the 100 graphs sampled at each new iteration.

- Synchronization ratio decreases the quickest for UCLA, moderately for NWS and in the case of Caltech, remains almost the same (above $\sim 90\%$)

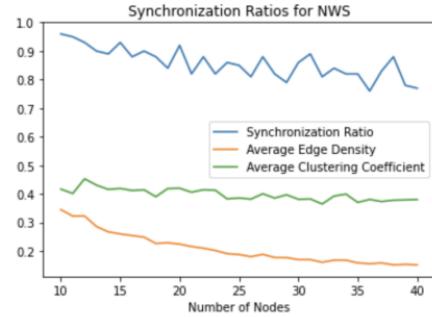
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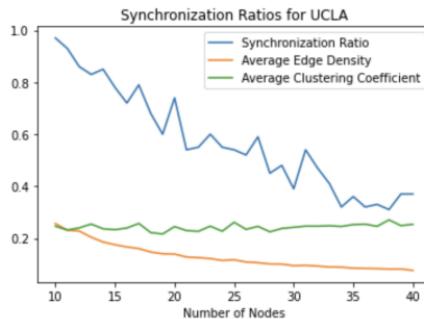


(c) NWS Synchronization Ratio

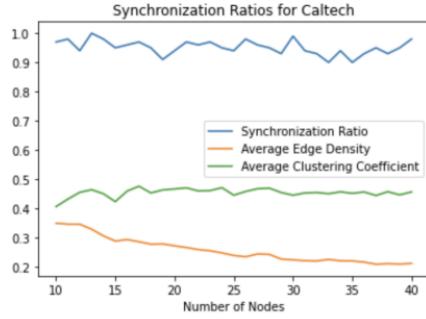
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- The average clustering coefficient roughly remains the same for each network sub-graphs

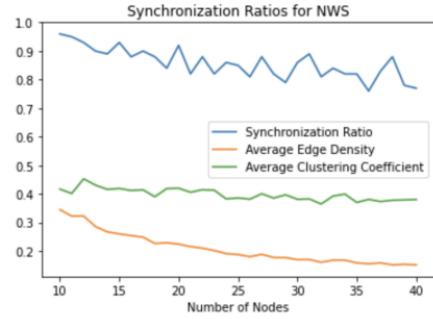
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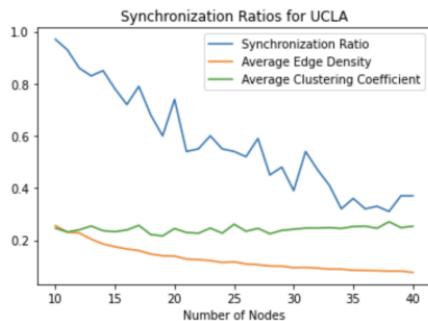


(c) NWS Synchronization Ratio

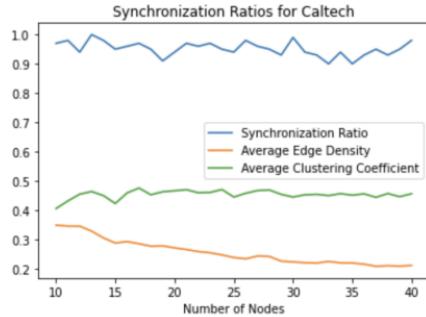
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- Synchronization ratio decreases the quickest for UCLA, moderately for NWS and in the case of Caltech, remains almost the same (above $\sim 90\%$)
- The average clustering coefficient roughly remains the same for each network sub-graphs
- The average edge density of the network sub-graphs, decay in an asymptotic fashion

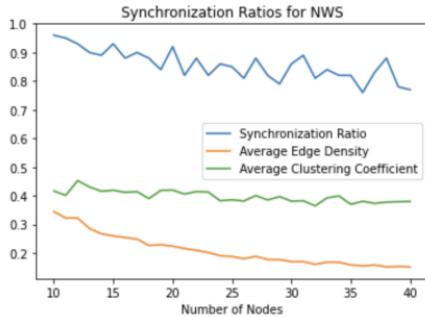
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- Inference:

- UCLA: Sparse – 0.35% edge density (**low**) and 0.25 Average Clustering Coefficient (**low**)
- NWS: Quite dense – 8.5% edge density (**high**) and 0.31 Average Clustering Coefficient (**moderate**)
- Caltech: Quite dense – 5.5% edge density (**moderate to high**) and 0.41 Average Clustering Coefficient (**high**)

Non-negative Matrix Factorization – Experimental Setup

- For each of the three networks, we sample 1600 50-node sub-graphs and simulate the Kuramoto dynamics on them.

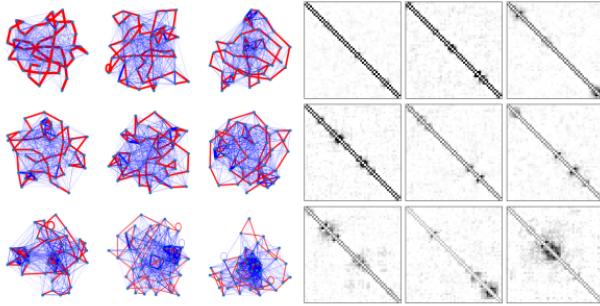
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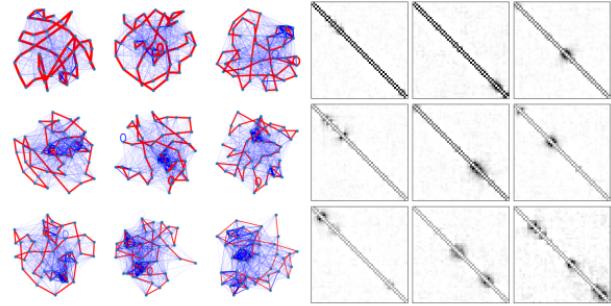
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- Next, we separate out the cases of synchronization and non-synchronization into two separate matrices while ensuring a balanced split. We learn 9 dictionary atoms using non-negative matrix factorization on these matrices containing feature spaces for synchronized and non-synchronized cases separately.

Non-negative Matrix Factorization – UCLA Results



(a) UCLA Synchronization Dictionaries

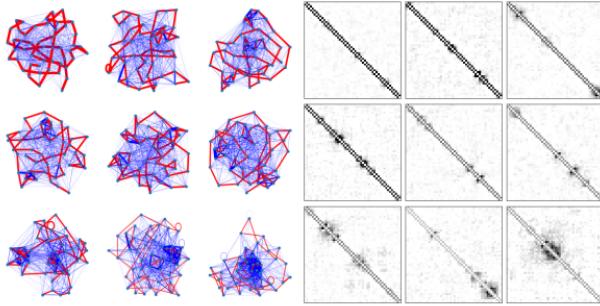


(b) UCLA Non-Synchronization Dictionaries

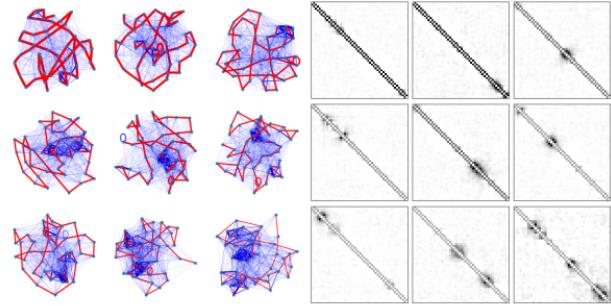
Figure: Figures showing the Dictionary atoms learned using Non-negative Matrix Factorization and their Graphical Representations for UCLA network.

- Dictionaries have “communities” lying along the Hamiltonian path

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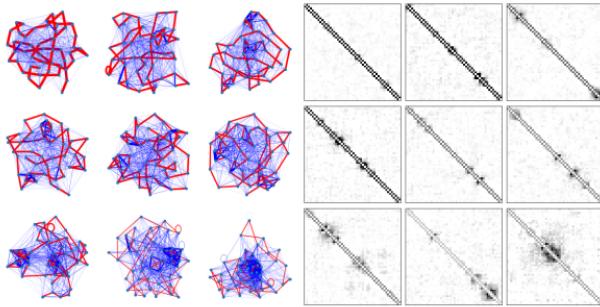


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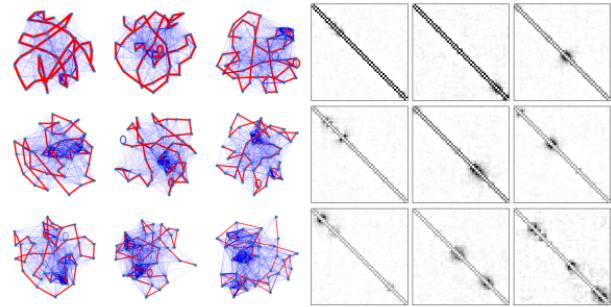
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- Dictionaries have “communities” lying along the Hamiltonian path
- Feature space for UCLA contains sparse graphs

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- Dictionaries have “communities” lying along the Hamiltonian path
- Feature space for UCLA contains sparse graphs
- Distinguishable edge density (**Graphs look denser for synchronizing case**)

Non-negative Matrix Factorization – UCLA Results

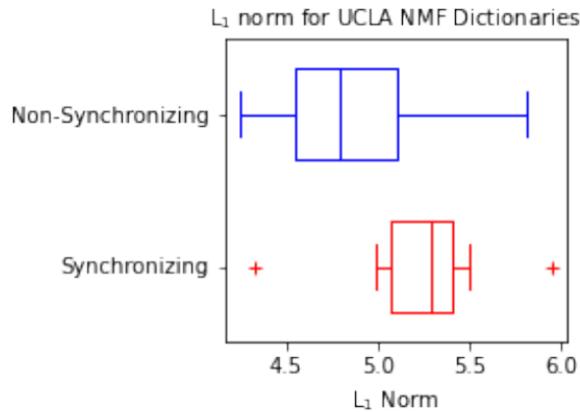
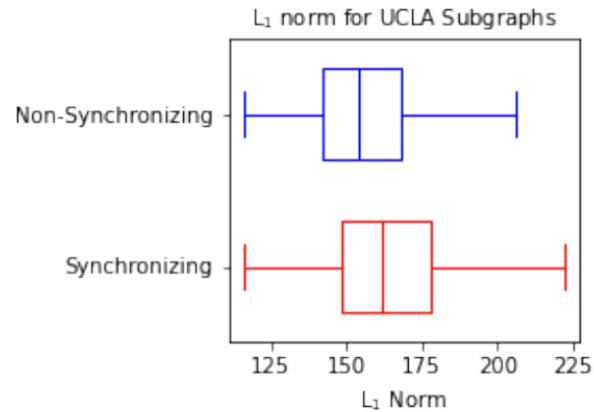
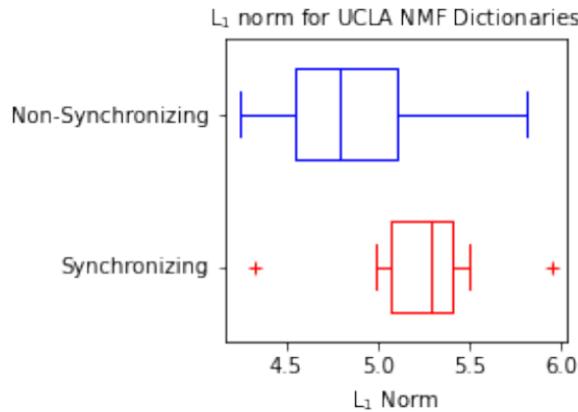
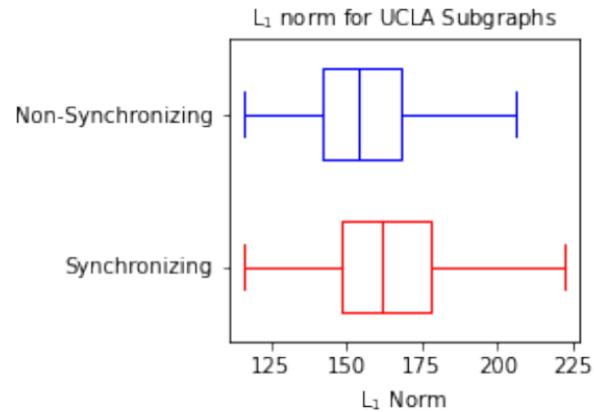
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Figure: UCLA Dictionaries L₁ norm Box Plot in comparison to the L₁ norm Box Plot for the Sub-Graphs for UCLA

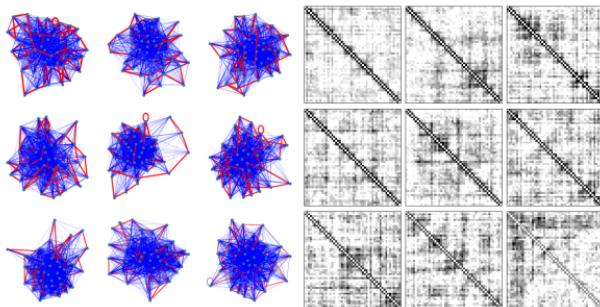
- Median for **synchronizing** higher than median and even 75th percentile for **non-synchronizing**

