MAIN 2019

Montreal Artificial Intelligence & Neuroscience
From machine intelligence to brain science and back

Montréal Intelligence Artificielle & Neurosciences
De l'intelligence des machines à la science des cerveaux

14-17 Nov 2019

Centre de Recherches Mathématiques (CRM)
Union Neurosciences et Intelligence Artificielle - Québec (UNIQUE)

Université de Montréal

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Tutorial on Graph Convolutional Networks in Brain Imaging

NEUROMOD
THE COURTOIS PROJECT ON NEURONAL MODELLING

IVADO

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https://simexp.github.io/lab-website/

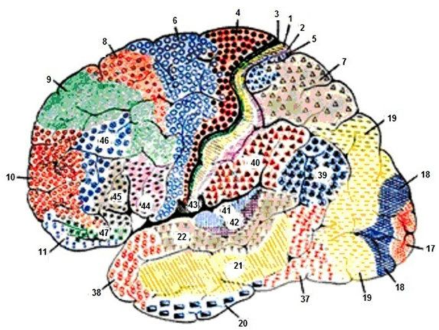
Outline

- **Brain graphs:**
  - **Brain atlas & connectome**
- **Graph signal processing and Graph Laplacian**
  - **Graph Laplacian**
  - **Spectral Decomposition**
  - **Graph Fourier Transform**
- **Graph Convolutional Network**
  - **Spectral GCN**
  - **ChebNet and 1stGCN**
  - **applications**
- **Practice on Notebook**

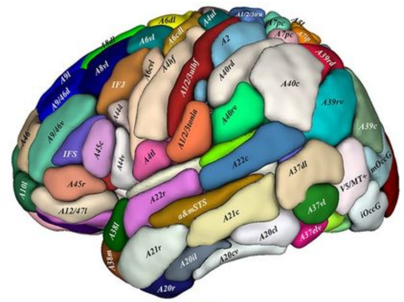
Brain Graphs
--to understand brain organization

- **brain atlas**

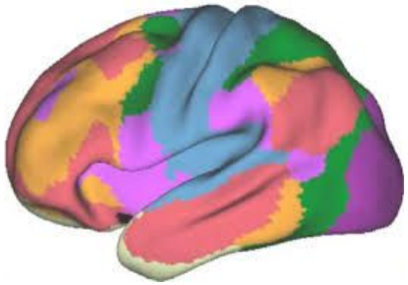
Brodmann atlas



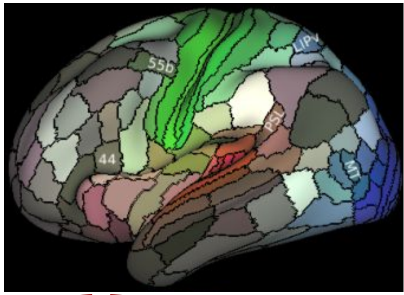
Brainnectome Atlas



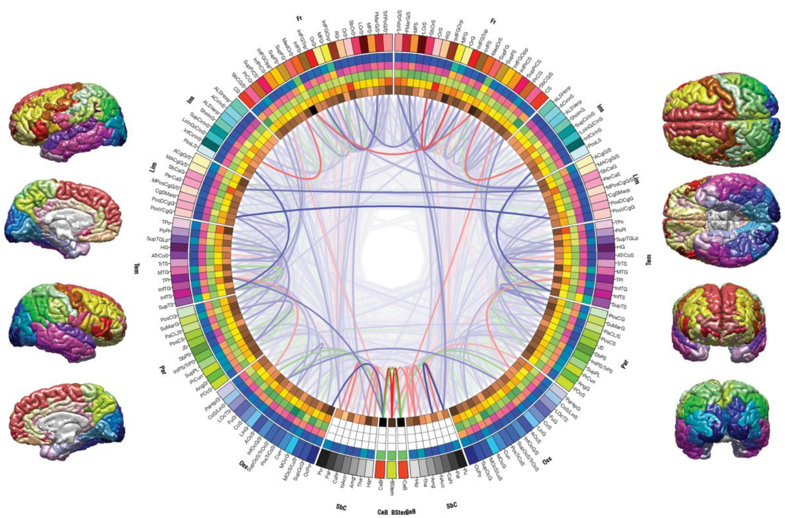
Yeo Atlas

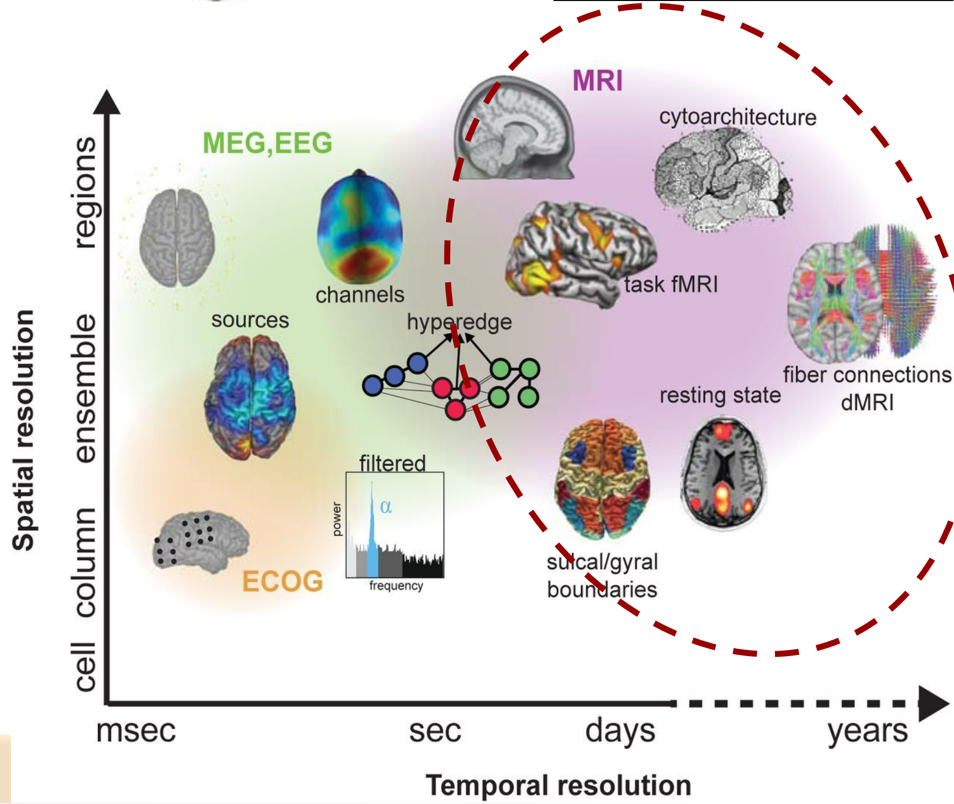


Glasser atlas



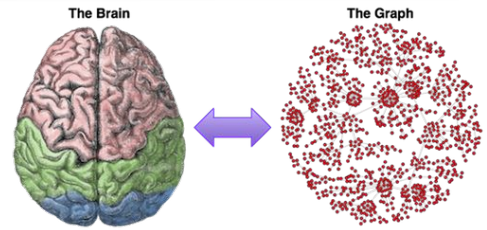
- **brain connectome**





Fan et al. 2016; Yeo et al. 2011; Glasser et al. 2016; Garcia et al. 2017.

