Spectral Graph Convolutions for Population-based Disease Prediction

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Paper overview



Disease prediction



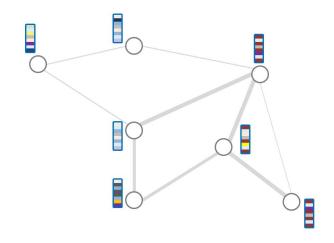
Contribution: Graph Convolution Networks [*]



Datasets: ABIDE → Autism | ADNI → Alzheimer

Population graph

- O Nodes = Patients
- Edges = Similarity between patients
 - Feature vector

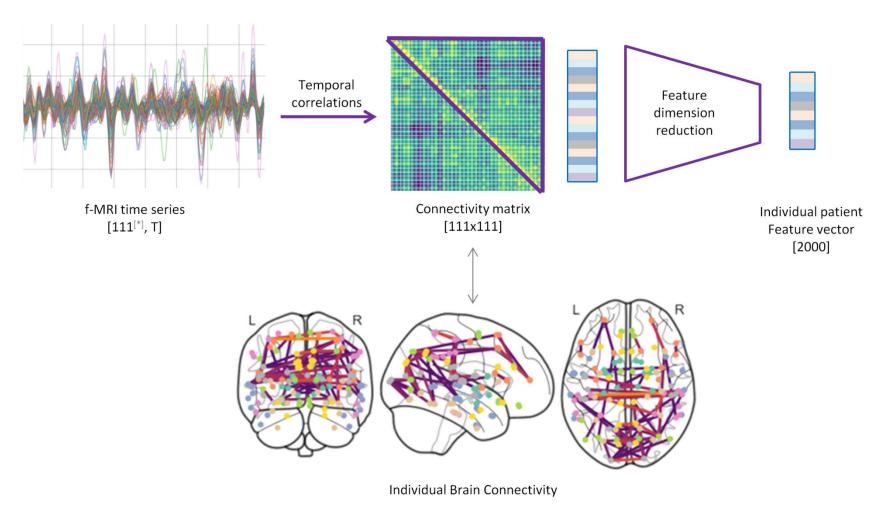


[*] Semi-Supervised Classification with Graph Convolutional Networks - Thomas N. Kipf, Max Welling ICLR 2017