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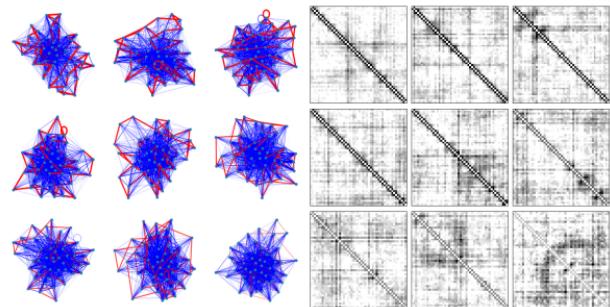
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- Median for **synchronizing** higher than median and even 75th percentile for **non-synchronizing**
- Box plot for the original sub-graphs – higher median L₁ norm for **synchronizing**

Non-negative Matrix Factorization – Caltech Results



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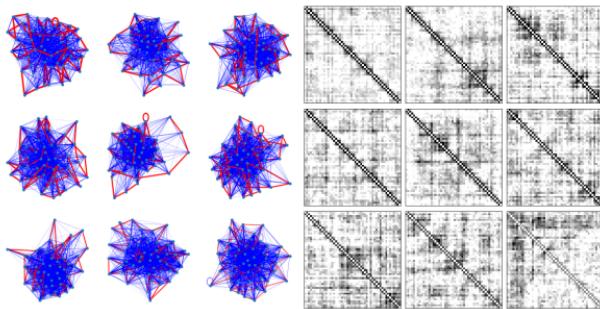


(b) Caltech Non-Synchronization Dictionaries

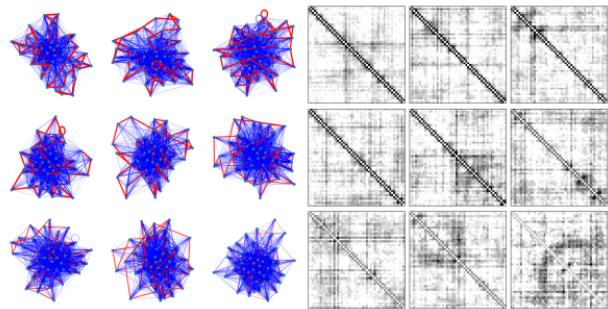
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- No significant communities like UCLA

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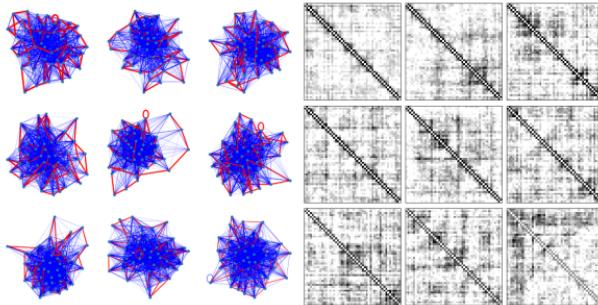


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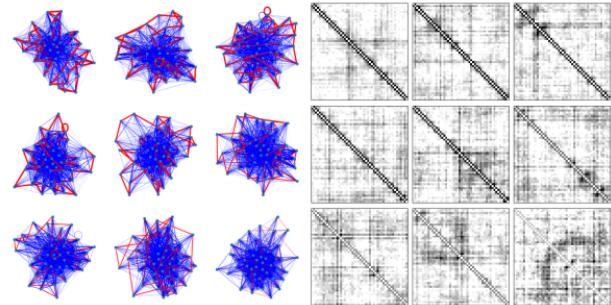
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- “Pivot nodes” lying along the Hamiltonian path.

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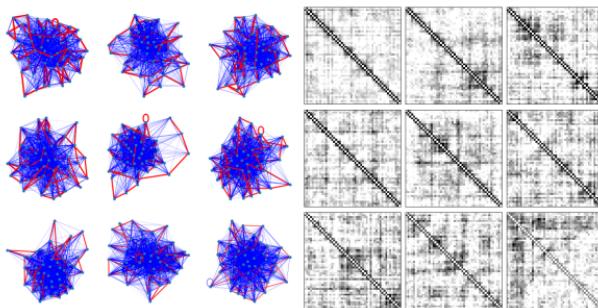


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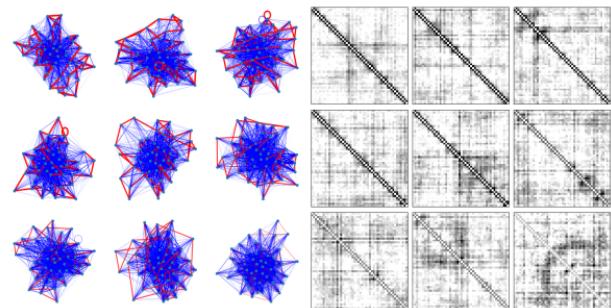
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- No significant communities like UCLA
- “Pivot nodes” lying along the Hamiltonian path.
- Feature space for Caltech contains dense graphs

Non-negative Matrix Factorization – Caltech Results



(a) Caltech Synchronization Dictionaries



(b) Caltech Non-Synchronization Dictionaries

Figure: Figures showing the Dictionary atoms learned using Non-negative Matrix Factorization and their Graphical Representations for Caltech network.

- No significant communities like UCLA
- “Pivot nodes” lying along the Hamiltonian path.
- Feature space for Caltech contains dense graphs
- Hard to distinguish edge density; **synchronizing** cases arguably contain more pivot nodes

Non-negative Matrix Factorization – Caltech Results

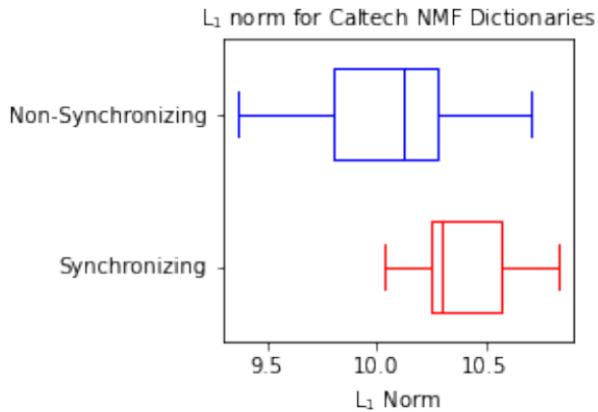
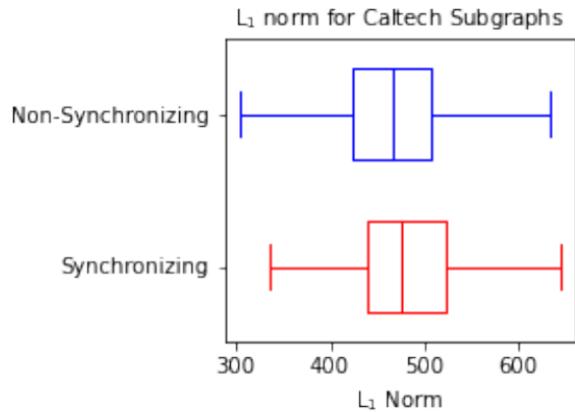
(a) Caltech Dictionaries L₁ norm Box Plot(b) Caltech Subgraphs L₁ norm Box Plot

Figure: Caltech Dictionaries L₁ norm Box Plot in comparison to the Box Plot for the Sub-Graphs for Caltech

- Median for **synchronizing** higher than median and even 75th percentile for **non-synchronizing**

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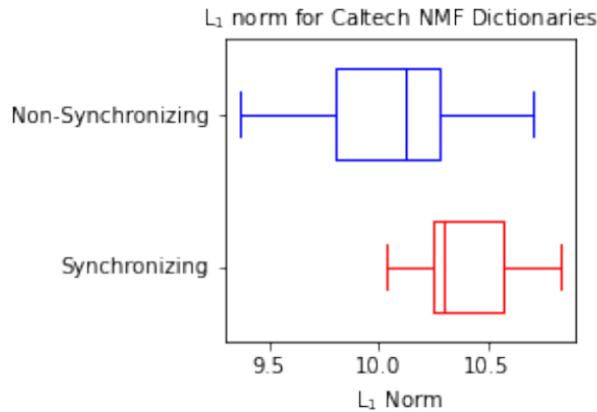
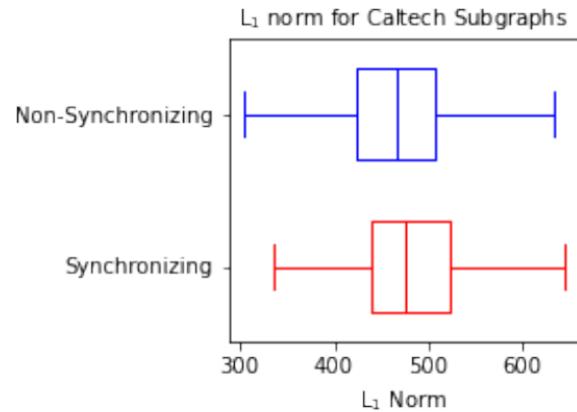
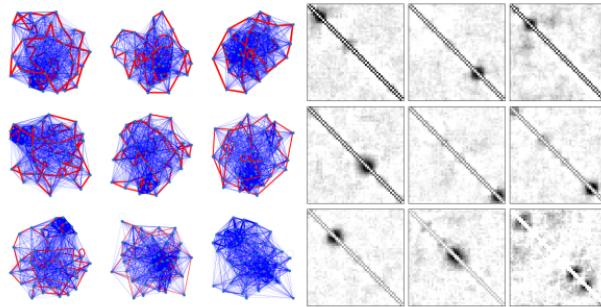
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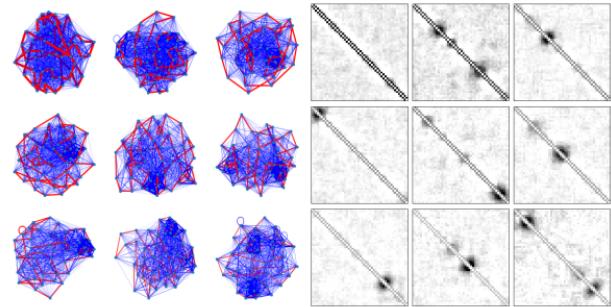
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Non-negative Matrix Factorization – NWS Results



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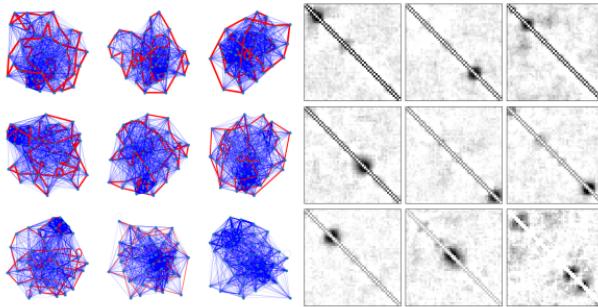


(b) NWS Non-Synchronization Dictionaries

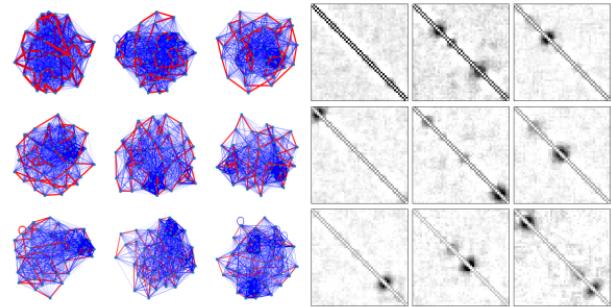
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Non-negative Matrix Factorization – NWS Results



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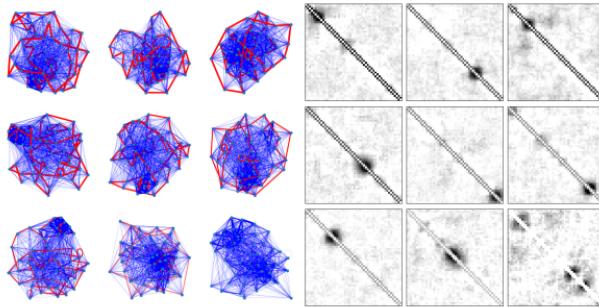


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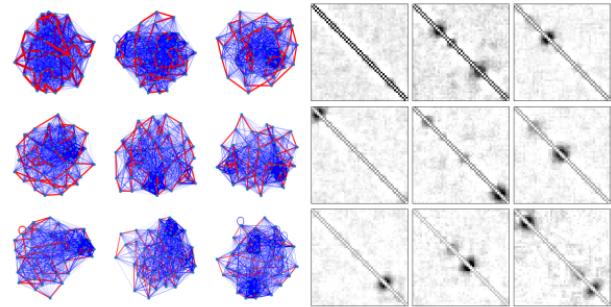
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Non-negative Matrix Factorization – NWS Results

