CS6208 : Advanced Topics in Artificial Intelligence
Graph Machine Learning

Lecture 5 : Graph Convolutional Networks
Spectral and Spatial Techniques

Semester 2 2022/23

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Outline

- Part 1 : Traditional ConvNets
  - Architecture
  - Graph Domain
  - Convolution
- Part 2: Spectral Graph ConvNets
  - Spectral Convolution
  - Spectral GCNs
- Part 3 : Spatial Graph ConvNets
  - Template Matching
  - Isotropic GCNs
  - Anisotropic GCNs
  - DGL : Implemented layers and lab demo
- Conclusion

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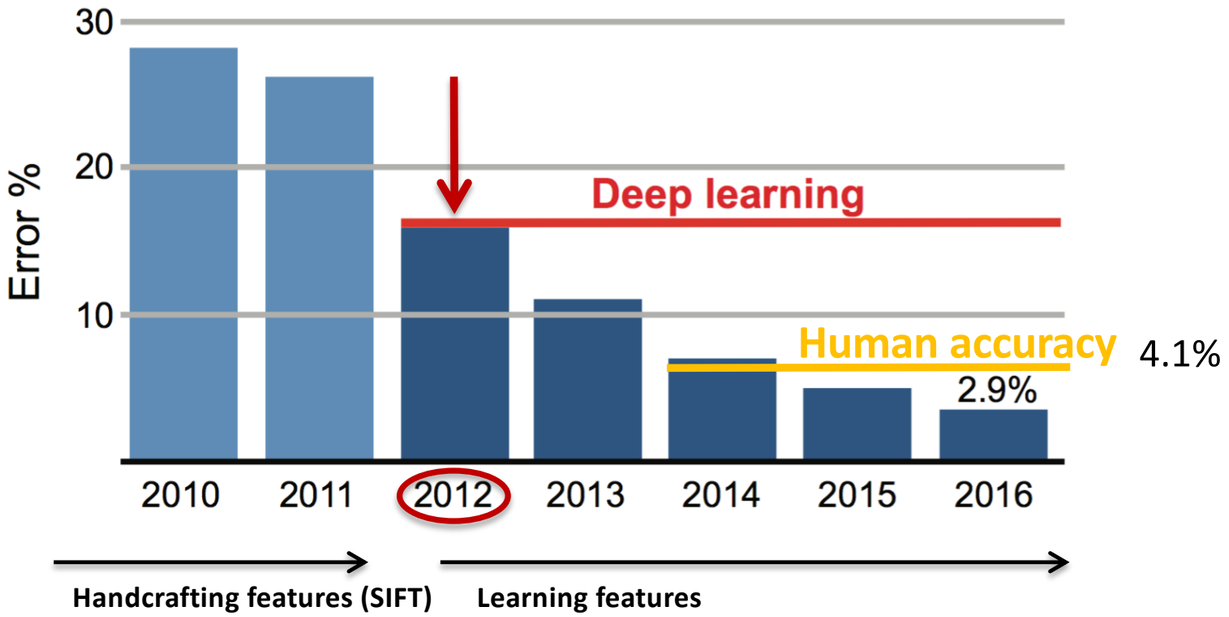
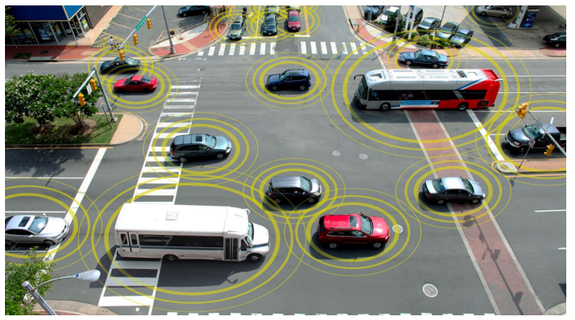
ConvNets

- A breakthrough in Computer Vision :

  LeCun, Bottou, Bengio, Haffner 1998
  Krizhevsky, Sutskever, Hinton, 2012

IMAGENET





- Also in Speech and Natural Language Processing.

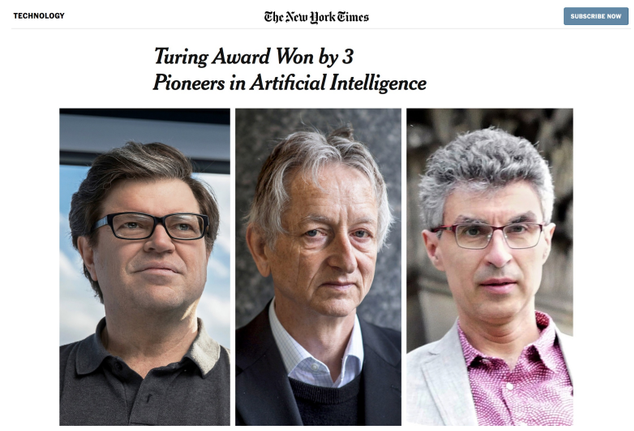
ConvNets

- ConvNets are powerful architectures to solve high-dimensional learning problems.

- Curse of dimensionality :

  dim(image) = 1024 x 1024 ≈ 10^6

  For N=10 samples/dim ⇒ $10^{1,000,000}$ points


TECHNOLOGY

The New York Times

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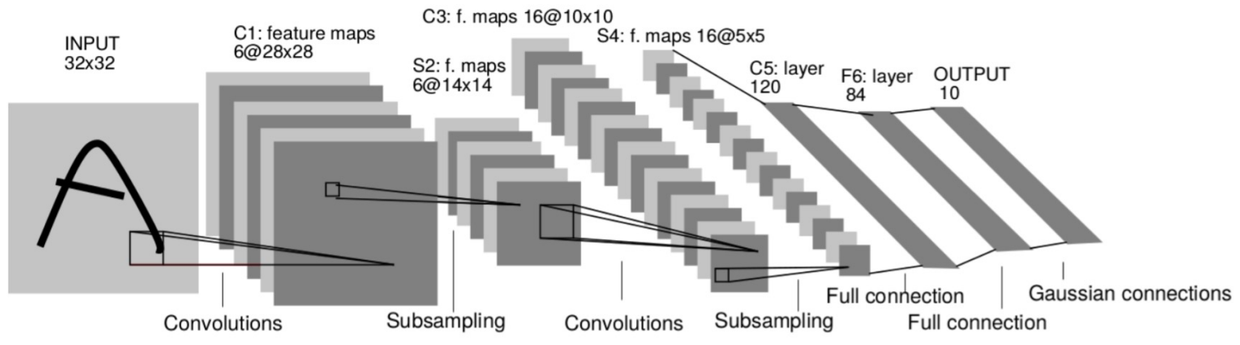
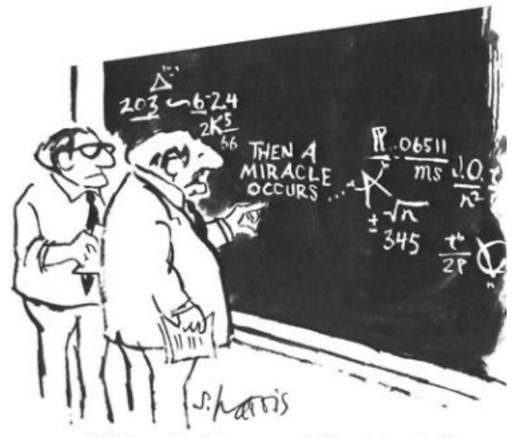
Turing Award Won by 3 Pioneers in Artificial Intelligence