Part #1:
Graph signal processing and Graph Laplacian



- **Graph Laplacian:**
  - **graph** $G = (V, E, W)$
  - **nodes** V **edges** E **weight matrix** W

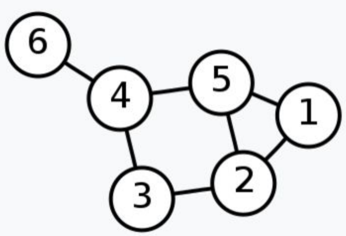
  - **Adjacency matrix**

$$a_{ij} = \begin{cases} 1, \text{ if } (v_i, v_j) \in E \\ 0, \text{ otherwise} \end{cases}$$

  - **Laplacian matrix**

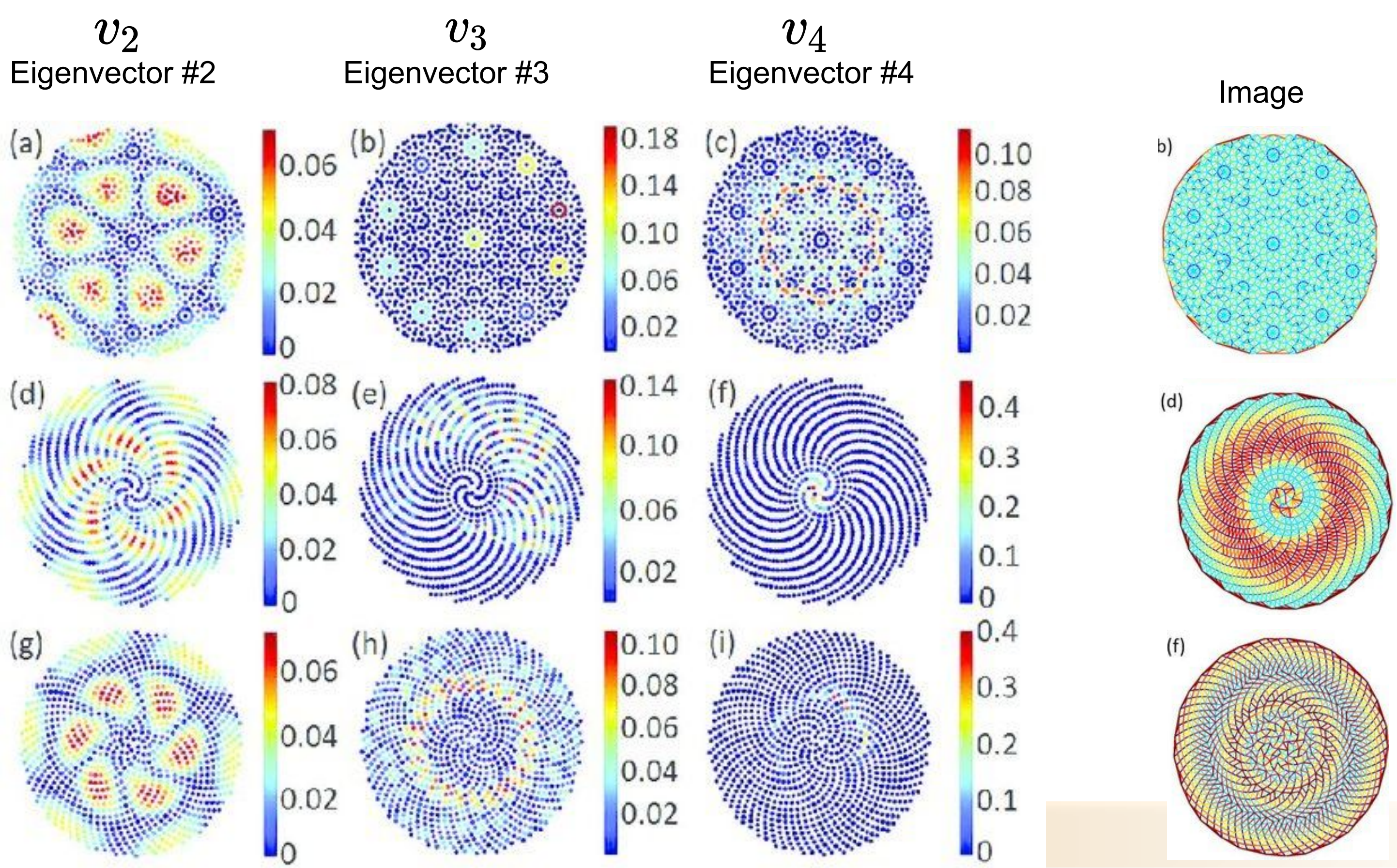
$$L = D - A, or L = D - W$$

  - **normalized Laplacian**

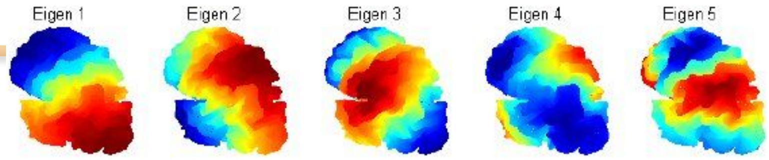
Labeled graph	Degree matrix D	Adjacency matrix A	Laplacian matrix L
	$\begin{pmatrix} 2 & 0 & 0 & 0 & 0 & 0 \\ 0 & 3 & 0 & 0 & 0 & 0 \\ 0 & 0 & 2 & 0 & 0 & 0 \\ 0 & 0 & 0 & 3 & 0 & 0 \\ 0 & 0 & 0 & 0 & 3 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix}$	$\begin{pmatrix} 0 & 1 & 0 & 0 & 1 & 0 \\ 1 & 0 & 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 & 1 & 1 \\ 1 & 1 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \end{pmatrix}$	$\begin{pmatrix} 2 & -1 & 0 & 0 & -1 & 0 \\ -1 & 3 & -1 & 0 & -1 & 0 \\ 0 & -1 & 2 & -1 & 0 & 0 \\ 0 & 0 & -1 & 3 & -1 & -1 \\ -1 & -1 & 0 & -1 & 3 & 0 \\ 0 & 0 & 0 & -1 & 0 & 1 \end{pmatrix}$