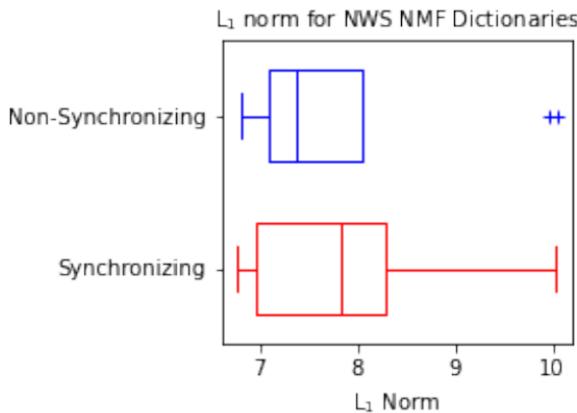
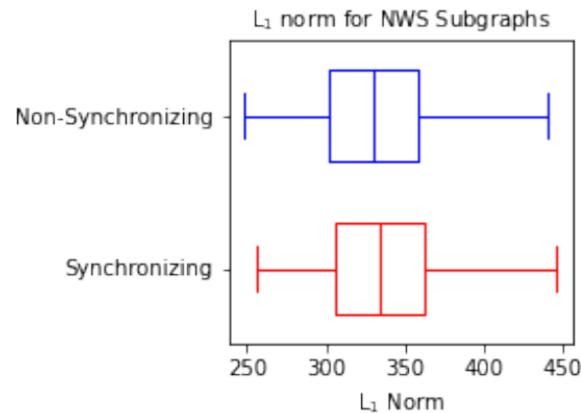
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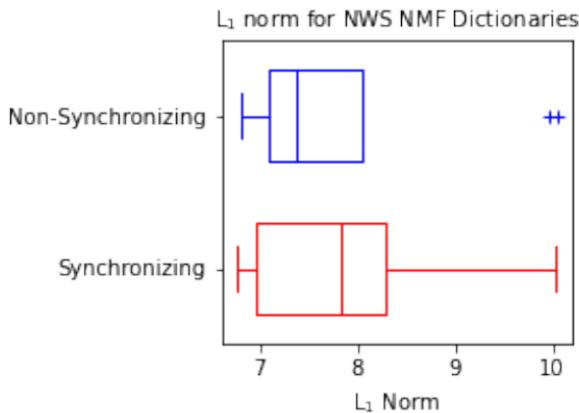
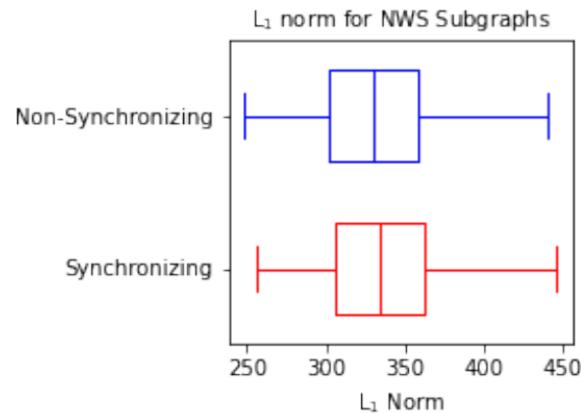
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- Moreover, on applying SDL to such a setting leads to unclear and uninterpretable results, which calls for some alternative approaches

Color-coded Adjacency Matrix at time t

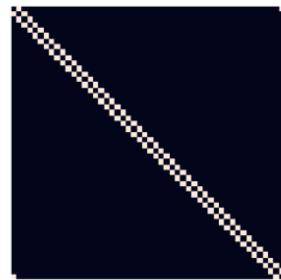
Consider the following two graphs - (1) 25-Node NWS Graph (Synchronizing) and (2) 50-Node Cycle Graph (Non-Synchronizing). Here's their adjacency matrix

Color-coded Adjacency Matrix at time t

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(a) 25-Node NWS Adjacency Matrix



(b) Cyclic Graph Adjacency Matrix

Figure: Adjacency matrices of the two graphs to illustrate the concept of Color-Coded Adjacency Matrix

NWS Color-Coded Adjacency Matrix – Synchronizing

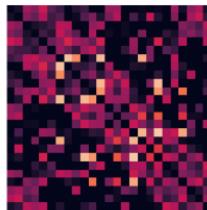
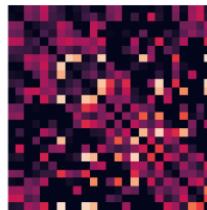
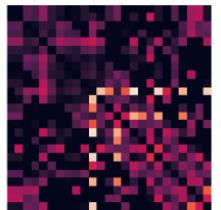
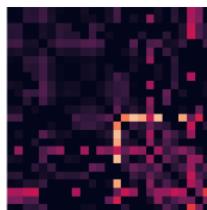
(a) $t = 0$ (b) $t = 50$ (c) $t = 100$ (d) $t = 150$ (e) $t = 200$ (f) $t = 250$

Figure: Kuramoto dynamics on NWS at different iterations mentioned below the figure

Cycle Graph Color-Coded Adjacency Matrix – Non-Synchronizing

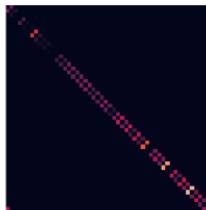
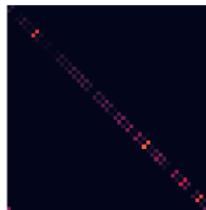
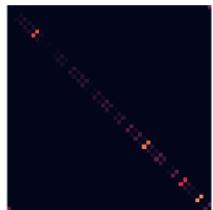
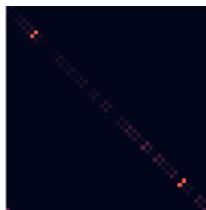
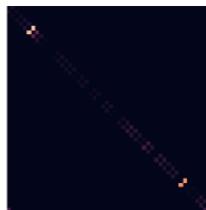
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FCA Dynamics Datasets

Datasets	NWS	UCLA26
# nodes	20	20
Avg of # edges	41.02	25.93
Std of # edges	9.53	4.75
Avg diameter	5.28	11.18
Std of diameter	1.22	3.47
r (training iter)	50	50
T (prediction iter)	200	200
# Sync.	7548	7553
# Nonsync.	2452	2447

Table: Dynamics datasets generated for FCA($\kappa = 8$) on 20-node connected sub-graphs of a large NWS graph and UCLA26. The large NWS graph is generated with 20000 nodes, nearest neighbors of 1000, and shortcut edge probability of 0.7. Each dataset contains 10000 underlying graph structures.

Black-Box Model: Random Forest

1 Dynamics

Black-Box Model: Random Forest

- ① Dynamics
- ② Width of dynamics

Black-Box Model: Random Forest

- ① Dynamics
- ② Width of dynamics
- ③ Shifted dynamics

Shifted Dynamics

Let $G = (V, E)$ be a graph, and let $X : V \rightarrow \mathbb{Z}_\kappa$ be a κ -configuration.

- $X_{shifted} = X + \operatorname{argmin}_{0 \leq a < \kappa} (\max(X + a) \bmod \kappa)$

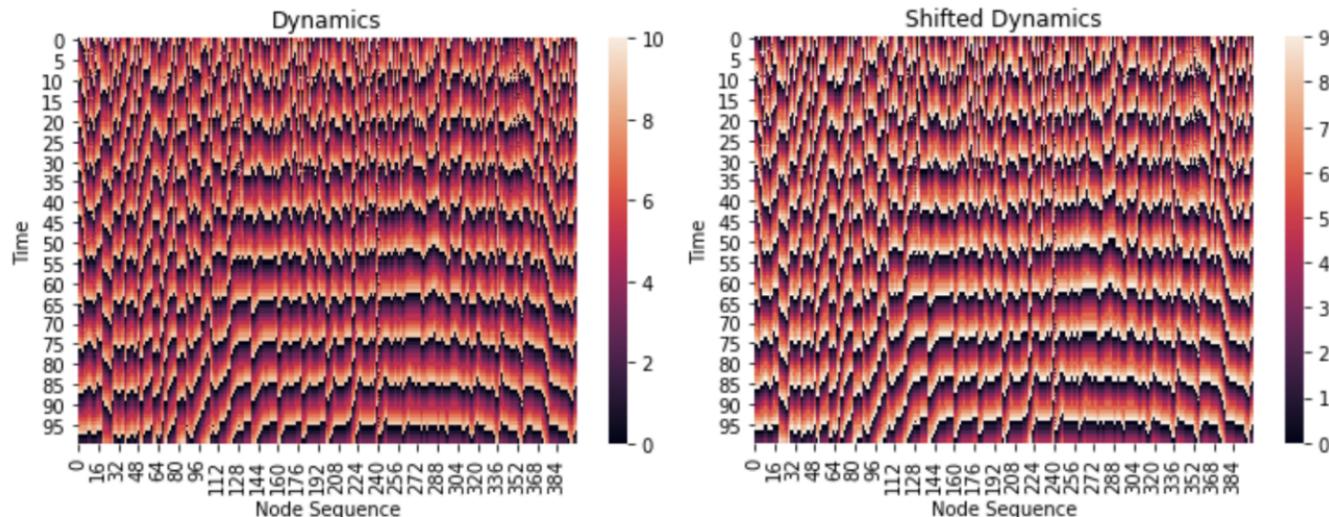


Figure: Left: Heatmap of dynamics from time 0 to time 100 on 20×20 2d grid networks. Right: Heatmap of shifted dynamics from time 0 to time 100 on 20×20 2d grid networks

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- ⑦ Dynamics + spectral embedding
- ⑧ Dynamics + Graph features

Graph Features

Features	
Graph-level	# edges, # nodes, min degree, max degree, diameter, degree assortativity coefficient, # cliques, average clustering coefficient, density
Node-level	Degree centrality, eigenvector centrality, betweenness centrality, closeness centrality, clustering coefficient, degree

Table: Graph features calculated for sub-graphs of a large NWS graph and UCLA26. The graph-level feature is applied to each underlying graph. The node-level feature is applied to each node of each underlying graph.

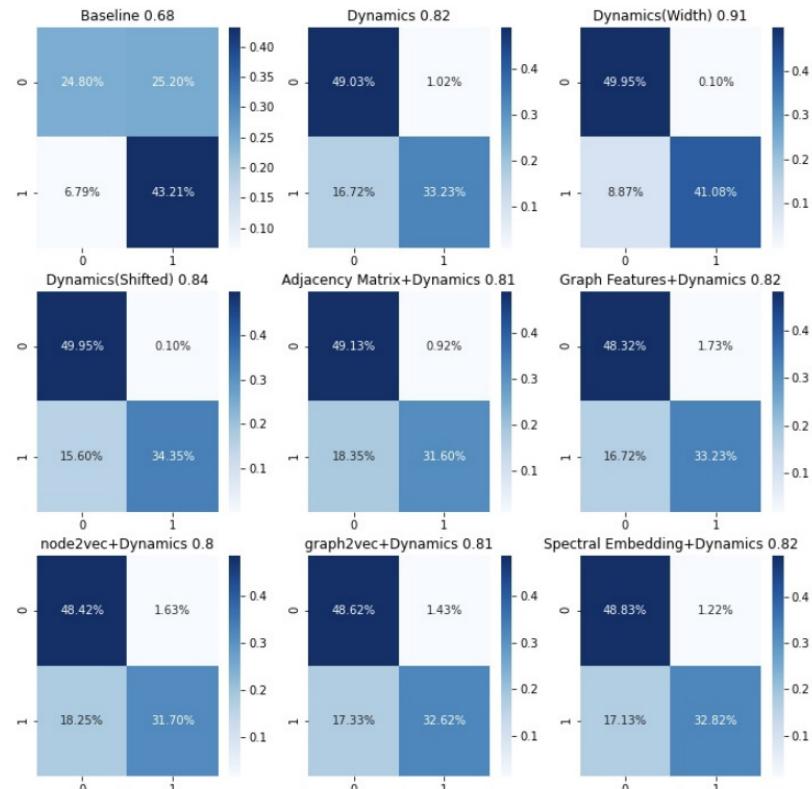


Figure: RF performance on different feature inputs for sub-graphs of a large NWS network. The number in the title is the accuracy score. For each confusion matrix, the x-axis is the predicted value and the y-axis is the actual value. If it is labeled as 0, then it is non-synchronizing. If it is labeled as 1, then it is synchronizing.