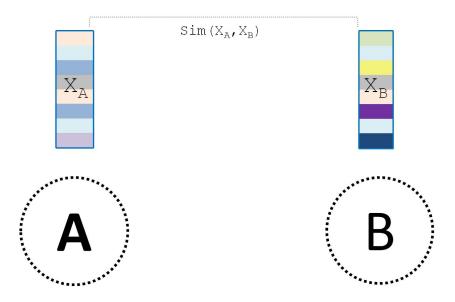


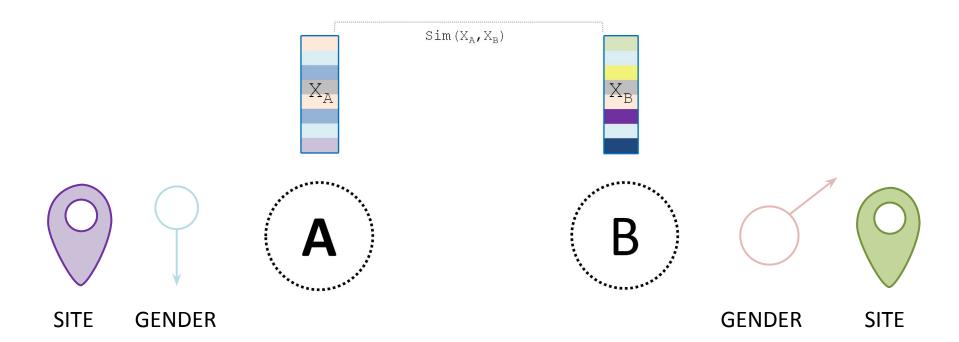
Defining graph nodes

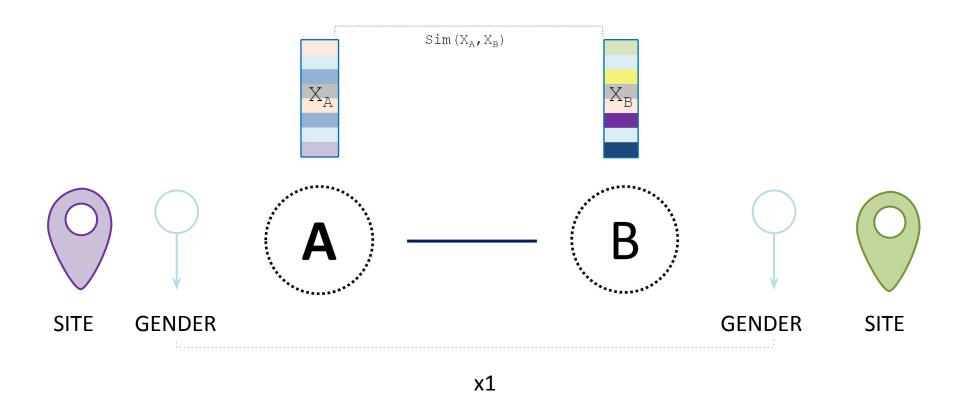
1 patient \leftrightarrow 1 node

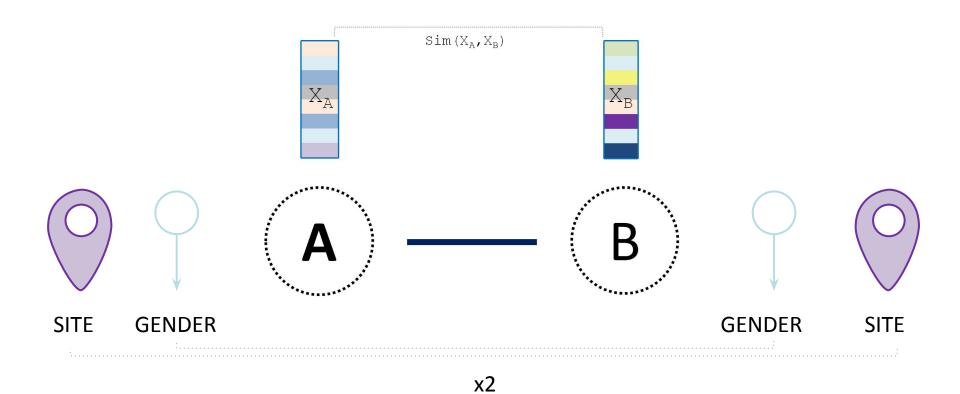


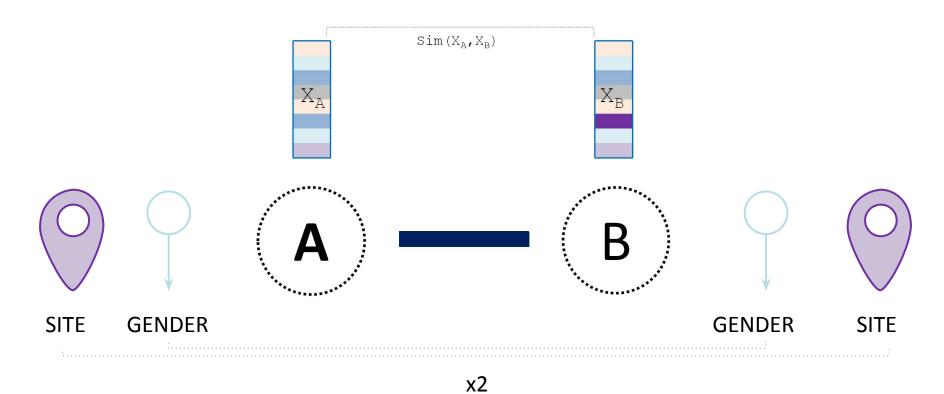
[*] 111: Harvard-Oxford cortical and subcortical structural atlases