1.1 Graph Laplacian

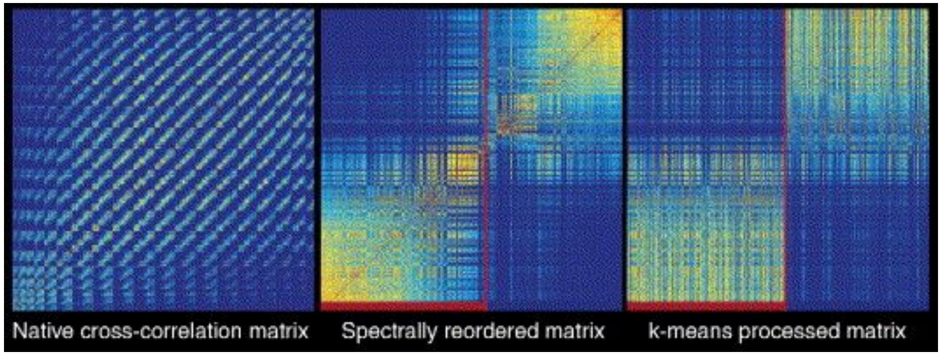
- **Spectral decomposition:** $Lv = \lambda v$
  - **assume W is undirected and symmetric**
  - **eigenvalues are non-negative (descending order):** $\{\lambda_i, i = 1...k\}$
  - **eigenvectors are real and orthogonal** $\{v_i, i = 1...k\}$

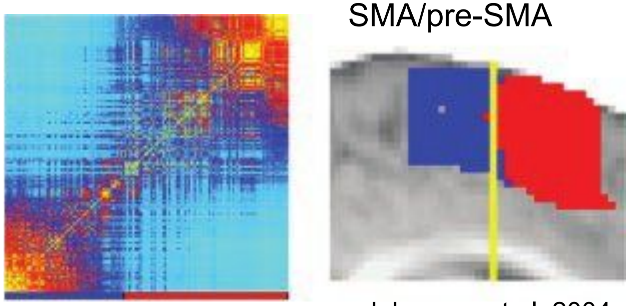


Graph Laplacian in Brain imaging



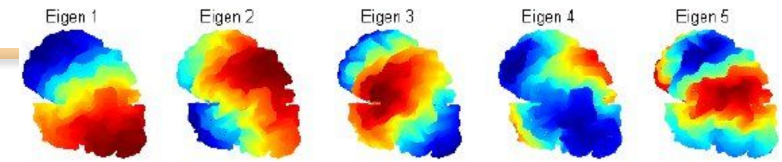
- **brain parcellation**
  - ***spectral reordering (2nd eigenvector)*** v_2
  - **spectral clustering (first k eigenvectors)** $\{v_i, i = 1...k\}$





Johansen et al. 2004

Graph Laplacian in Brain imaging



- **brain parcellation**
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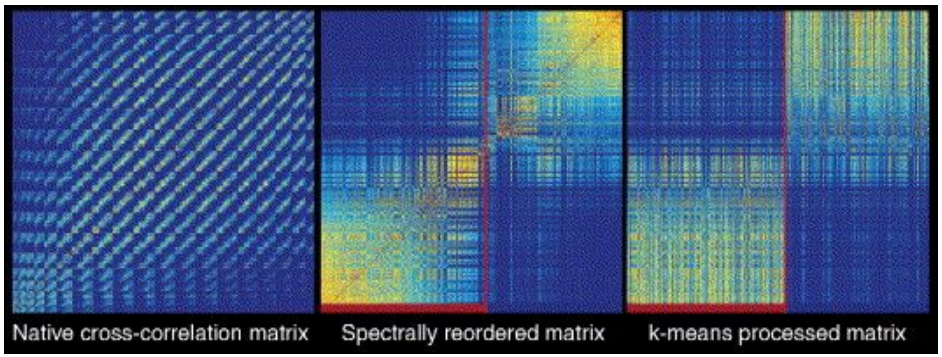
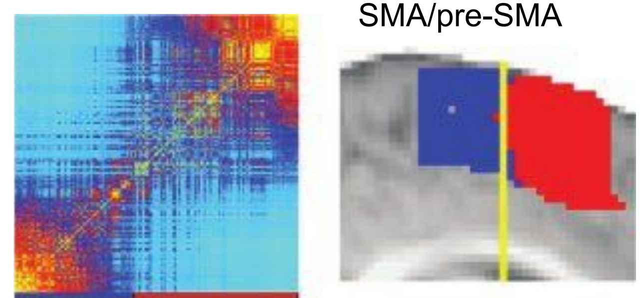
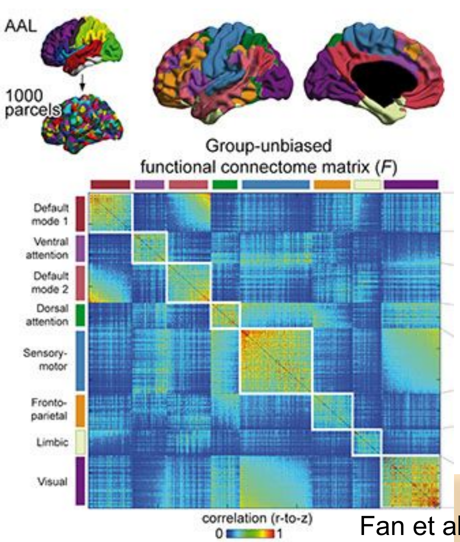