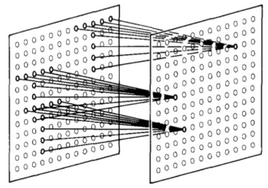


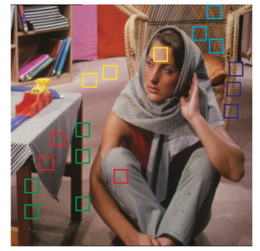


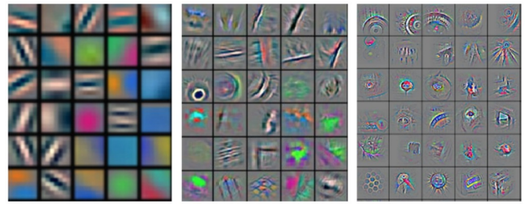
"I think you should be more explicit here in step two."

ConvNets

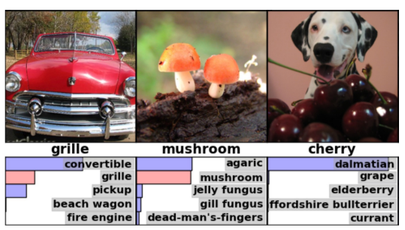
- Main assumption :
  - Data (image, video, speech) is compositional, it is formed of patterns that are:
    - Local (Hubel-Wiesel 1962)
    - Stationary (shared patterns)
    - Hierarchical (multi-scale)



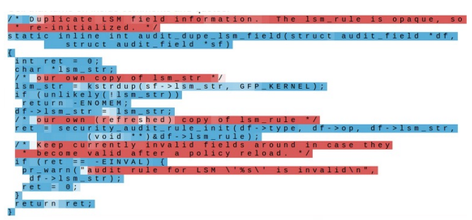




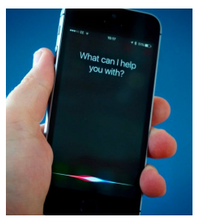
- ConvNets leverage the compositionality structure :
  - They extract compositional features and feed them to classifier, recommender, etc (end-to-end systems).



Computer Vision



NLP



Speech

Game of Go

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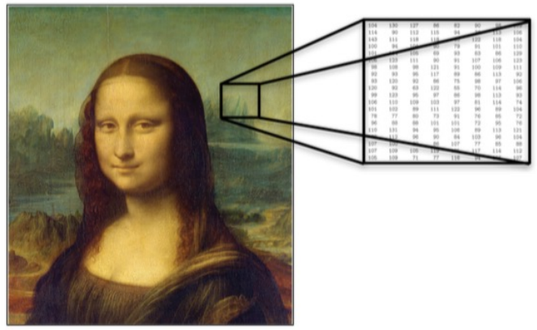
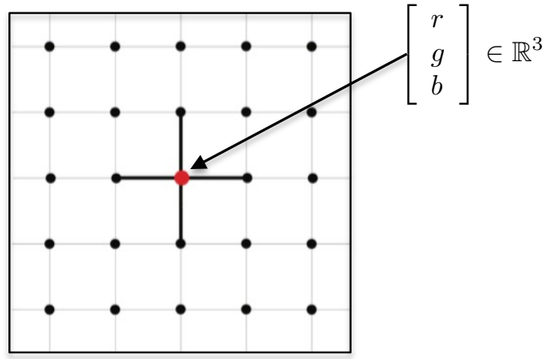
Data Domain

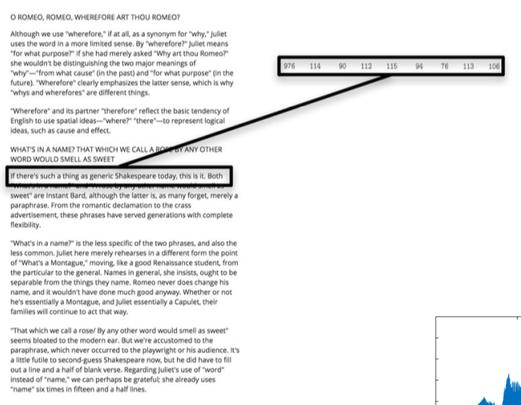
- Images, volumes, videos lie on
  2D, 3D, 2D+1 Euclidean domains (grids)

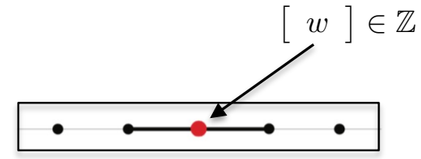




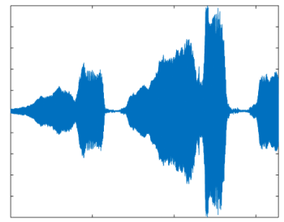
2D grid

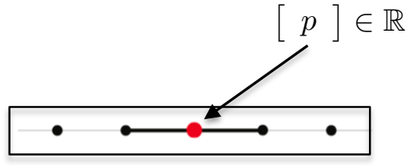
- Sentences, words, speech lie on
  1D Euclidean domain





1D grid





1D grid

- These domains have strong regular spatial structures.
  - All ConvNet operations are mathematically well defined and fast (convolution, pooling).