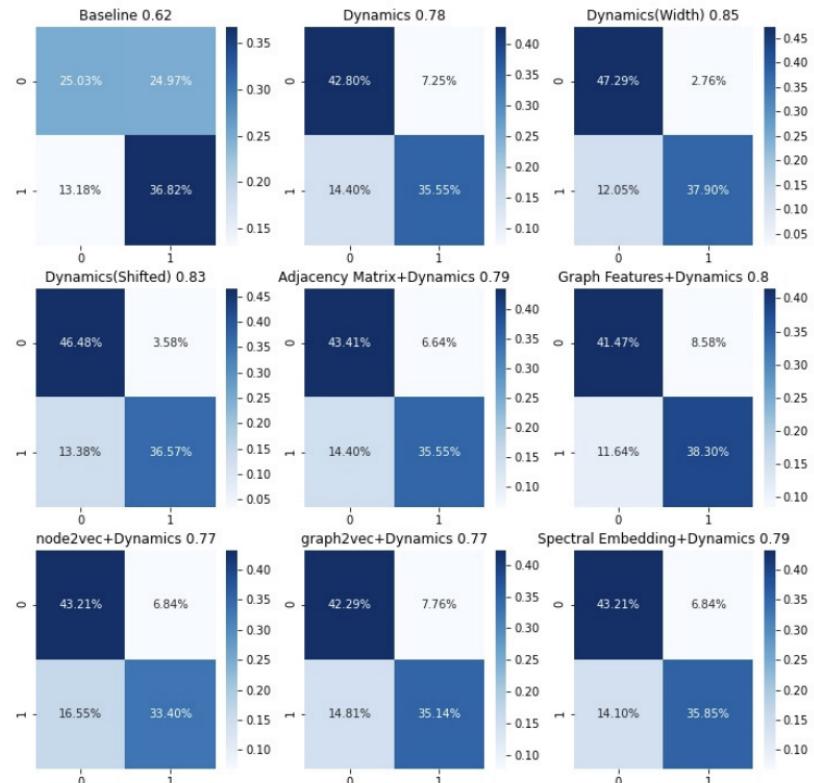
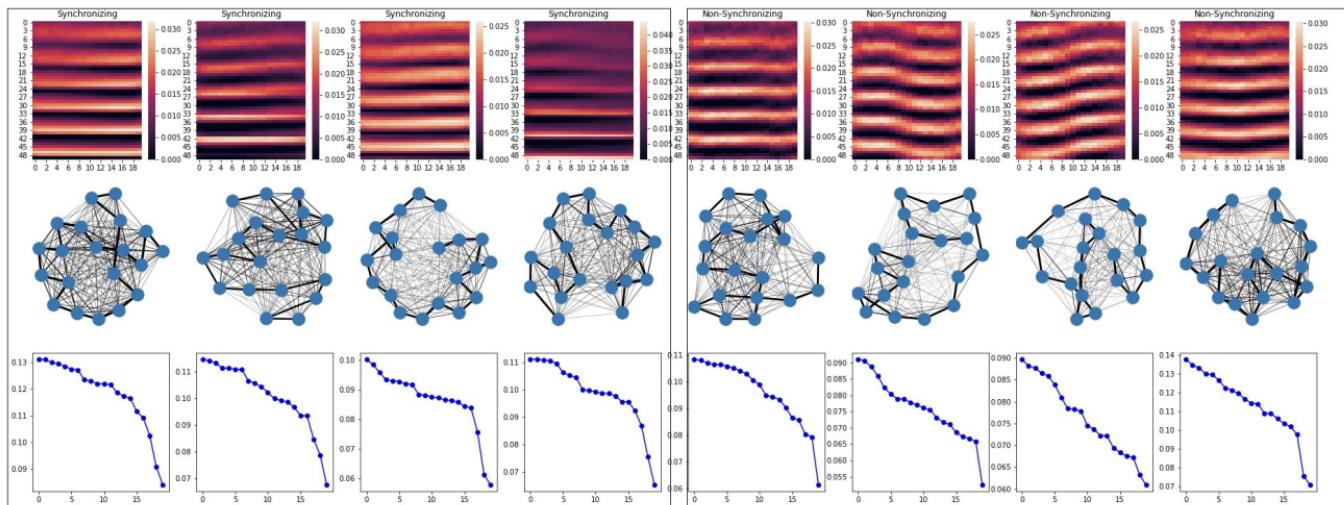


Figure: RF performance on different feature inputs for sub-graphs of UCLA26. The number in the title is the accuracy score. For each confusion matrix, the x-axis is the predicted value and the y-axis is the actual value. If it is labeled as 0, then it is non-synchronizing. If it is labeled as 1, then it is synchronizing.

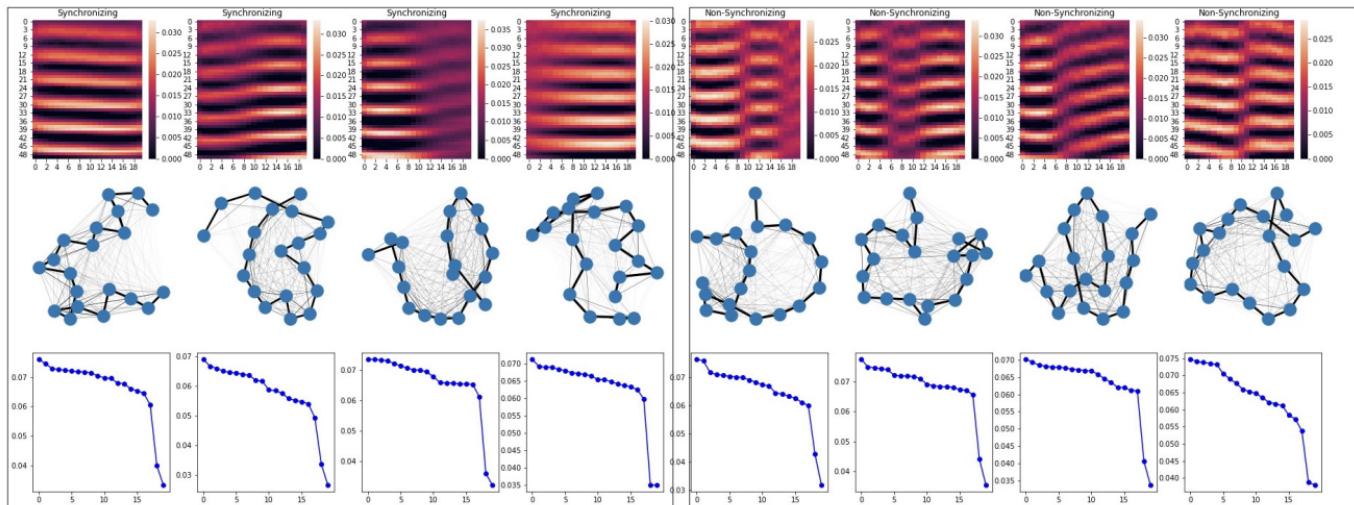
NMF to compare synchronizing and nonsynchronizing pairs

- Dynamics + Adjacency matrix
- apply separately on synchronizing and nonsynchronizing pairs

NMF to compare synchronizing and nonsynchronizing pairs



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SDL on predicting synchronization

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SDL on predicting synchronization

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- ④ Colored adjacency matrix

SDL on predicting synchronization

Feature	Baseline	RF	SDL
Dynamics	0.68	0.82	0.68
Shifted dynamics	0.68	0.84	0.68
Dynamics + adjacency matrix	0.68	0.81	0.61
Colored adjacency matrix	0.68	0.83	0.80

Table: The classification accuracy of the baseline model, RF model, and SDL model based upon different feature inputs from the dataset of NWS

SDL on predicting synchronization

Feature	Baseline	RF	SDL
Dynamics	0.61	0.78	0.63
Shifted dynamics	0.61	0.83	0.68
Dynamics + adjacency matrix	0.61	0.79	0.50
Colored adjacency matrix	0.61	0.82	0.74

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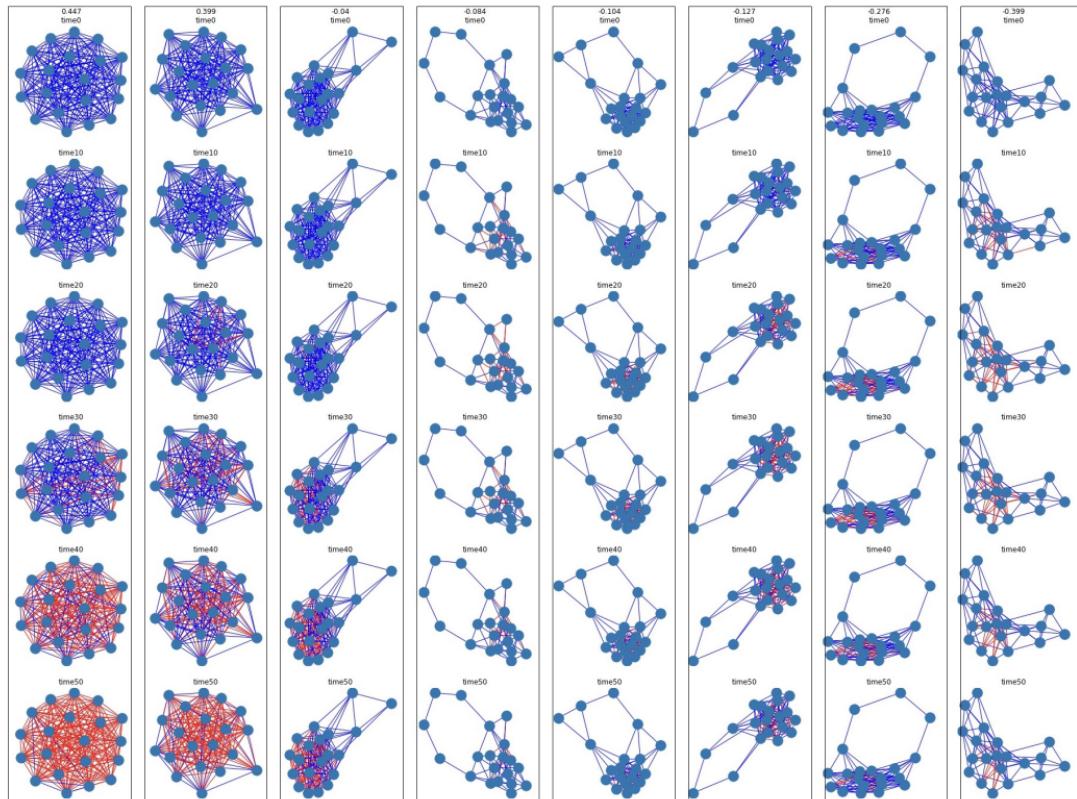


Figure: The dictionary elements learned from SDL on the colored adjacency matrix from dataset of NWS.