SMA/pre-SMA

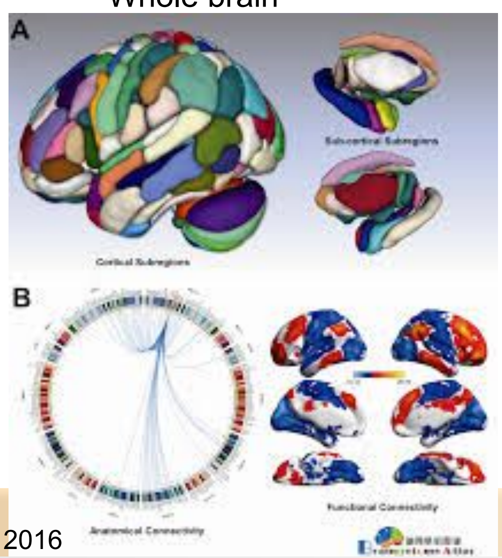


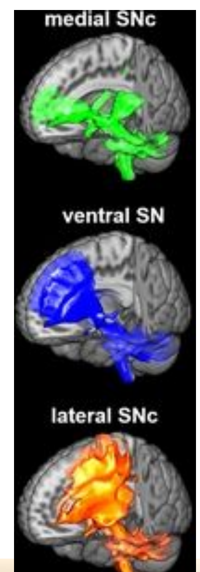
Johansen et al. 2004



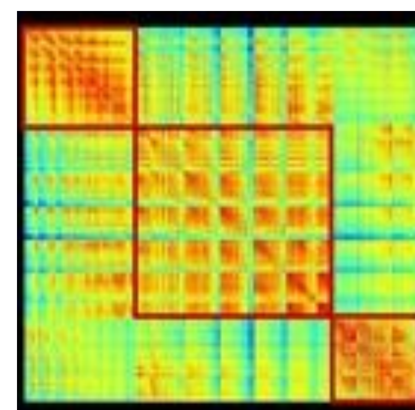
Fan et al. 2016

Whole brain



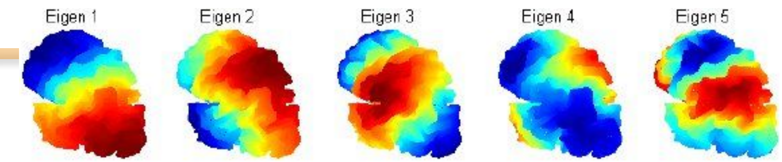


Substantia Nigra



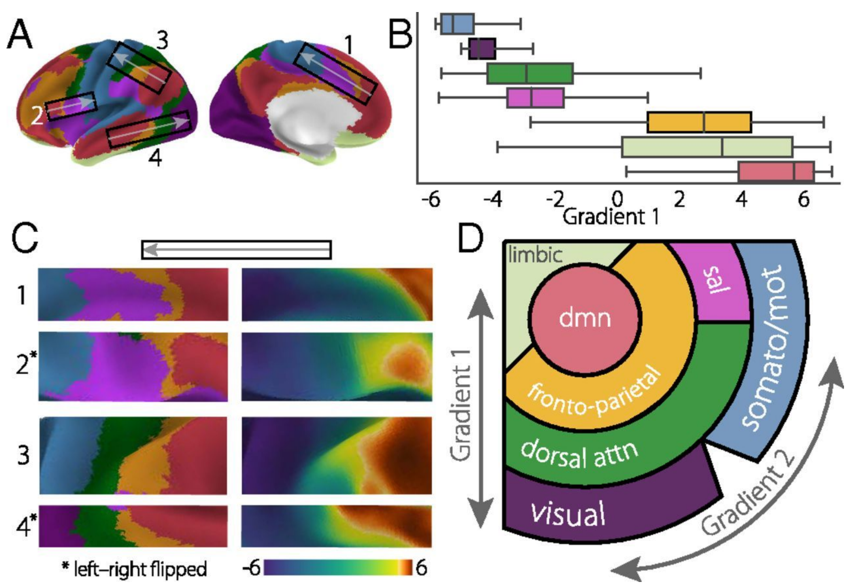
Zhang et al. 2017

Graph Laplacian in Brain imaging



- **brain organization**
  - **mapping of *2nd-eigenvector* or higher orders**

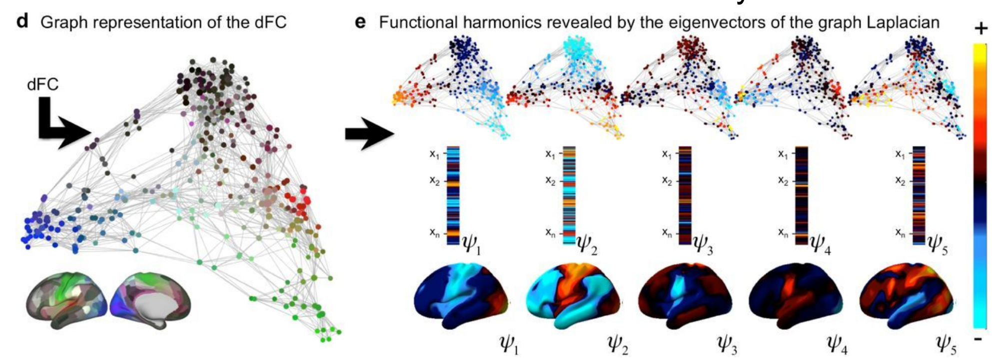
- **Connectivity Gradients**



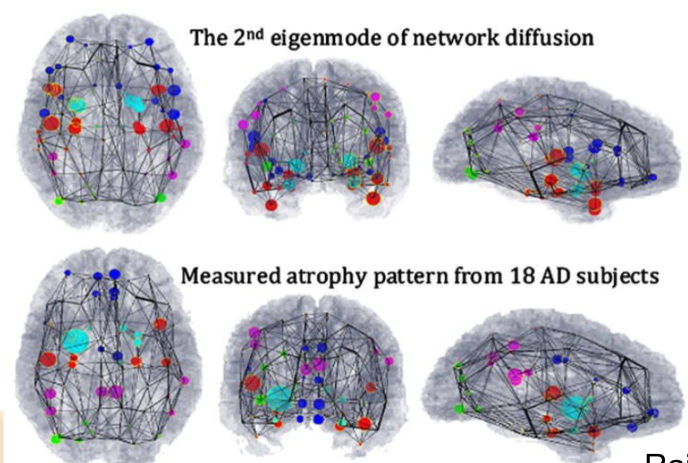
Margulies et al. 2016

- **Harmonics**

Atasoy et al. 2017



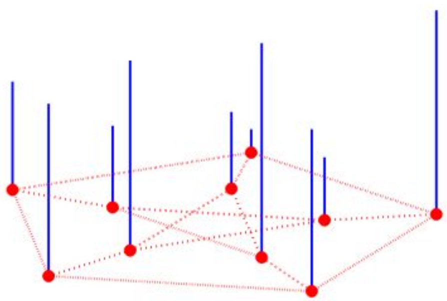
- **Disease propagation**



Raj et al. 2012

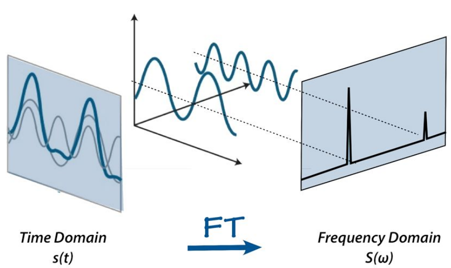
1.2 Graph signal processing

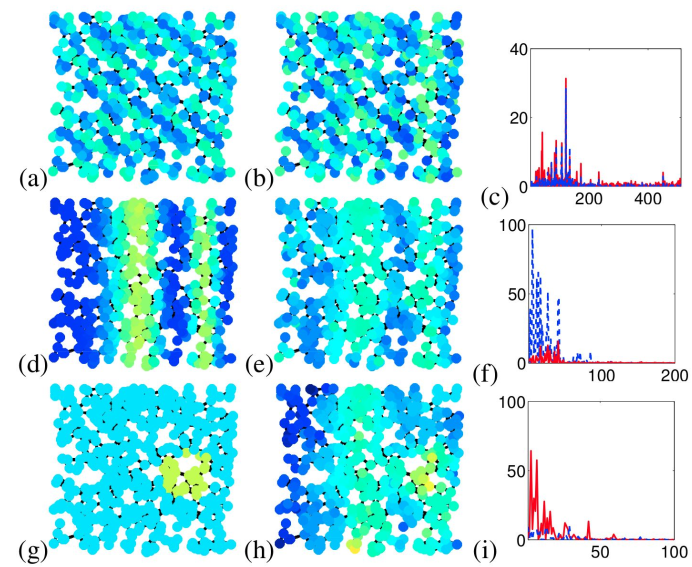
- **Graph Fourier transform:**
  - **graph signals: signal on each node**
  - **spatial domain to spectral domain**
  - **low frequency vs high frequency**