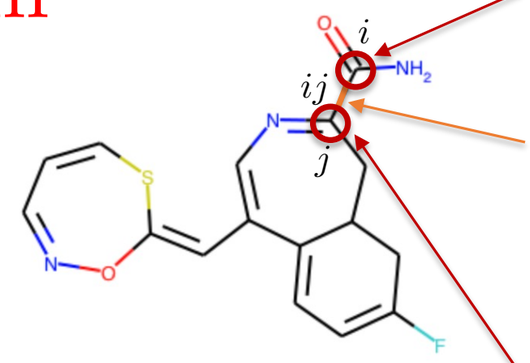
Graph Domain

Social networks
(Advertisement/
recommendation)

$$\textbf{User}_\textbf{i} \begin{bmatrix} \text{messages} \\ \text{images} \\ \text{videos} \end{bmatrix}_i \in \mathbb{R}^d$$

$$\textbf{User connection}_\textbf{ij} \quad A_{ij} = \begin{cases} 1 & \text{if ij friends} \\ 0 & \text{otherwise} \end{cases}$$

$$\textbf{User}_\textbf{j} \begin{bmatrix} \text{messages} \\ \text{images} \\ \text{videos} \end{bmatrix}_j \in \mathbb{R}^d$$



Quantum Chemistry
(novel molecules for drugs
and materials)

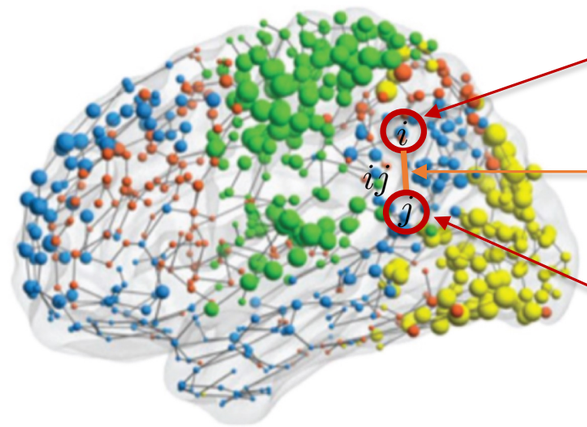
$$\textbf{Atom}_\textbf{i} \begin{bmatrix} \text{type} \\ \text{coordinates} \\ \text{charge} \end{bmatrix}_i \in \mathbb{R}^{d_v}$$

$$\textbf{Bond}_\textbf{ij} \quad A_{ij} = \begin{cases} 1 & \text{if ij bond} \\ 0 & \text{otherwise} \end{cases}$$

$$\begin{bmatrix} \text{type} \\ \text{energy} \end{bmatrix}_{ij} \in \mathbb{R}^{d_e}$$

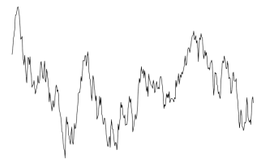
$$\textbf{Atom}_\textbf{j} \begin{bmatrix} \text{type} \\ \text{coordinates} \\ \text{charge} \end{bmatrix}_j \in \mathbb{R}^{d_v}$$

Brain connectivity
(sMRI)



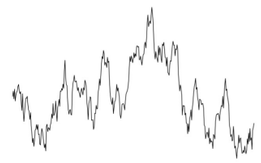
Brain analysis
(Neuroscience/neuro-diseases)

$$\textbf{ROI}_\textbf{i} \begin{bmatrix} a_1 \\ \vdots \\ a_T \end{bmatrix}_i \in \mathbb{R}^T$$



$$\textbf{Cerebral connection}_\textbf{ij} \quad A_{ij} \in \mathbb{R}_+$$

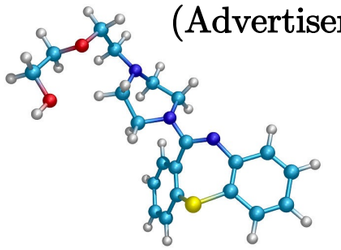
$$\textbf{ROI}_\textbf{j} \begin{bmatrix} a_1 \\ \vdots \\ a_T \end{bmatrix}_j \in \mathbb{R}^T$$



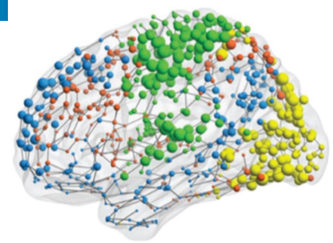
Functional
activations (fMRI)

Graph Domain

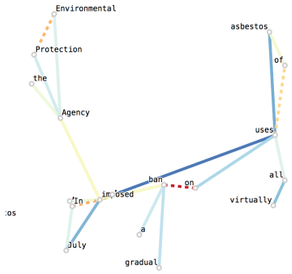
Social networks (Advertisement)



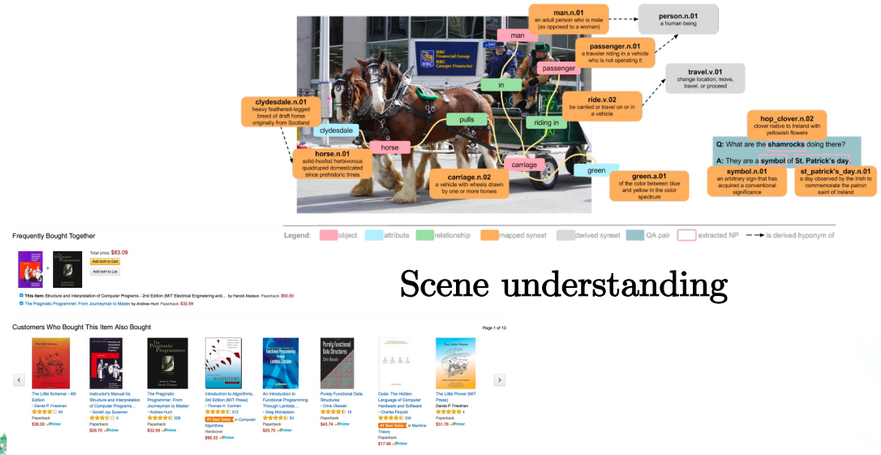
Drug/Material molecules (Chemistry)



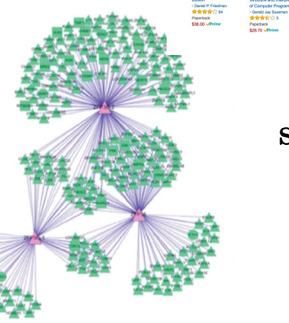
Brain connectivity (Neuroscience)