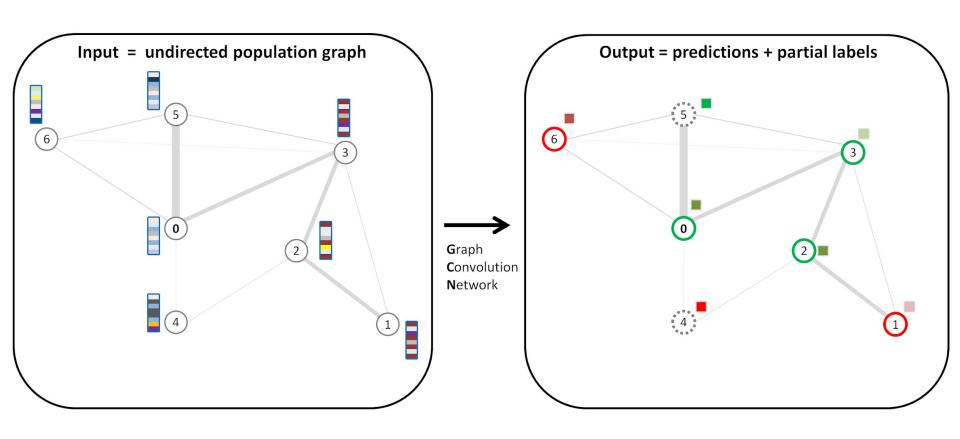










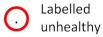


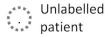






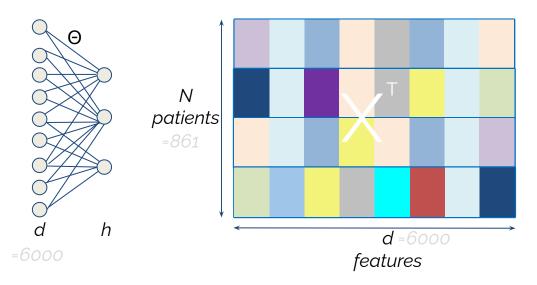








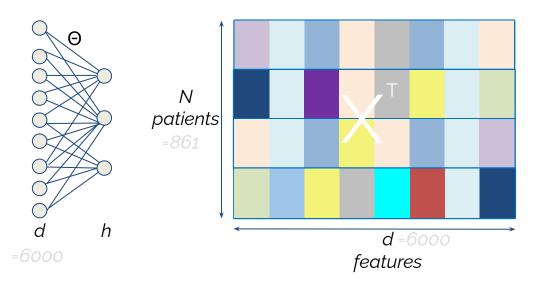
$$\underbrace{Y}_{h,N} = \underbrace{\Theta}_{h,d} \underbrace{X}_{N,d}^T$$



Fully connected [h,d]

Input features [N, d]

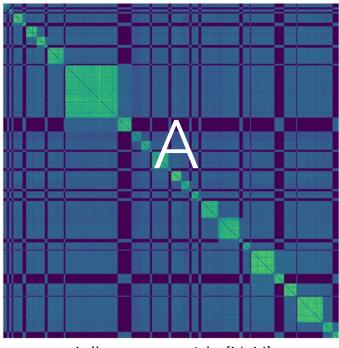
$$\underbrace{Y}_{h,N} = \underbrace{\Theta}_{h,d} \underbrace{X}_{N,d}^T \underbrace{A}_{N,N}$$



Fully connected [h,d]

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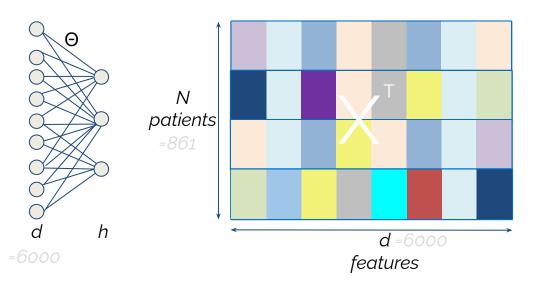
Basic message passing



Adjacency matrix [N, N]

Analogy: Non Local means - denoise similar colors on images

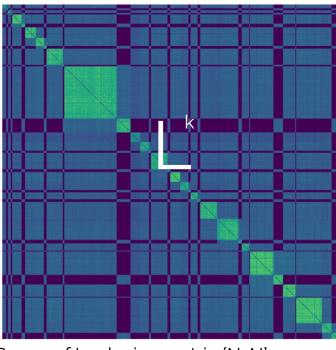
$$\underbrace{Y}_{h,N} = \underbrace{\Theta}_{h,d} \underbrace{X}_{N,d}^T \underbrace{A}_{N,N}$$



Fully connected [h,d]

Input features [N, d]

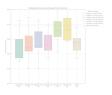
Basic message passing



Power of Laplacian matrix [N, N]