$$\hat{x} = \mathcal{L}\{x\} = U^T x$$
$$x = U\hat{x}$$

$$U = [v_0, v_1, \ldots v_N]$$





https://persagen.com/resources/graph_signal_processing.html

Graph signal processing in Brain imaging

- **Graph Fourier transform:**
  - **graph signals: signal on each node**
  - **spatial domain to spectral domain**
  - **low frequency vs high frequency**

$$\hat{x} = \mathcal{L}\{x\} = U^T x$$
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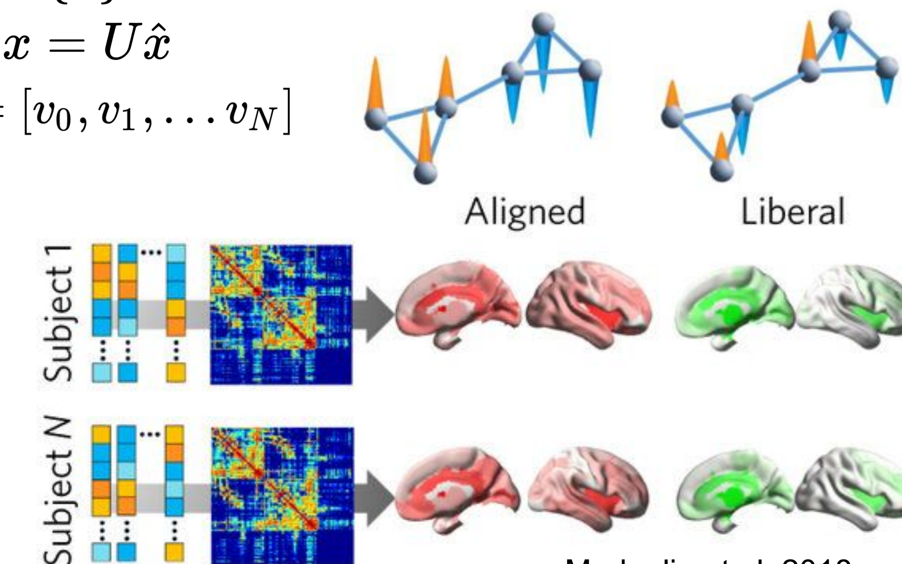
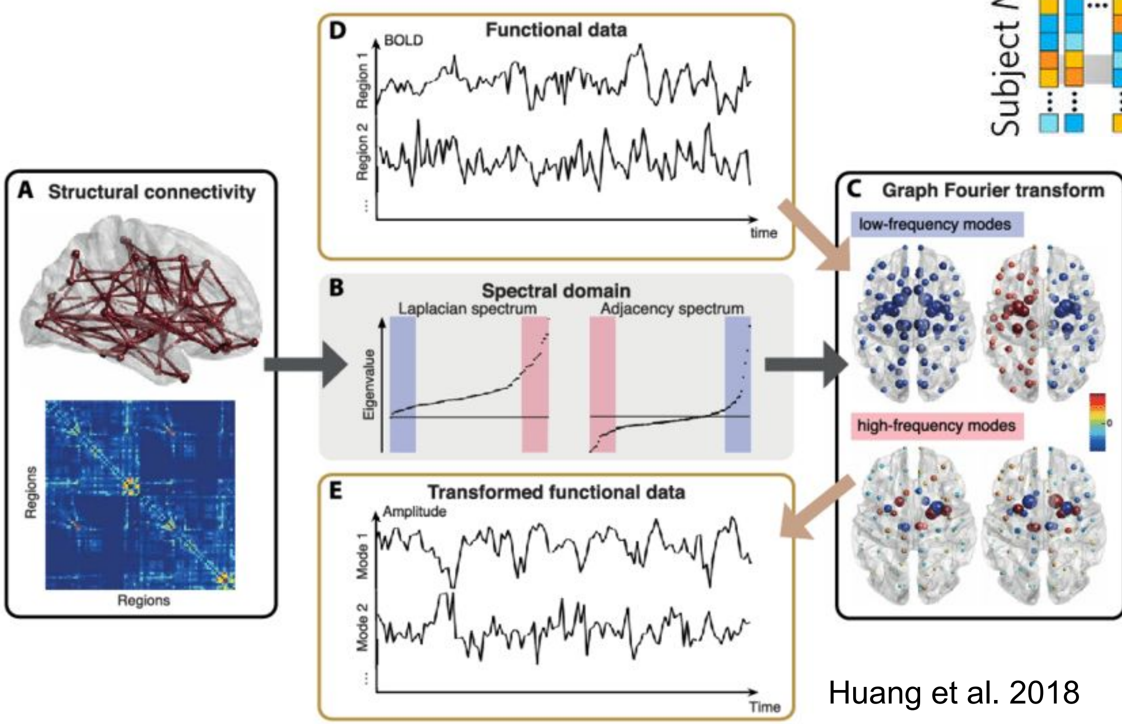
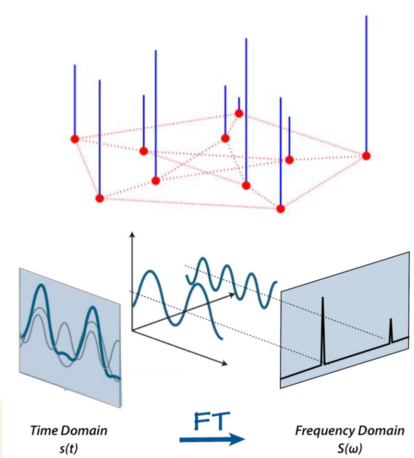