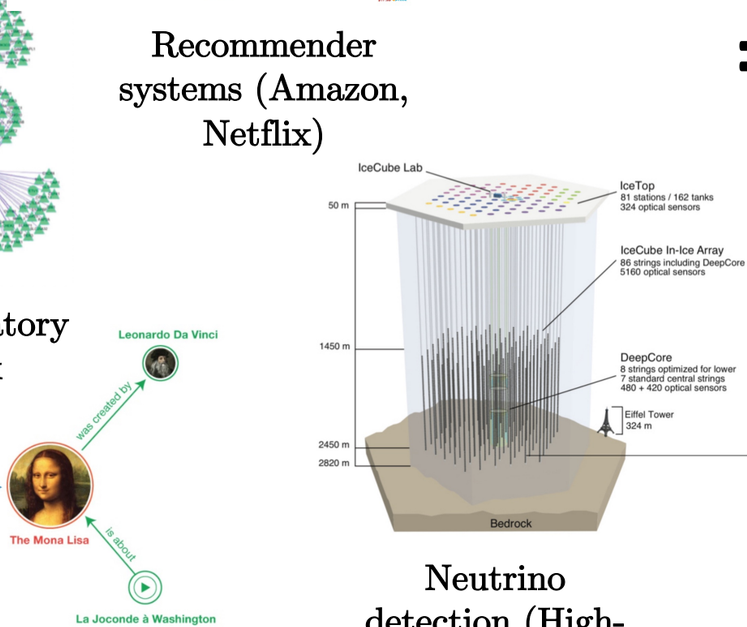
Words relationships (NLP)



Scene understanding



Gene Regulatory Network



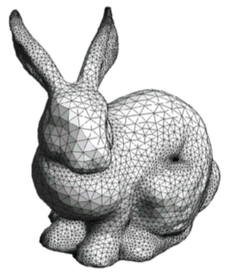
Knowledge graphs

Recommender systems (Amazon, Netflix)

Neutrino detection (High-energy Physics)

=

Graph

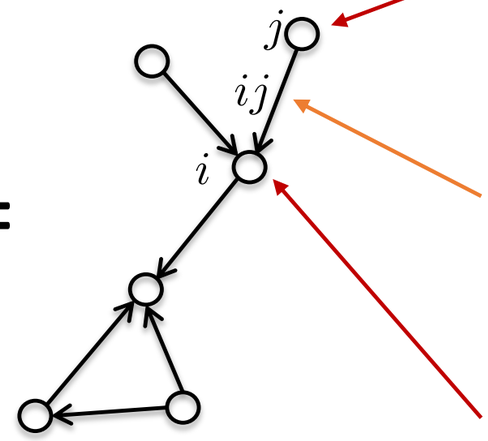


3D Meshes (Computer Graphics)

Transportation networks

Graph Domain

- Graphs G are defined by :
  - Vertices V
  - Edges E
  - Adjacency matrix A



$$h_j = \begin{bmatrix} \vdots \end{bmatrix} \in \mathbb{R}^{d_v}$$

$$e_{ij} = \begin{bmatrix} \vdots \end{bmatrix} \in \mathbb{R}^{d_e}$$

$$h_i = \begin{bmatrix} \vdots \end{bmatrix} \in \mathbb{R}^{d_v}$$

$$\mathcal{G} = (V, E, A)$$

$$V = \{1, .., n\}$$

- Graph features :
  - Node features : h_i, h_j (atom type)
  - Edge features : e_{ij} (bond type)
  - Graph features : g (molecule energy)

$$g = \begin{bmatrix} \vdots \end{bmatrix} \in \mathbb{R}^{d_g}$$

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Convolution

- Convolutional layer (for grids) :

$$h^{\ell+1} = w^{\ell} * h^{\ell}$$

$$n_1 \times n_2 \times d \qquad\qquad n_1 \times n_2 \times d$$

$$3 \times 3 \times d$$

h^{ℓ}

Image/Hidden features

$*$

w^{ℓ}

Pattern/kernel (learned by backpropagation)

$=$

$h^{\ell+1}$

Convolution

- How to define convolution ?
  - Definition #1 : Convolution as template matching
  - O(n) by parallelization and for compact support patterns

$$h_i^{\ell+1} = w^\ell * h_i^\ell$$

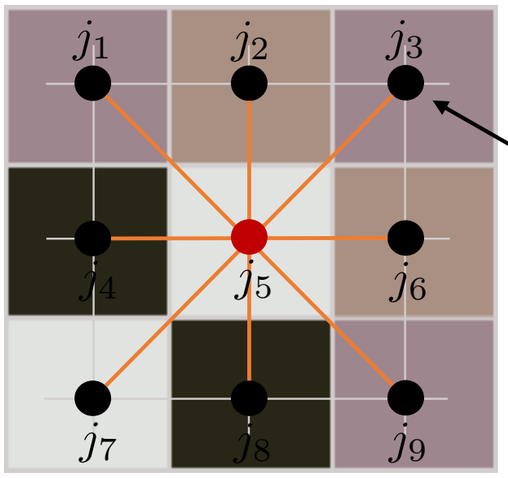
$$= \sum_{\underbrace{j \in \Omega}_{j \in \mathcal{N}_i}} \langle w_j^\ell, \underbrace{h_{i-j}^\ell}_{h_{i+j}^\ell = h_{ij}^\ell} \rangle$$

$$= \sum_{j \in \mathcal{N}_i} \langle w_j^\ell, h_{ij}^\ell \rangle$$

$$= \sum_{j \in \mathcal{N}_i} \left\langle \begin{bmatrix} \\ w_j^\ell \\ \\ \end{bmatrix}, \begin{bmatrix} \\ h_{ij}^\ell \\ \\ \end{bmatrix} \right\rangle$$

$3 \times 3 \times d$

$n_1 \times n_2 \times d$



Node j_3 is always located at the top-right corner of the pattern.

All nodes of the template w^l are always ordered/positioned the same way !