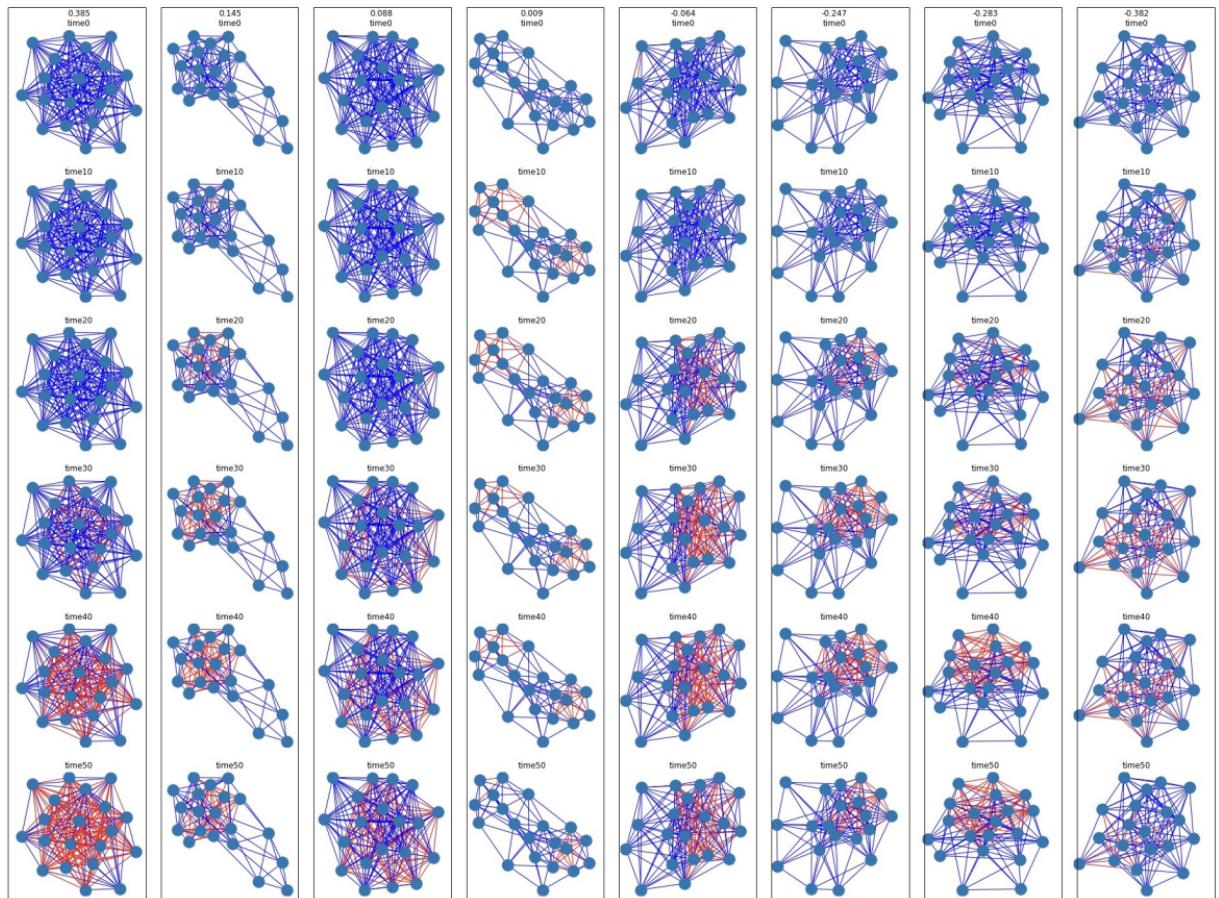


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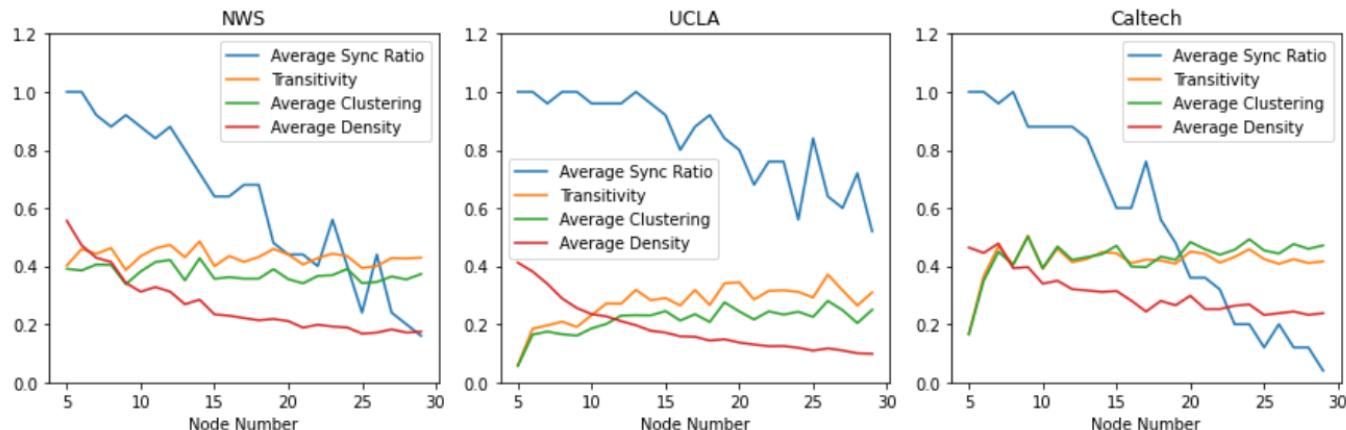


Figure: Synchronization ratio, average clustering coefficient, average transitivity, and average density trend with different node number in NWS, UCLA, and Caltech networks

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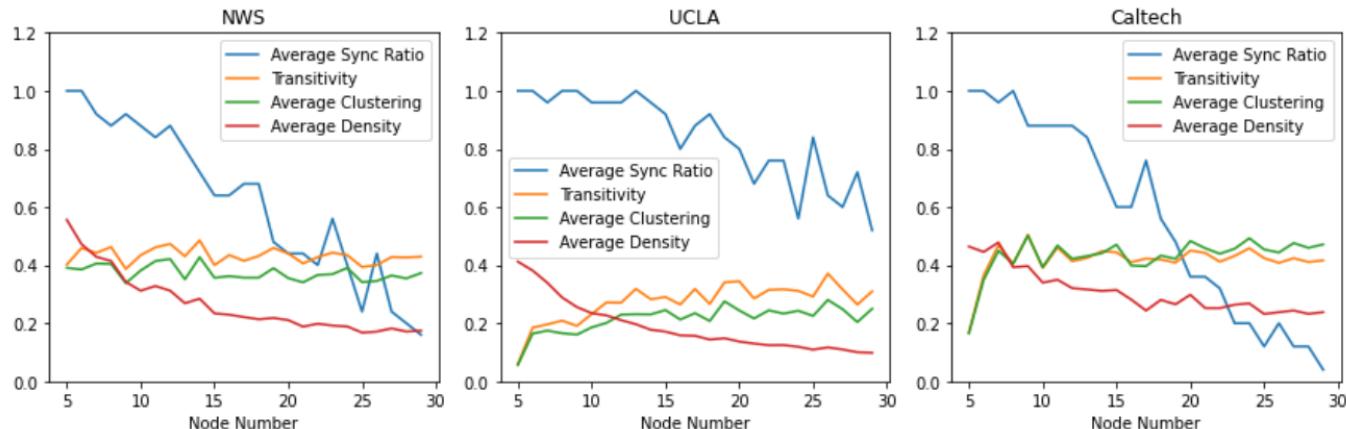


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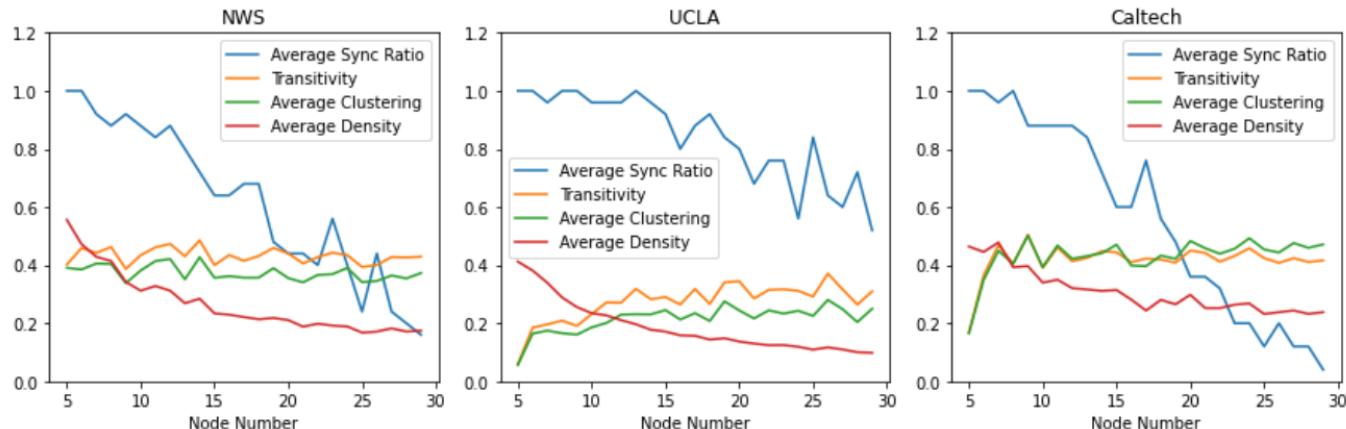


Figure: Synchronization ratio, average clustering coefficient, average transitivity, and average density trend with different node number in NWS, UCLA, and Caltech networks

Preliminary experiment II: Adding randomness to GHM

- ① GHM in general synchronizes very fast or falls into periodic wave-like behavior.

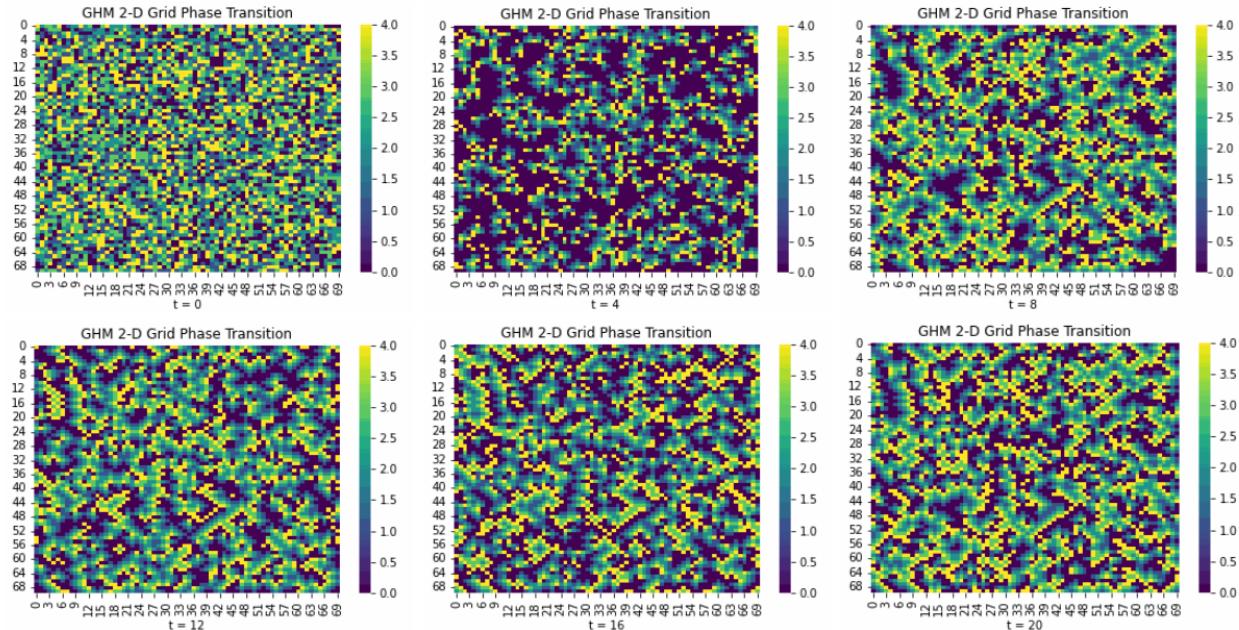


Figure: Time evolution of GHM dynamics on 70-by-70 grid

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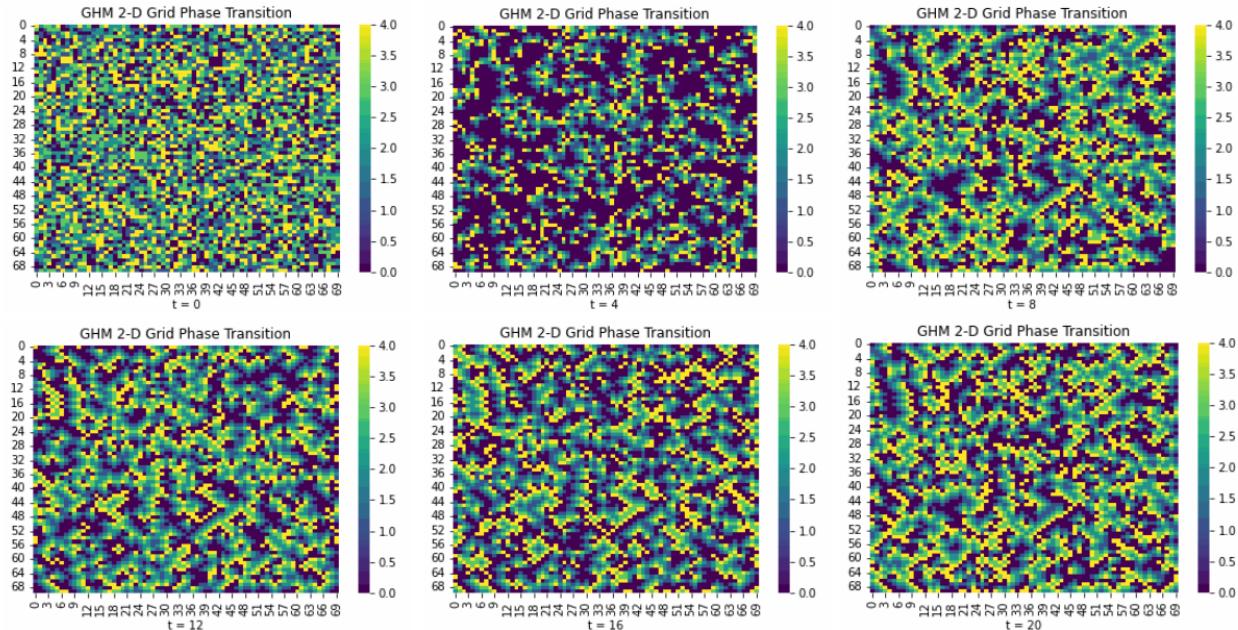