Medaglia et al. 2018

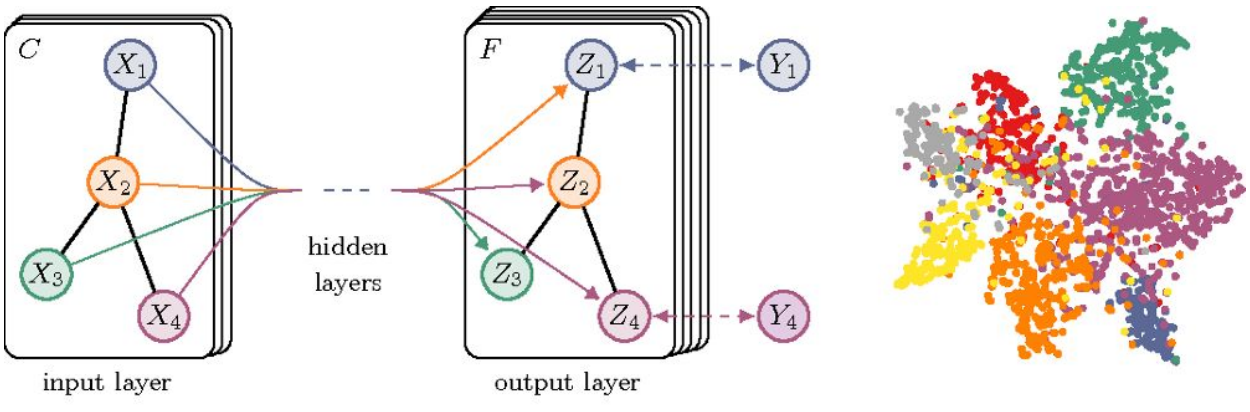


Huang et al. 2018



Part #2:
Graph Convolutional networks (GCN)

- **graph filters g_θ and graph convolutions $x * g_\theta$**

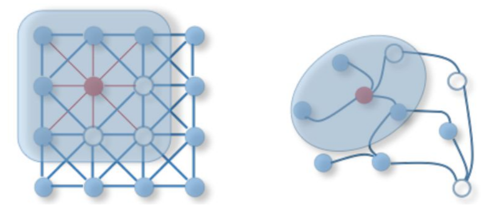


(a) Graph Convolutional Network

(b) Hidden layer activations

- graph Fourier transform

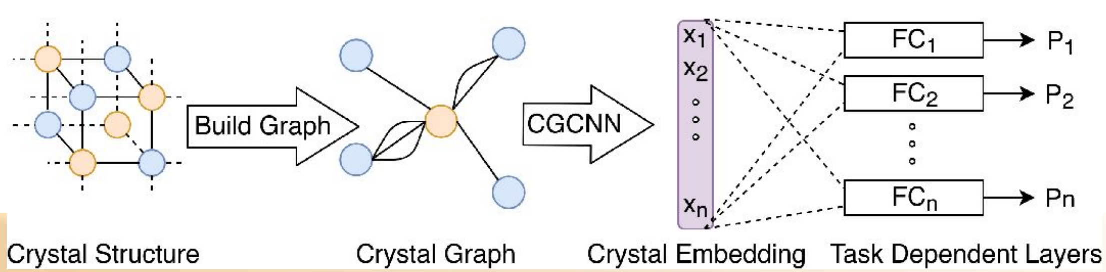
$$\mathbf{x} *_G \mathbf{g}_\theta = \mathbf{U}\mathbf{g}_\theta\mathbf{U}^T\mathbf{x}$$



Defferrard et al. 2016; Kipf et al. 2016; Wu et al. 2019;

- **two types of graph convolutions**
  - **spectral GCN: based on graph Laplacian**
  - **spatial methods: approximation using neighbors, for instance ChebyNet; 1stGCN**

- **Applications**



Graph Convolutional networks (GCN)

--merging graph signal processing with neural networks

- **ChebyNet**
  - **use Chebychev polynomial expansion instead**

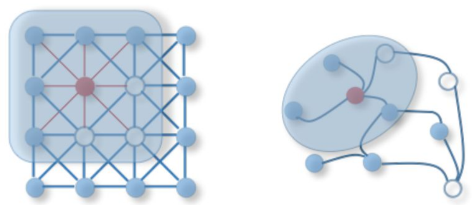
$$x * g_\theta = \sum_{k=0}^{K} \theta_k T_k(\widetilde{L})x \qquad \widetilde{L} = 2L/\lambda_{\max} - I$$

  - **a recursive formula to calculate Chebychev polynomials**

$T_k(x) = 2T_{k-1}(x) - T_{k-2}(x)$ with $T_0(x) = 1, T_1(x) = x,$

- graph Fourier transform

$$\mathbf{x} *_G \mathbf{g}_\theta = \mathbf{U}\mathbf{g}_\theta \mathbf{U}^T \mathbf{x}$$



Defferrard et al. 2016

- **1stGCN**
  - **A simplified version with order** $k = 1,\ \lambda_{\max} \approx 2.0\ , \theta_0 = \theta_1$

$$x * g_\theta = \theta(I + D^{-1/2} W D^{-1/2})x$$

$$x * g_\theta = (\theta_0 I + \theta_1 \widetilde{L})x = (\theta_0 I - \theta_1 D^{-1/2} W D^{-1/2})x$$

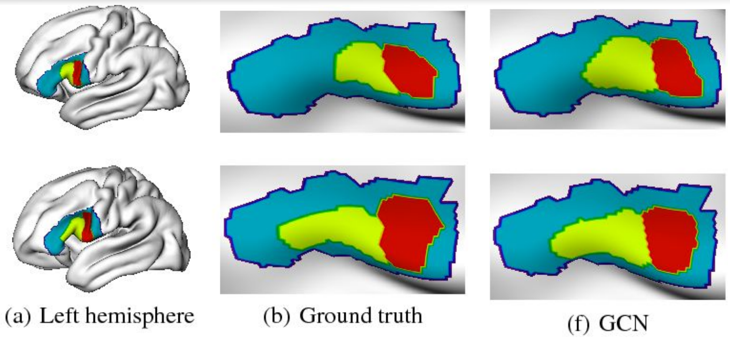
  - **a graph convolution layer:**

$$X^{l+1} = \sigma(\widetilde{W} X^l \Theta^l), \quad \widetilde{W} = I + D^{-1/2} W D^{-1/2}$$