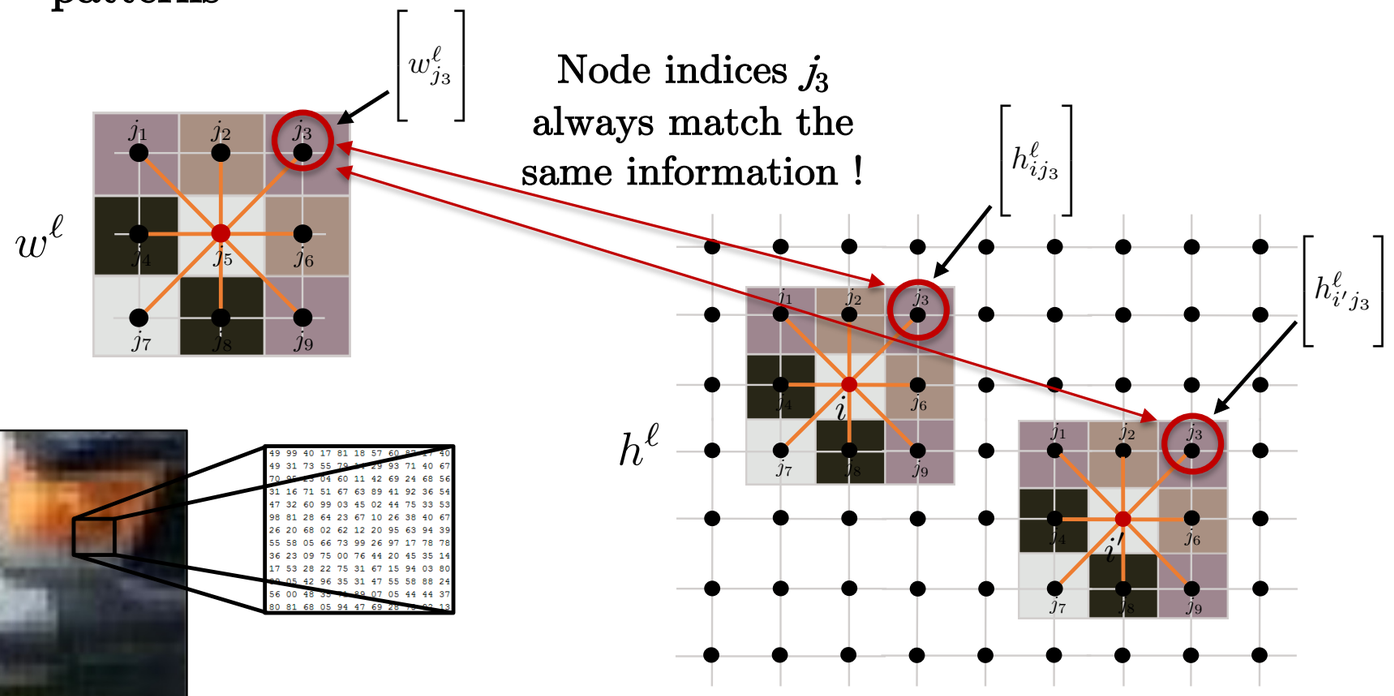
w^ℓ

$$\begin{bmatrix} \\ w_{j_3}^\ell \\ \\ \end{bmatrix} \in \mathbb{R}^d$$

Template features at j_3

Convolution

- How to define convolution ?
  - Definition #1 : Convolution as template matching
  - O(n) by parallelization for compact support patterns



Same node ordering $\forall i$
j_3 is always positioned at the top-right corner of the template.

$$h^{\ell+1}_i = w^\ell * h^\ell_i$$
$$= \sum_{j \in \mathcal{N}_i} \langle w^\ell_j, h^\ell_{ij} \rangle$$
$$= \sum_{j \in \mathcal{N}_i} \left\langle \begin{bmatrix} w^\ell_j \end{bmatrix}, \begin{bmatrix} h^\ell_{ij} \end{bmatrix} \right\rangle$$

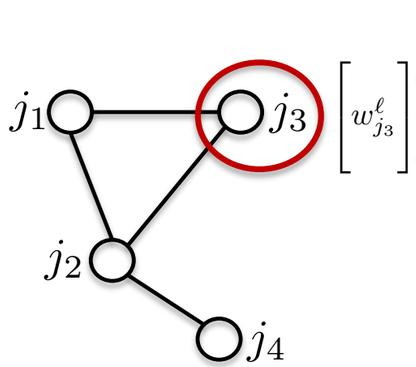
$$\left\langle \begin{bmatrix} w^\ell_{j_3} \end{bmatrix}, \begin{bmatrix} h^\ell_{ij_3} \end{bmatrix} \right\rangle$$

$$\left\langle \begin{bmatrix} w^\ell_{j_3} \end{bmatrix}, \begin{bmatrix} h^\ell_{i'j_3} \end{bmatrix} \right\rangle$$

These matching scores are always for the top-right corner between the template and the image patches.

Graph Convolution

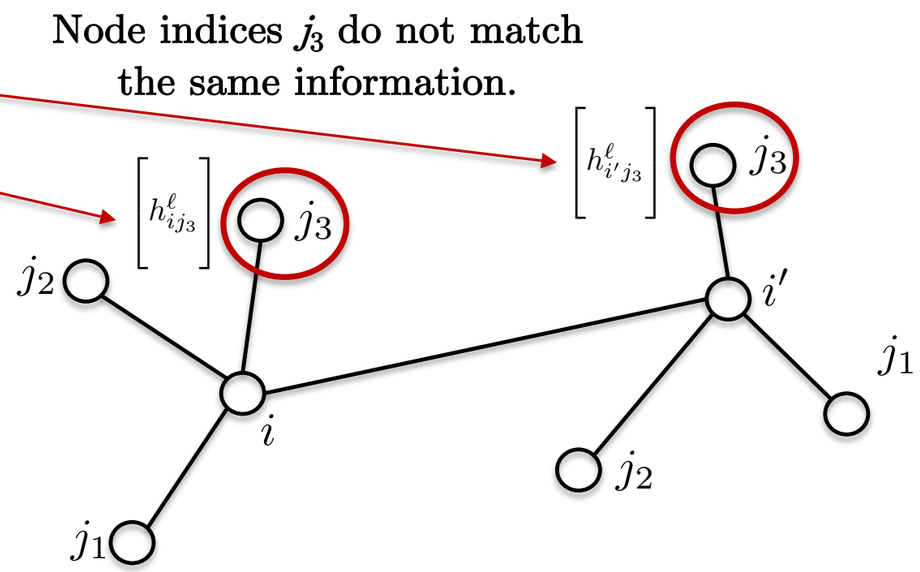
- Can we extend template matching for graphs ?
  - Main issues :
    - No node ordering : How to match template features with data features when nodes have no given position (index is not a position) ?



w^ℓ

Node j_3 has no specific position. It is just an (arbitrary) index.