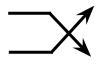
Variant in the paper : ChebConv - polynomial of the Laplacian L=I-A ⇒ gives access to a larger neighborhood

Experimental setup



Accuracy 68.9% +/- 4% on ABIDE (Autism Disorder Spectrum) Ability to reproduce results (~69.5%)

 \rightarrow Compare various models



Cross validation over 10 runs

80% train, 10% validation, 10% test



Frozen hyperparameters

Adam, LR 1E-4, Weight decay 0.1, no LR scheduler, 1000 epochs



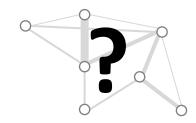
Reproducible results



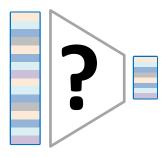
Code from scratch with documentation.

Results

- Is the use of graphs truly relevant? Compare
 - Dense Neural Networks
 - Graph Convolutional Networks +5%



- Is input dimension reduction relevant?
 - No significant differences between
 - Raw input features
 - Recursive Feature Elimination •0%
 - Auto Encoders' Latent vector -3%



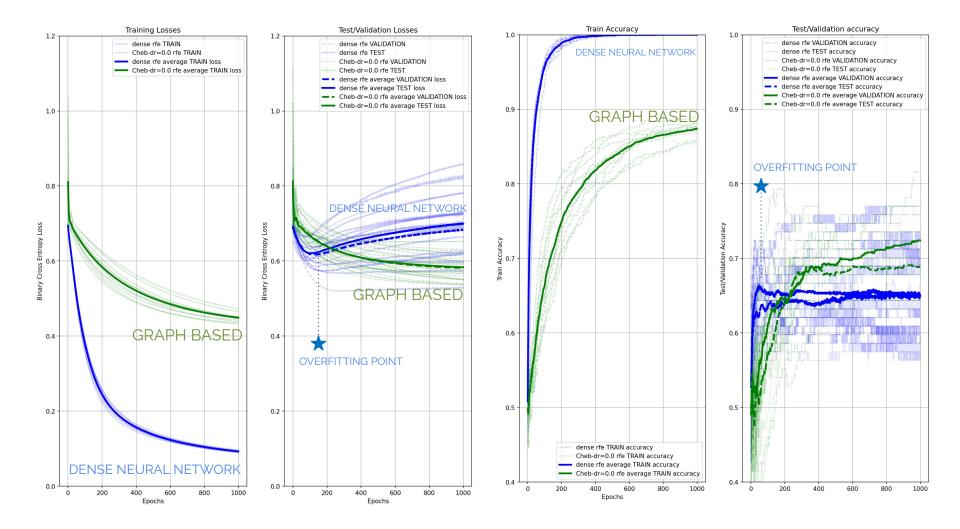
Conclusion

- A good introduction to the difficult domain of medical data analysis
- Curse of dimensionality
- Personal insights
 - Data type : time series , not 4D f-MRI volumes
 - Memory requirements: laptop GPU Nvidia T500 4Gb
 - « Spectral graph convolutions »