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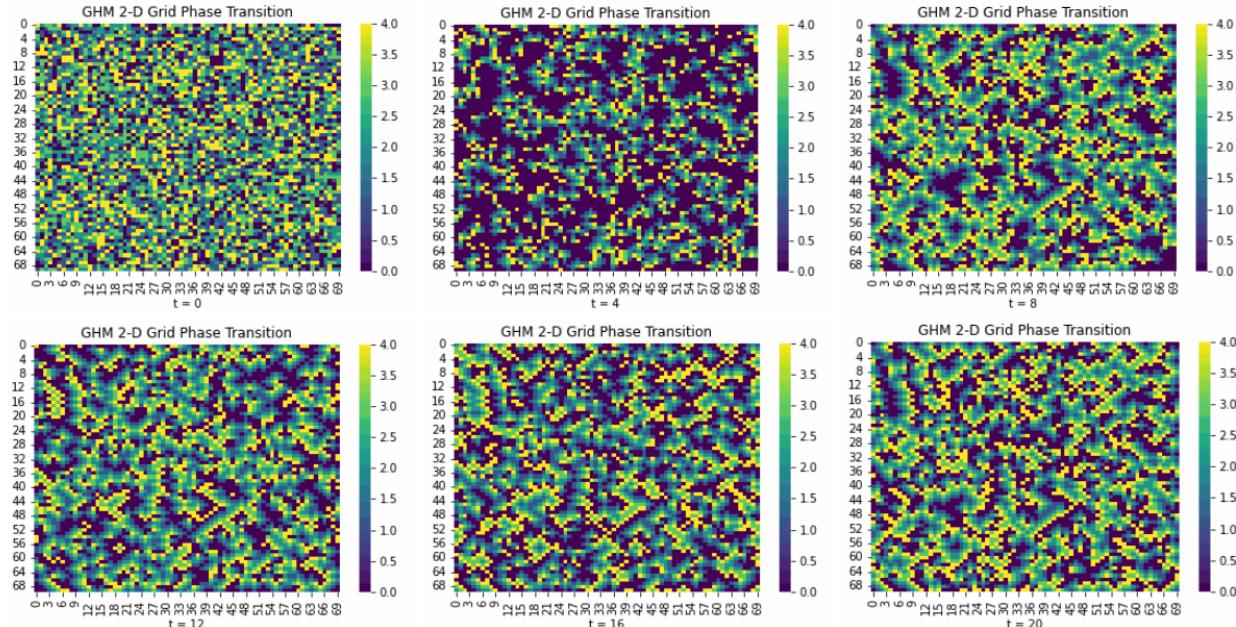


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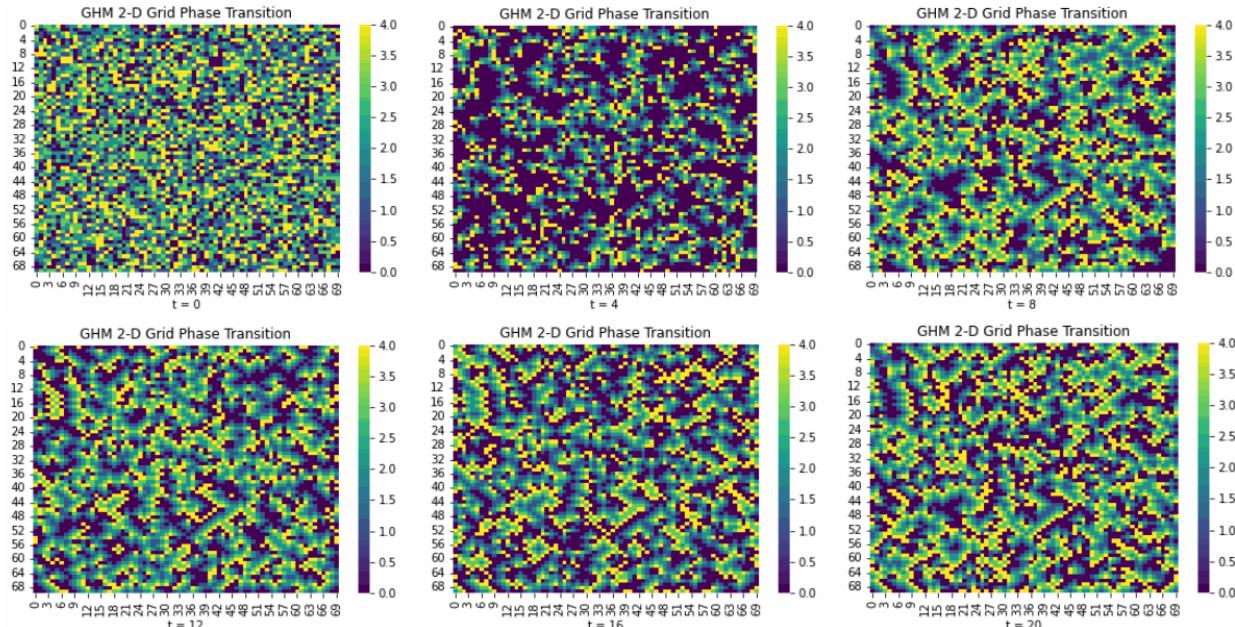


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Stochasticity for GHM transition on 2-D

- ① Add stochasticity to the original updating rule of GHM

$$X_{t+1}(v) = \begin{cases} 0 & \text{if } X_t(v) = 0 \quad \& \quad X_t(u) \neq 1 \forall u \in N(v) \\ 1 & \text{if } X_t(v) = 0 \quad \& \quad \exists u \in N(v) \text{ s.t. } X_t(u) = 1 \\ (X_t(v) + 1)mod(\kappa) & \text{otherwise} \end{cases} \quad (4)$$

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- ➊ Add stochasticity to the original updating rule of GHM
- ➋ Is the quiescent or excited state more important for synchronization?
- ➌ Randomly generate $P_{tv} \in [0, 1]$ at t-th iteration for node v. Tuning the threshold probability H to see different synchronizing behaviors.

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Stochasticity for GHM transition on 2-D

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Result

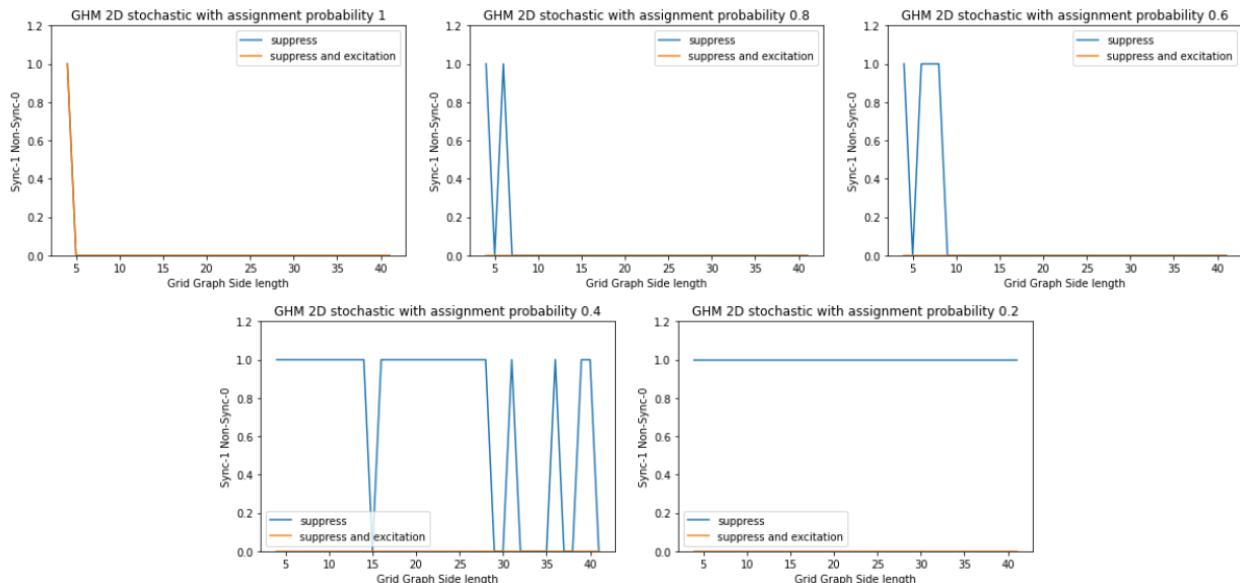


Figure: Synchronizing behavior for different transition probability applied to suppressing excitation only and both boosting and suppressing excitation on grid with side length 2 to 40

GHM NMF Setup

- 1 Perform Non-Negative Matrix Factorization over subgraphs of NWS with rank-16 approximation. Those 16 dictionary elements are latent factors for reconstructing the initial data matrix. Here the features used are adjacency matrix only

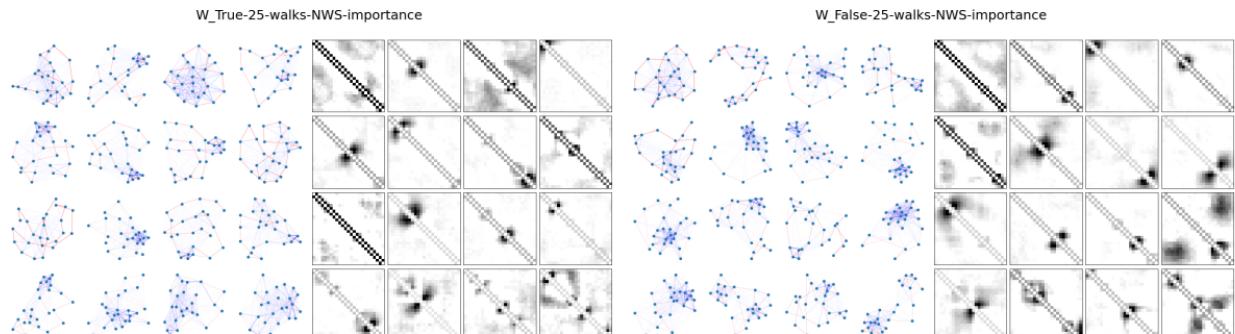


Figure: GHM NMF dictionary plots and box plots for dictionary elements and real graph adjacency matrices on NWS subgraphs

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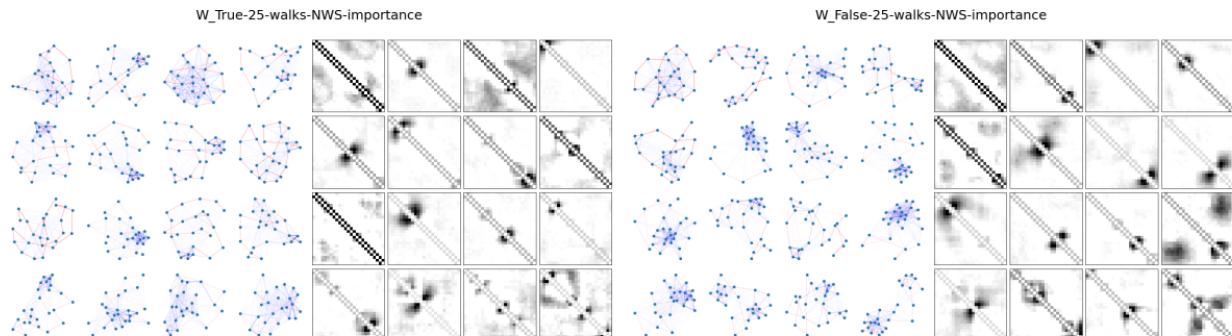


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- ② Generate the dictionary elements as symmetric adjacency matrix plot, then their corresponding graph visualization.
- ③ Box plot the distribution of the L-1 norm of dictionary graphs and original adjacency matrices for all the graphs, split by sync or non-sync

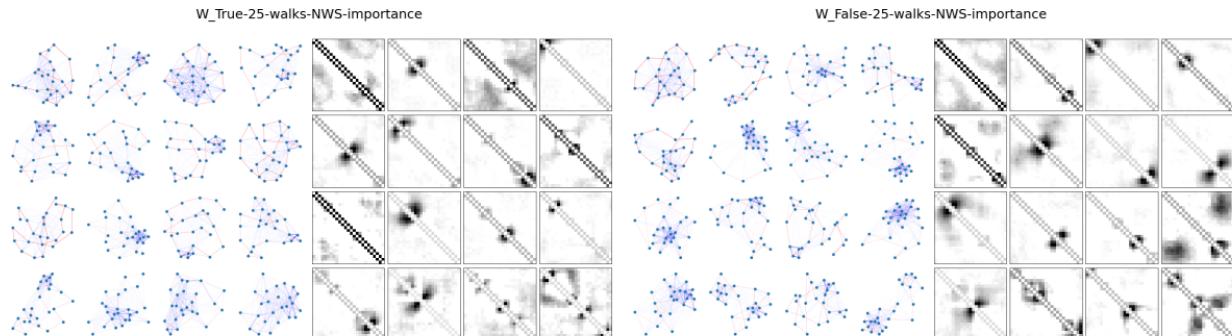
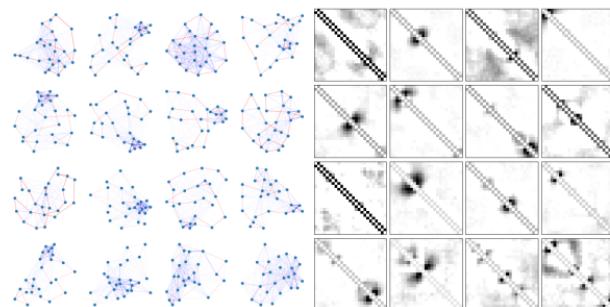