Node indices j_3 do not match the same information.



h^ℓ

No node ordering on graphs :
The correspondence of nodes is lost on graphs.
There is no up, down, right and left on graphs.

$$\left\langle \begin{bmatrix} w^\ell_{j_3} \end{bmatrix}, \begin{bmatrix} h^\ell_{ij_3} \end{bmatrix} \right\rangle$$

$$\left\langle \begin{bmatrix} w^\ell_{j_3} \end{bmatrix}, \begin{bmatrix} h^\ell_{i'j_3} \end{bmatrix} \right\rangle$$

These matching scores have no meaning as they do not compare the same information.

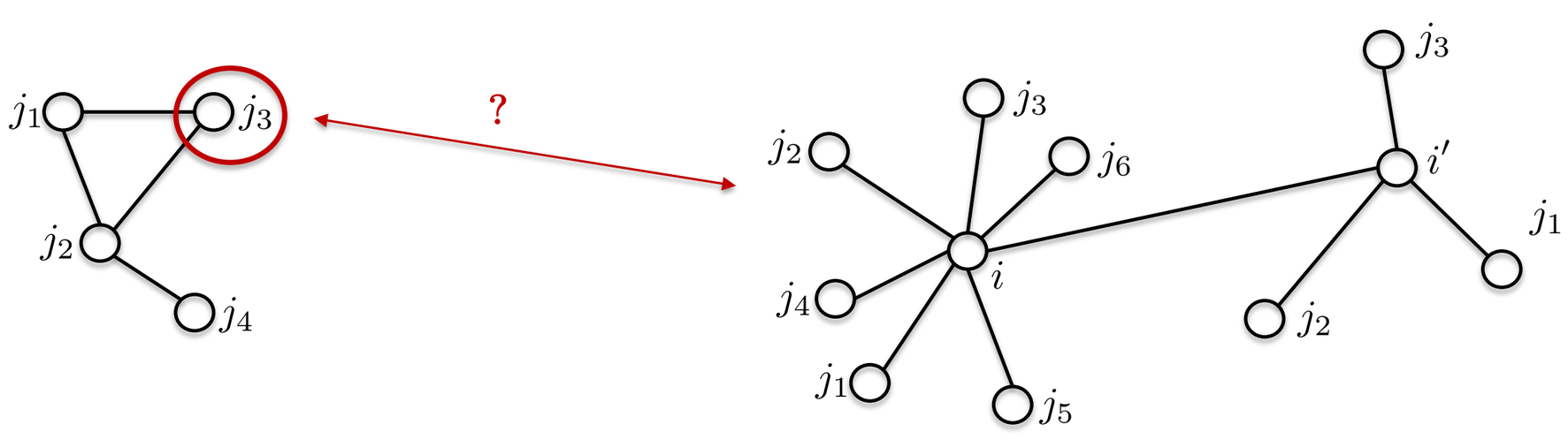
$$h^{\ell+1}_i = w^\ell *_{\mathcal{G}} h^\ell_i$$

$$= \sum_{j \in \mathcal{N}_i} \langle w^\ell_j, h^\ell_{ij} \rangle$$

$n \times d$

Graph Convolution

- Can we extend template matching for graphs ?
  - Main issues :
    - No node ordering : How to match template features with data features ?
    - Heterogeneous neighborhood : How to deal with different neighborhood sizes ?



Graph Convolution

- How to define convolution ?
  - Definition #1 : Template matching
  - Definition #2 : Convolution theorem
    - Fourier transform of the convolution of two functions is the pointwise product of their Fourier transforms

$$\mathcal{F}(w * h) = \mathcal{F}(w) \odot \mathcal{F}(h) \quad \Rightarrow \quad w * h = \mathcal{F}^{-1}(\mathcal{F}(w) \odot \mathcal{F}(h))$$

    - Generic Fourier transform has $O(n^2)$ complexity, but if the domain is a grid then complexity can be reduced to $O(n \log n)$ with FFT[1].

- Can we extend the Convolution theorem to graphs ?
  - How to define Fourier transform for graphs ?
  - How to compute fast spectral convolutions in $O(n)$ time for compact kernels ?

$$w *_{\mathcal{G}} h \stackrel{?}{=} \mathcal{F}_{\mathcal{G}}^{-1}(\mathcal{F}_{\mathcal{G}}(w) \odot \mathcal{F}_{\mathcal{G}}(h))$$

[1] JW Cooley, JW Tukey, An algorithm for the machine calculation of complex Fourier series, 1965

Outline

- Part 1 : Traditional ConvNets
  - Architecture
  - Graph Domain
  - Convolution
- Part 2: Spectral Graph ConvNets
  - Spectral Convolution
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  - Template Matching
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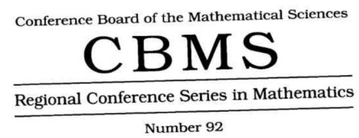
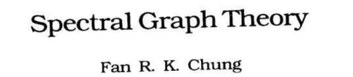
  - Anisotropic GCNs
  - DGL : Implemented layers and lab demo
- Conclusion

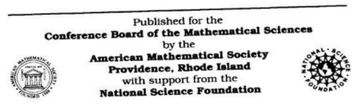
Spectral Convolution

- Spectral graph theory
  - Book of Fan Chung[1] (harmonic analysis, graph theory, combinatorial problems, optimization)



- How to perform spectral convolution ?
  - Graph Laplacian
  - Fourier functions
  - Fourier transform
  - Convolution theorem





[1] FRK Chung, Spectral graph theory, 1997

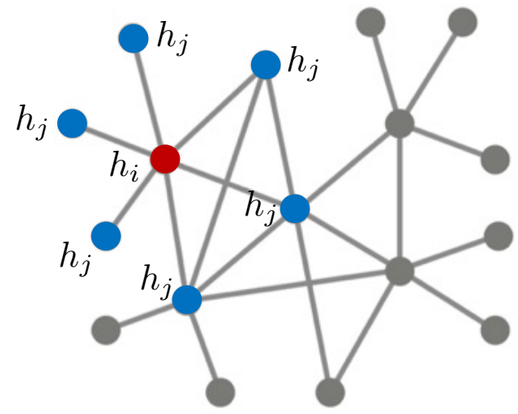
Graph Laplacian

- Core operator in Spectral Graph Theory

$$\mathcal{G} = (V, E, \underset{n \times n}{A}) \quad \rightarrow \quad \underset{n \times n}{\Delta} = \mathrm{I} - D^{-1/2} A D^{-1/2} \qquad \text{Normalized Laplacian}$$
$$\text{where } \underset{n \times n}{D} = \mathrm{diag}(\sum_{j \neq i} A_{ij})$$