Kipf et al. 2016

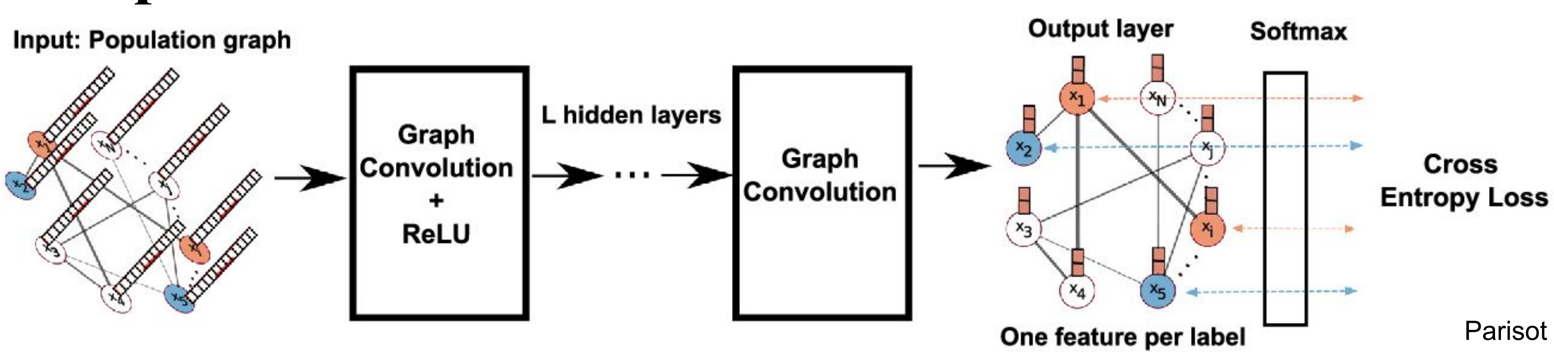
Graph Convolutional networks in Brain imaging