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GHM NWS NMF Visualization

W_True-25-walks-NWS-importance



W_False-25-walks-NWS-importance

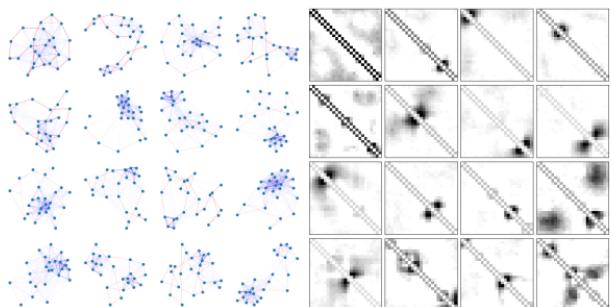
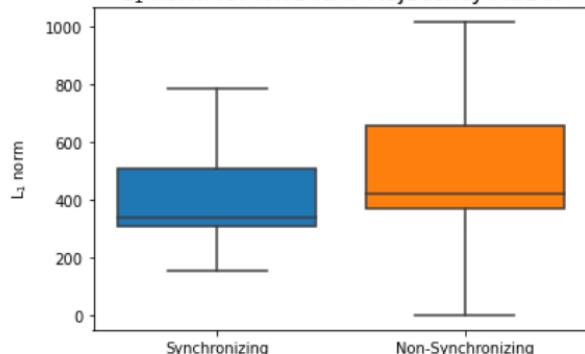
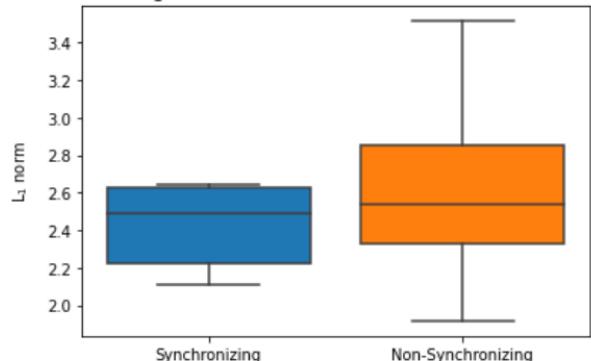
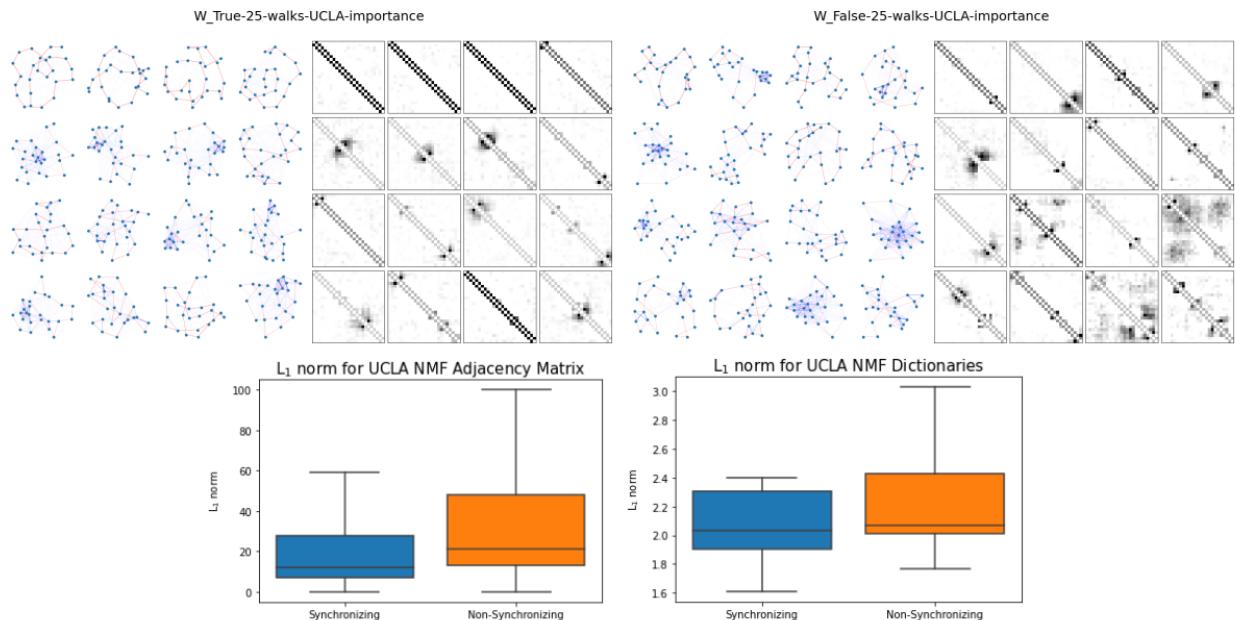
 L_1 norm for NWS NMF Adjacency Matrix L_1 norm for NWS NMF Dictionaries

Figure: GHM NMF dictionary plots and box plots for dictionary elements and real graph adjacency matrices on NWS subgraphs

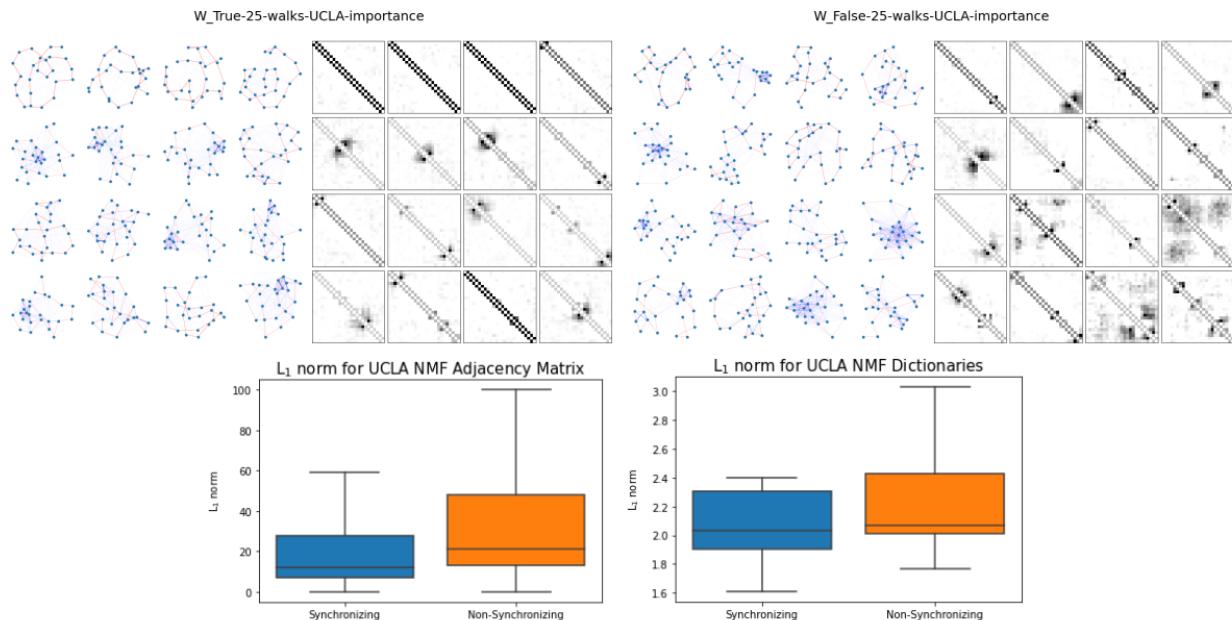
GHM UCLA NMF Visualization

- ① Communities occur on both synchronizing and non-synchronizing graphs. Dense area around the main path.



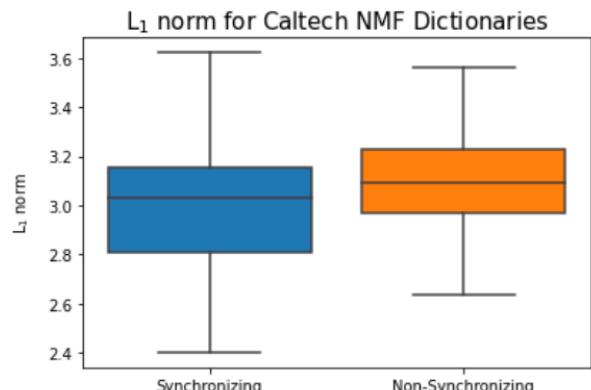
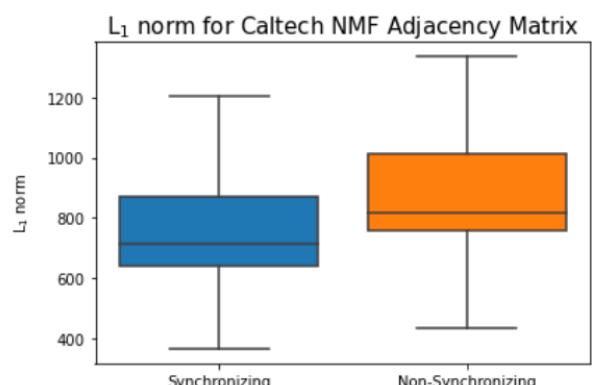
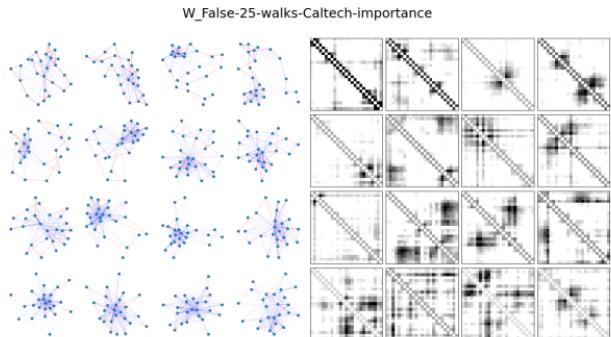
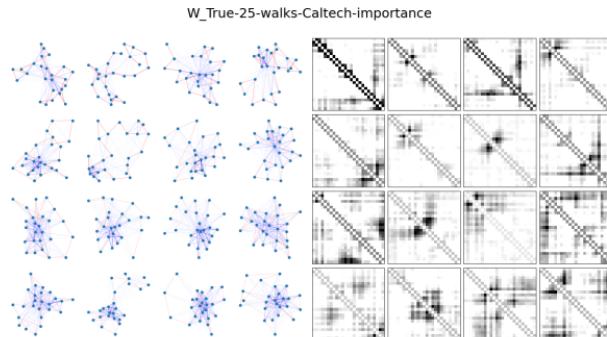
GHM UCLA NMF Visualization

- ❶ Communities occur on both synchronizing and non-synchronizing graphs. Dense area around the main path.
- ❷ Generally non-sync graphs are much denser than sync ones for real adjacency matrix L-1 norm distribution. Same trend for dictionary box plots



GHM Caltech NMF Visualization

- ① Similar trend as NWS graph. The real graph adjacency matrices' average densities are much lower than NWS.



GHM UCLA NMF Discussion

- ① Similar trend to both NWS and UCLA graphs such that with higher graph density, it leans towards non-synchronization.

GHM UCLA NMF Discussion

- ➊ Similar trend to both NWS and UCLA graphs such that with higher graph density, it leans towards non-synchronization.
- ➋ Caltech has the densest subgraphs of all three networks.