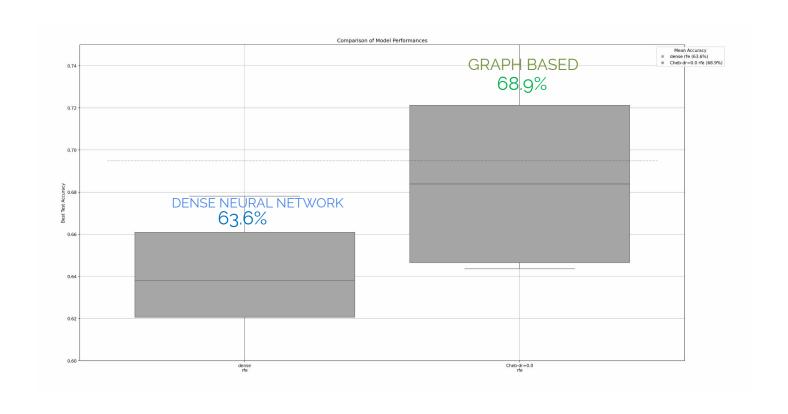
Thank you



Training curves

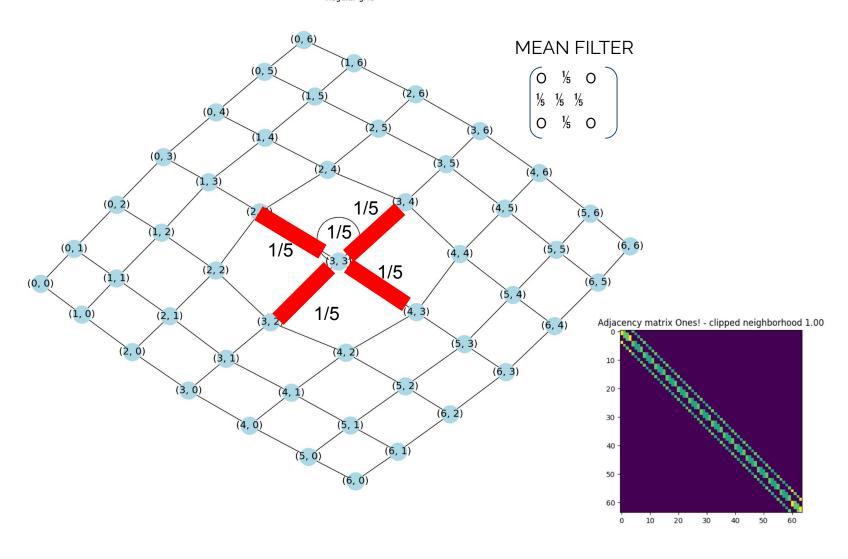


Dense Neural Network VS Graph Convolution



Analogy: Graph convolutions and Image denoising

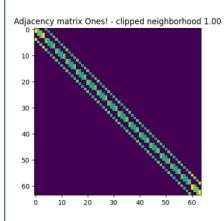
Feature smoothing using the normalized adjacency matrix
- Regular grid

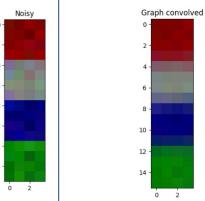


Analogy: Graph convolutions and Image denoising

CONSTANT WEIGHTS ON EDGES

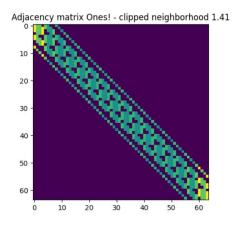


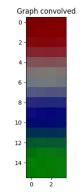




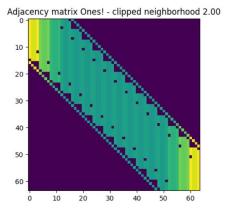
BOX FILTER

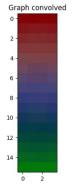
$$1/9 \begin{pmatrix} 1 & 1 & 1 \\ 1 & 1 & 1 \\ 1 & 1 & 1 \end{pmatrix}$$





1/13
$$\begin{pmatrix} 0 & 0 & 1 & 0 & 0 \\ 0 & 1 & 1 & 1 & 0 \\ 1 & 1 & 1 & 1 & 1 \\ 0 & 1 & 1 & 1 & 0 \\ 0 & 0 & 1 & 0 & 0 \end{pmatrix}$$