- **brain parcellation**



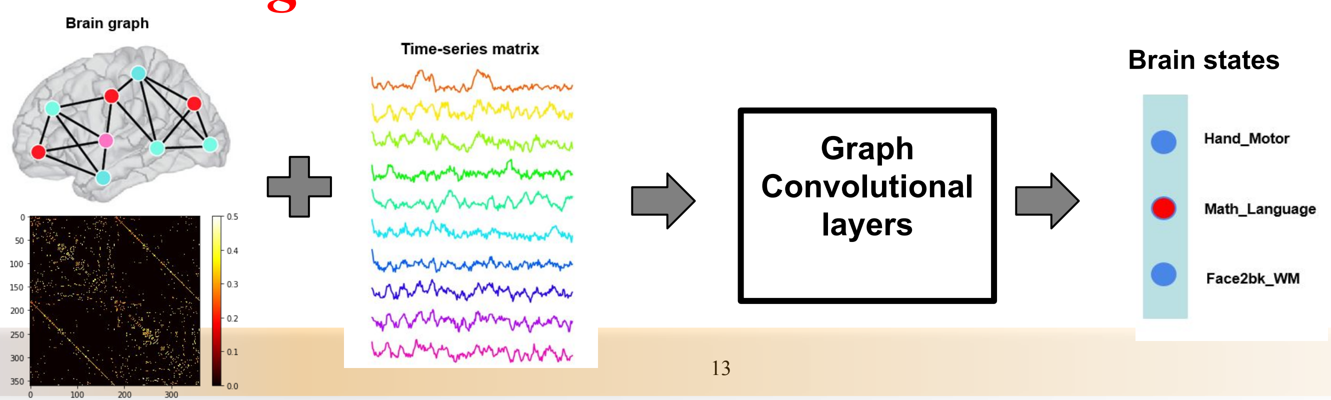
Cucurull et al. 2018

- **disease prediction**



Parisot et al. 2018

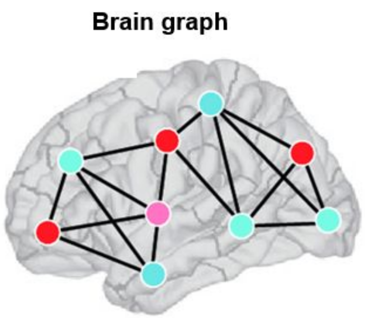
- ***brain decoding***



Zhang et al. 2019

Functional state annotation using Brain Graph Convolutions

- 6 graph convolutional layers + 2 fully connected layers

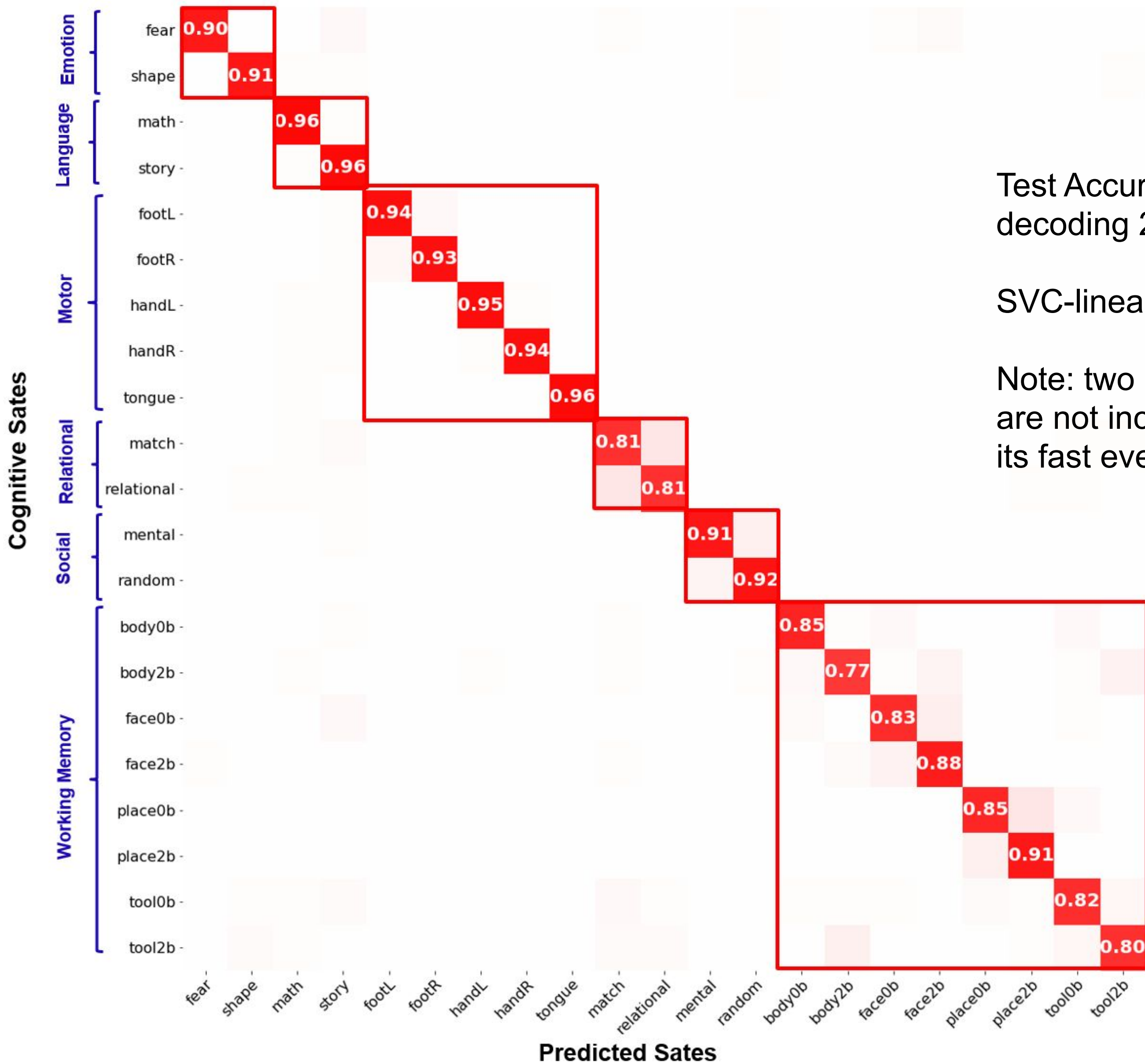


Multi-modal datasets: structural, diffusion, functional MRI, MEG

- **Subjects: 1200 healthy subjects with two runs**
- **7 cognitive domains and 23 conditions; detailed behavioral measures**
- **fMRI acquisition: TR=0.72s, 2mm iso-resolution**

Task Domains	#Subjects	#Runs	#Volumes per run	#Trials per run	#Conditions	Min trial duration (sec)
Working memory	1085	2	405	8	8	25
Motor	1083	2	284	10	5	12
Language	1051	2	316	8	2	12
Social Cognition	1051	2	274	5	2	23
Relational processing	1043	2	232	6	2	16
Emotion	1047	2	176	6	2	18

Brain state annotation using 10s of fMRI time series

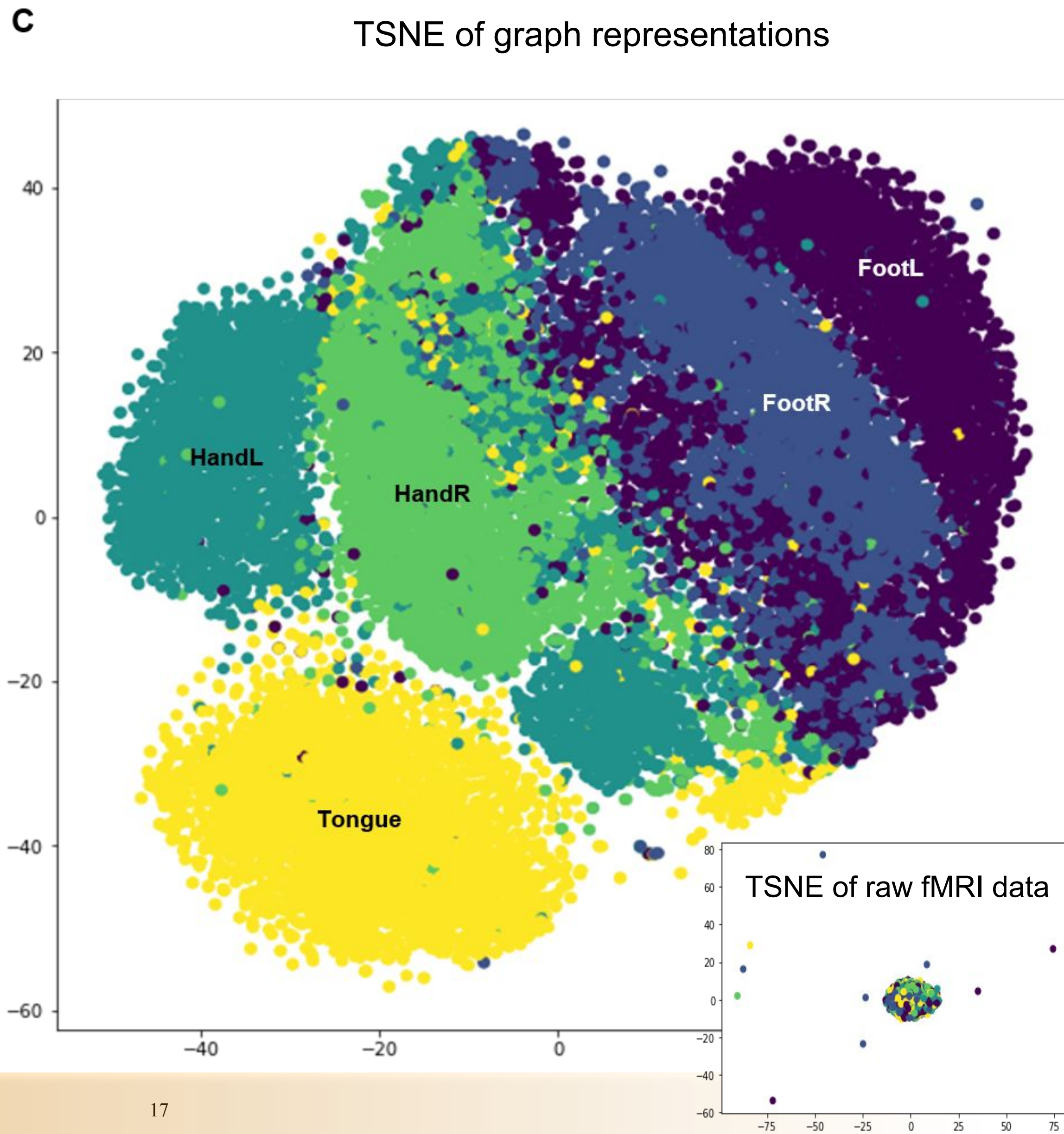


Test Accuracy (F1-score) in decoding 21 states: **89%**

SVC-linear: 63%

Note: two gambling conditions are not included here, due to its fast event-design nature

Representational Similarity Analysis of graph representations



Practice

- **github repo:**
  https://github.com/zhangyu2ustc/gcn_tutorial_test.git
- **binder projects:**
  https://mybinder.org/v2/gh/zhangyu2ustc/gcn_tutorial_test/master?filepath=notebooks%2F

- **Part #1: Graph Laplacian**
  - **brain graph -> Laplacian decomposition -> Graph Fourier Transform**

- **Part #2: Graph Convolutional Networks for brain decoding**
  - **Pytorch**
  - **Dataset and DataLoader**
  - **build a simple MLP -> train and evaluate the model**
  - **1stGCN and ChebyNet**

Acknowledgements
-SIMEXP lab

IVADO

NEUROMOD
THE COURTOIS PROJECT
ON NEURONAL MODELLING

Université de Montréal

Centre de recherche
iugm
Institut universitaire
de gériatrie de Montréal

Brain state annotation using 10s of fMRI time series

- **Summarize to 6 cognitive domains (averaging)**