- Interpretation :
  - Measure of smoothness : Difference between local value h_i and its neighborhood average values h_j.

$$(\Delta h)_i = h_i - \sum_{j \in \mathcal{N}_i} \frac{1}{\sqrt{d_i d_j}} A_{ij} h_j$$



Fourier Functions

- Eigen-decomposition of graph Laplacian :

Lap Eigenvalues/ Spectrum

Lap Eigenvectors/ Fourier functions

$$\underset{n \times n}{\Delta} = \Phi^T \Lambda \Phi$$

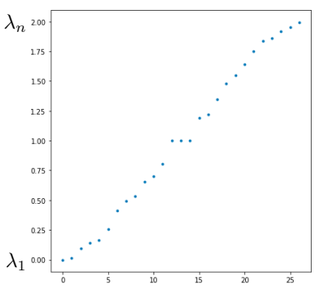
Fourier functions form an orthonormal basis

$$\text{where } \underset{n \times n}{\Phi} = [\phi_1, ..., \phi_n] = \begin{bmatrix} | & & | \\ \phi_1 & ... & \phi_n \\ | & & | \end{bmatrix} \text{ and } \Phi^T \Phi = \mathrm{I}, \ \langle \phi_k, \phi_{k'} \rangle = \delta_{kk'}$$

$$\text{where } \underset{n \times n}{\Lambda} = \mathrm{diag}(\lambda_1, ..., \lambda_n) = \begin{bmatrix} \lambda_1 & & 0 \\ & \ddots & \\ 0 & & \lambda_n \end{bmatrix} \text{ and } 0 \leq \lambda_1 \leq ... \leq \lambda_n = \lambda_{\max} \leq 2$$

$$\text{and } \underset{n \times 1}{\Delta \phi_k} = \lambda_k \phi_k, \quad k = 1, ..., n$$

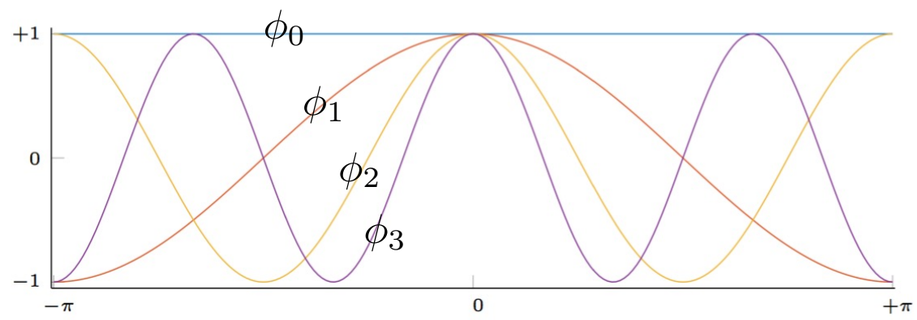
$n = 27$



Spectrum

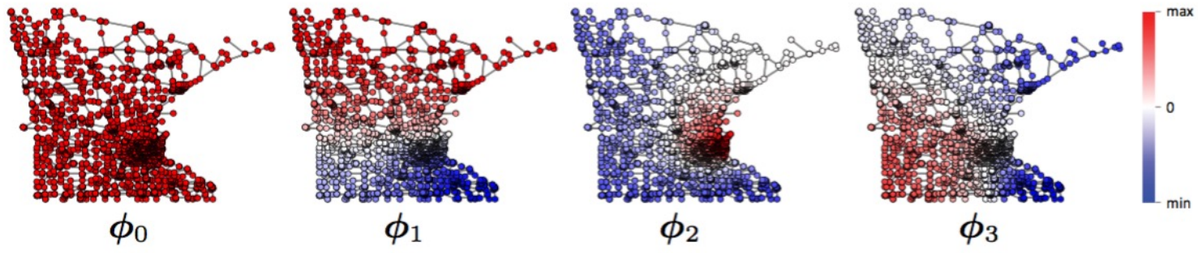
Fourier Functions

- Grid/Euclidean domain :



First eigenvectors of 1D Euclidean Laplacian = standard Fourier basis

- Graph domain :



First Laplacian eigenvectors of a graph

Fourier functions related to graph geometry
(s.a. communities, hubs, etc)
Spectral graph clustering[1]

[1] Von Luxburg, A tutorial on spectral clustering, 2007

Fourier Transform

- **Fourier series : Decompose function h with Fourier functions[1] :**

$$
\begin{aligned}
\underset{n \times 1}{h} &= \sum_{k=1}^{n} \underbrace{\langle \phi_k, h \rangle}_{\substack{\mathcal{F}(h)_k = \hat{h}_k = \phi_k^T h \\ \text{scalar}}} \underset{n \times 1}{\phi_k} \\
&= \sum_{k=1}^{n} \hat{h}_k \phi_k \\
&= \underbrace{\Phi \hat{h}}_{\mathcal{F}^{-1}(\hat{h})}
\end{aligned}
$$

Fourier transforms are one line of code (linear operations)

$$
\begin{cases}
\underset{n \times 1}{\mathcal{F}(h)} = \Phi^T h = \hat{h} & \text{Fourier Transform/ coefficients of Fourier Series} \\
\underset{n \times 1}{\mathcal{F}^{-1}(\hat{h})} = \Phi \hat{h} & \text{Inverse Fourier Transform} \\
\qquad\qquad = \Phi \Phi^T h = h \text{ as } \mathcal{F}^{-1} \circ \mathcal{F} = \Phi \Phi^T = \mathrm{I} & \text{Orthonormal basis/ Invertible transformation}
\end{cases}
$$

[1] K. Hammond, P. Vandergheynst, R. Gribonval, Wavelets on graphs via spectral graph theory, 2011