GHM Supervised Setup

- For supervised learning of GHM synchronization behavior, SVM and random forest methods will first be set as benchmarks of traditional classification algorithms. They will be used to train the data for the three networks and be compared to supervised dictionary learning techniques of SNMF and SDL-BCD.
- The random forest algorithm will spit out feature importance rank as an ordered list and we will visualize them using bar plot. The standard is based on mean decrease in impurity or known as Gini.
- Then we study the dictionary elements of the dictionary learning methods along with their regression coefficients.
- Apply color difference to the adjacency matrix and perform SDL

GHM Supervised Training

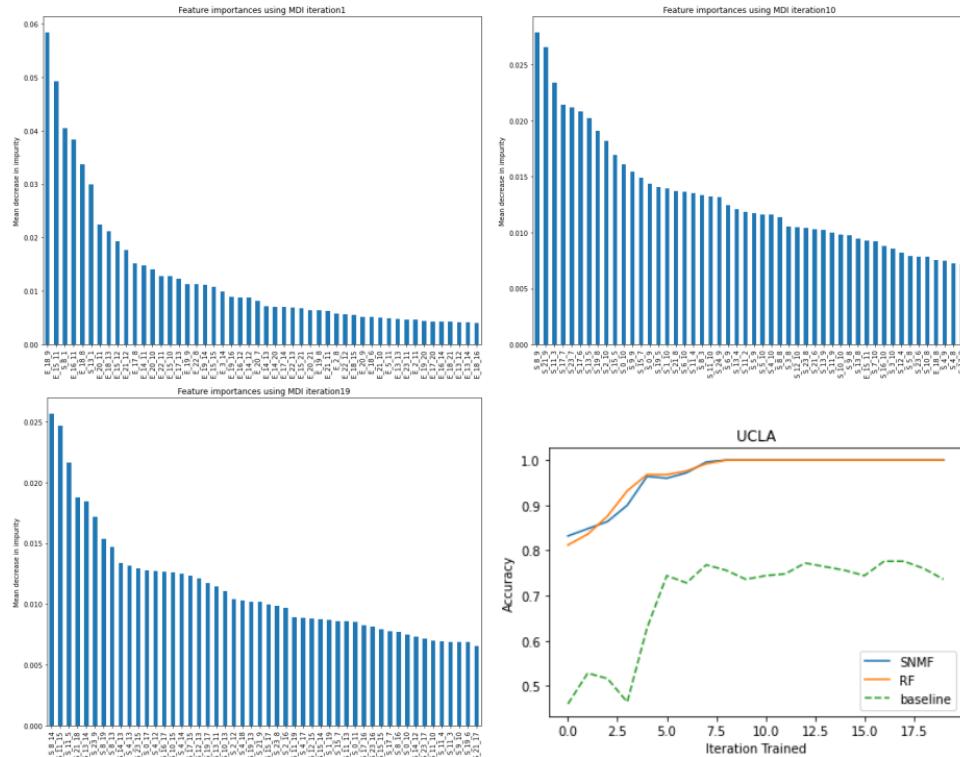


Figure: GHM feature importance and classification accuracy plot

GHM Supervised Training

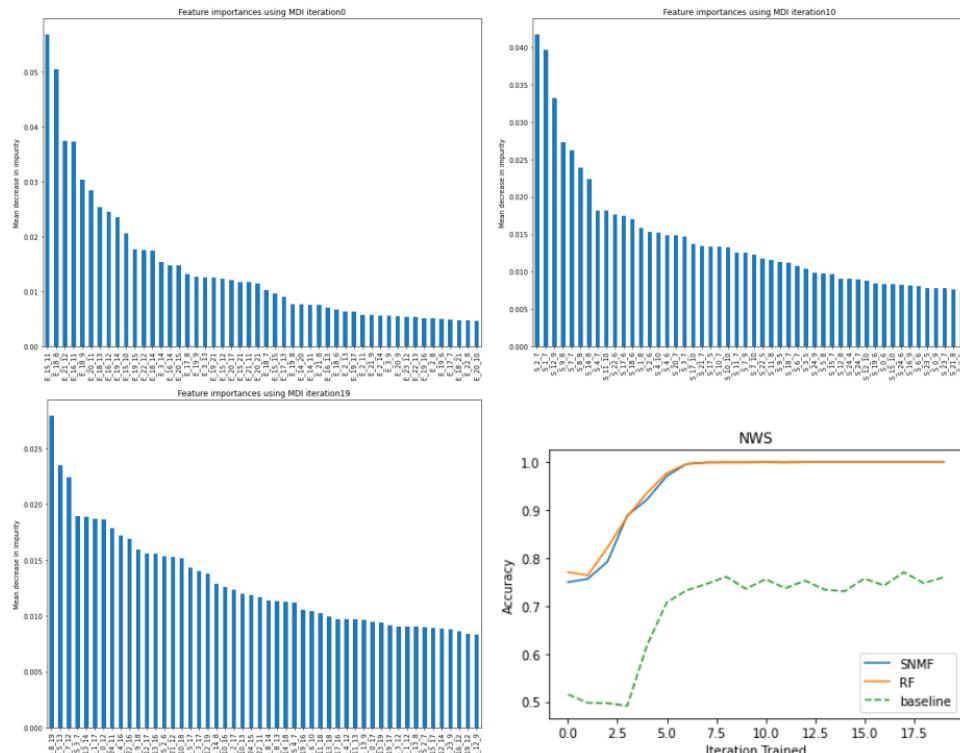


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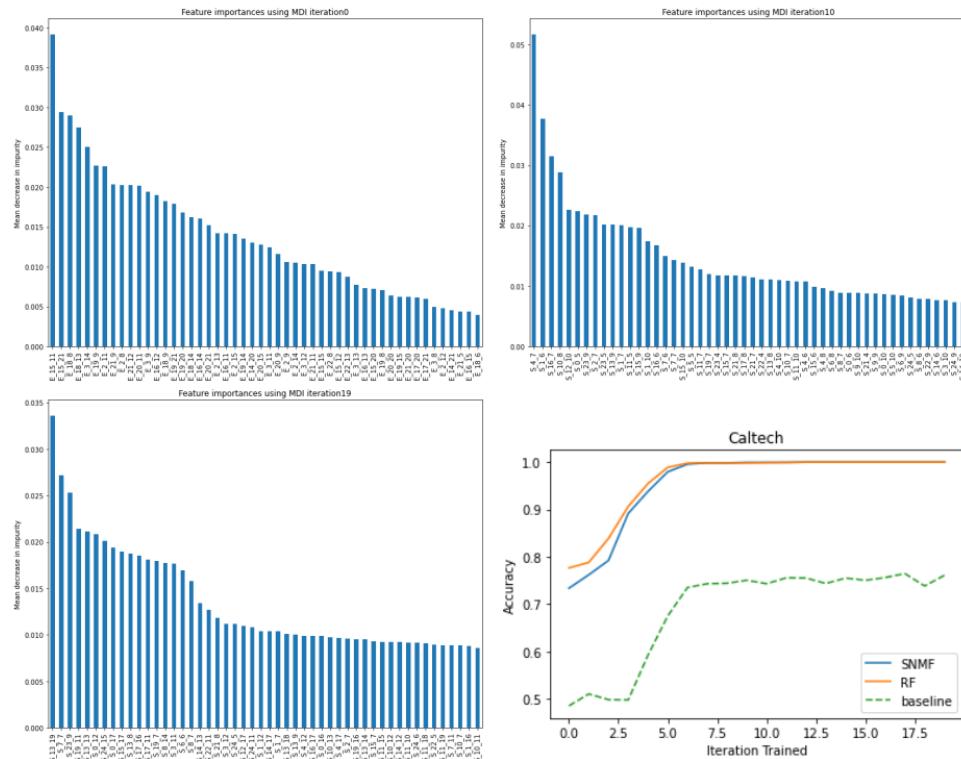
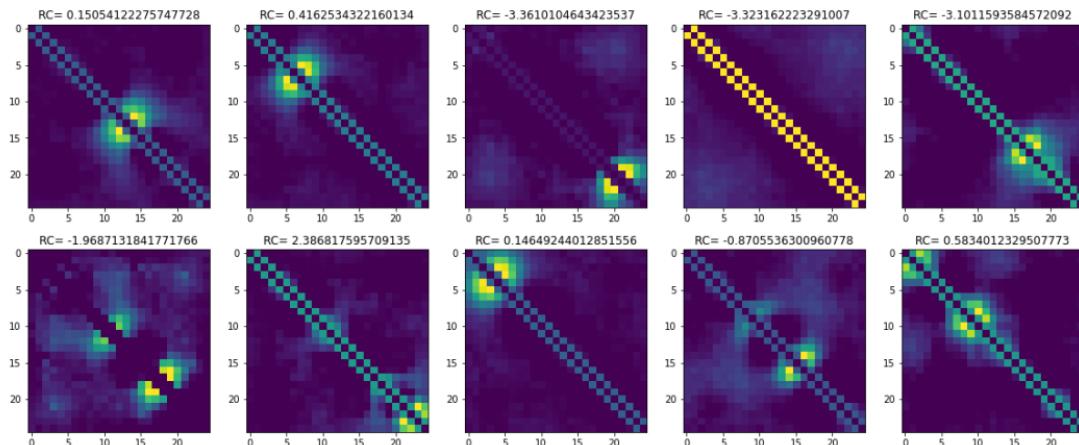


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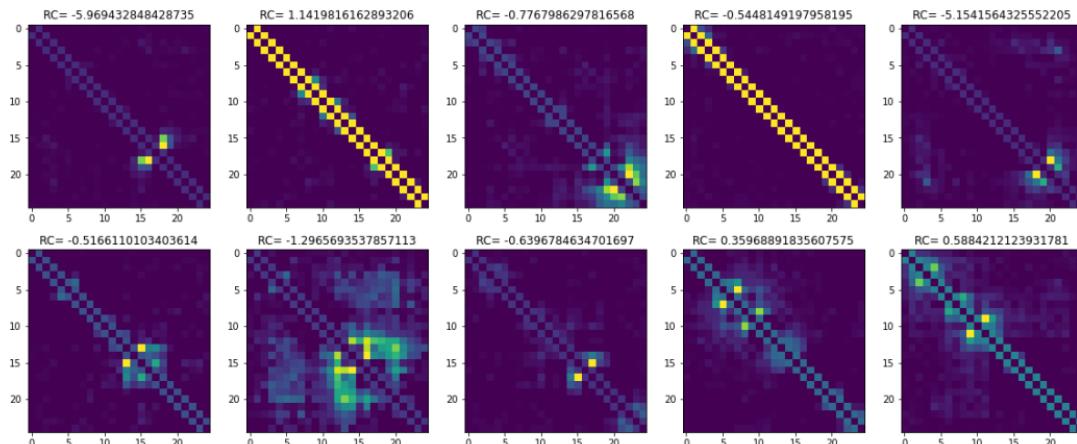
GHM SNMF Dictionary

NWS



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UCLA



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Caltech

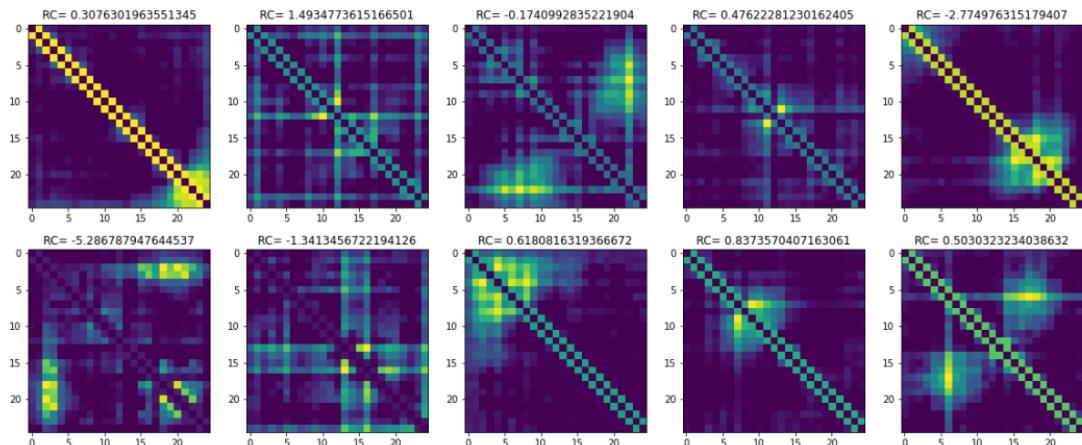


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Action Plan - I

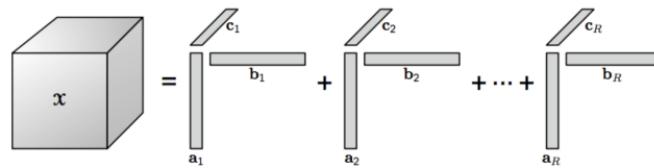
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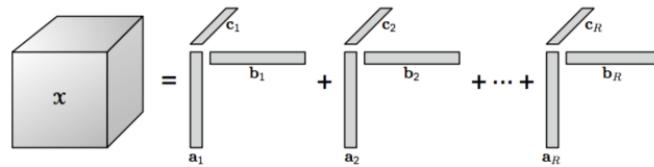


[Figure:](#) Illustrating CP-decomposition for a 3D tensor

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- Used it on weighted adjacency-matrices in L2PSync, might prove to be useful here

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