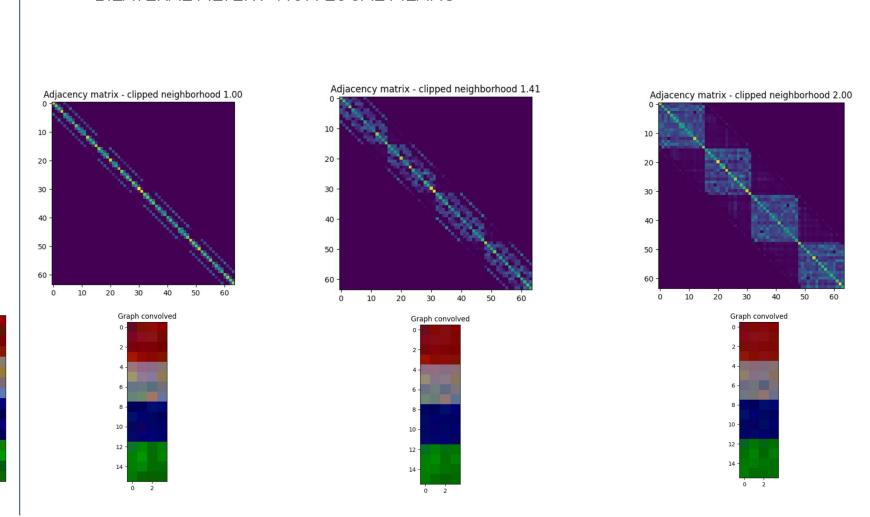




Analogy: Graph convolutions and Image denoising

SIMILARITY WEIGHTS ON EDGES

→ BILATERAL FILTER / NON LOCAL MEANS *

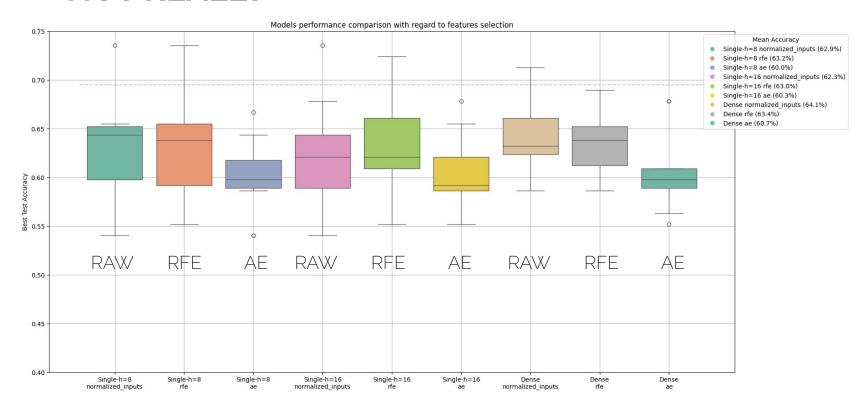


[*] Antoni Buades, Bartomeu Coll, and Jean-Michel Morel, Non-Local Means Denoising, Image Processing On Line, 1 (2011), pp. 208-212.

Results

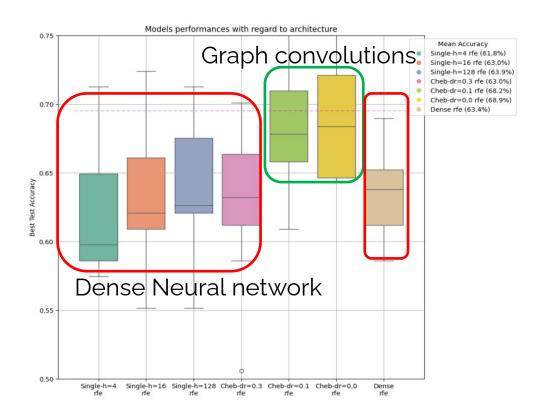
Relevance of reduce feature dimension?

- NOT REALLY



Results

- Relevance of using graph?
 - YES ~ +5% accuracy



Extra questions

A the beginning of the project, we asked ourselves a few questions on the paper:

- Does the graph structure bring anything?
 -> yes
- What does feature reduction do?
 -> nothing significant
- Would adding metadata to the input feature help a dense NN do better?
- How does the research world process MRI?
- Can we think of a toy example?
 - -> not trivial, focus on ABIDE dataset

Medical domain Expectations V.S. Reality

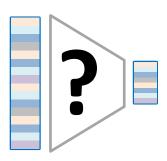
Expectation	Reality
f-MRI 4D volumes	Time series
Graph, big memory requirement	GPU laptop Nvidia T500 4Gb
« Spectral graph convolutions »	Message passing

Investigation

- Is the use of graphs truly relevant?



- Is input dimension reduction relevant?

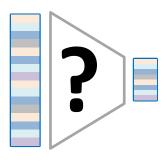


Investigation

- Is the use of graphs truly relevant?
 - Dense Neural Networks
 - Graph Convolutional Networks +5%



- Is input dimension reduction relevant? No significant differences between
 - Raw input features
 - Recursive Feature Elimination
 - Auto Encoder's Latent vector



Overview

- Paper summary Overview
 - Node
 - Edges
 - GCN
- Our contributions
 - Graph relevance
 - Feature dimension reduction
- Discussion

Medical domain Expectations V.S. Reality

Expectation	Reality
MRI 3D volumes ?	Time series
Huge medical dataset	861 patients – curse of dimensionality
Graph, big memory requirement	Nvidia T500 4Gb ~ enough
« Spectral graph convolutions »	Message passing, analogy NL-means