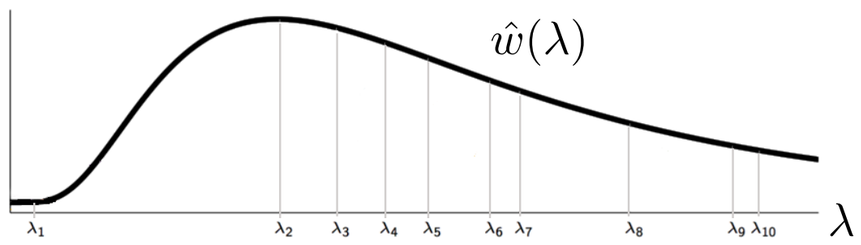
Convolution Theorem

- Fourier transform of the convolution of two functions is the pointwise product of their Fourier transforms :

$$
\begin{aligned}
\underset{n\times 1}{w * h} &= \underbrace{\mathcal{F}^{-1}}_{\Phi}\big(\underbrace{\mathcal{F}(w)}_{\Phi^T w=\hat{w}} \odot \underbrace{\mathcal{F}(h)}_{\Phi^T h}\big) \\
&= \underset{n\times n}{\Phi}\big(\underset{n\times 1}{\hat{w}} \odot \underset{n\times 1}{\Phi^T h}\big) \\
&= \Phi\ \big(\underset{n\times n}{\hat{w}(\Lambda)}\ \underset{n\times 1}{\Phi^T h}\big) \\
&= \Phi\ \hat{w}(\Lambda)\ \Phi^T h \\
&= \hat{w}(\underbrace{\Phi\Lambda\Phi^T}_{\Delta})\ h \\
&= \underset{n\times n}{\hat{w}(\Delta)}\underset{n\times 1}{h}
\end{aligned}
$$

$$
\underset{n\times 1}{\hat{w}} = \begin{bmatrix} \hat{w}(\lambda_1) \\ \vdots \\ \hat{w}(\lambda_n) \end{bmatrix}
$$

$$
\underset{n\times n}{\hat{w}(\Lambda)} = \mathrm{diag}(\hat{w}) = \begin{bmatrix} \hat{w}(\lambda_1) & & 0 \\ & \ddots & \\ 0 & & \hat{w}(\lambda_n) \end{bmatrix}
$$



Expensive computation O(n^2)
No FFT

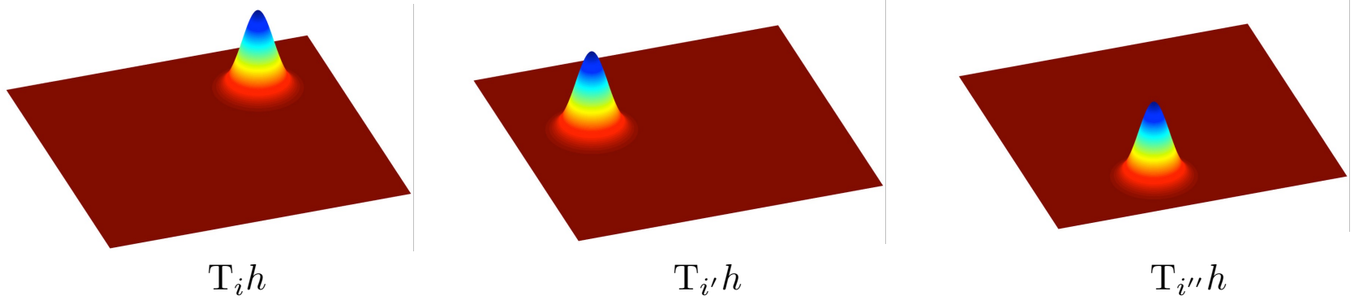
Spectral function/filter

No Shift Invariance for Graphs

- A signal h on graph can be translated to vertex *i* as follows :

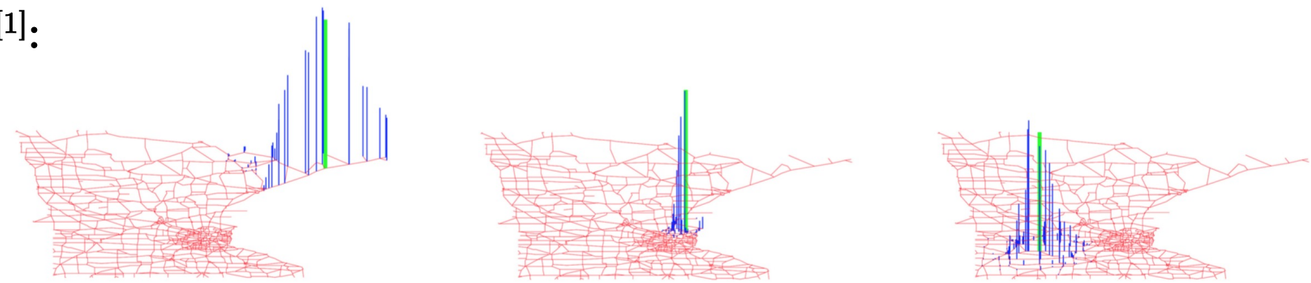
$$\mathrm{T}_i h = \delta_i * h$$

- Grid/Euclidean domain :



$\mathrm{T}_i h$ $\mathrm{T}_{i'} h$ $\mathrm{T}_{i''} h$

- Graph domain[1]:



$\mathrm{T}_i h$ $\mathrm{T}_{i'} h$ $\mathrm{T}_{i''} h$

[1] K. Hammond, P. Vandergheynst, R. Gribonval, Wavelets on graphs via spectral graph theory, 2011

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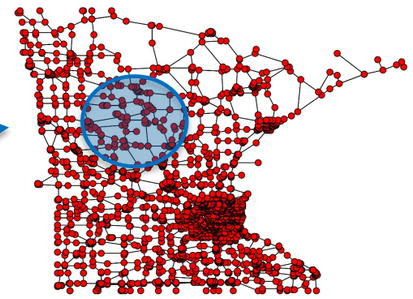
Vanilla Spectral GCN[1]

- Graph spectral convolutional layer :

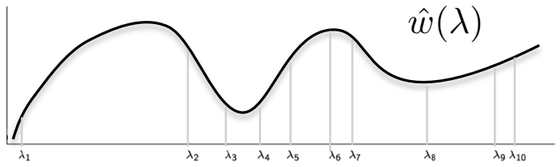
$$
\begin{aligned}
\underset{n \times d}{h^{\ell+1}} &= \eta(\ w^{\ell} * h^{\ell}\ ) \\
&= \eta(\ \hat{w}^{\ell}(\Delta) h^{\ell}\ ) \\
&= \eta(\ \underset{n \times n}{\Phi \hat{w}^{\ell}(\Lambda) \Phi^{T}} \underset{n \times d}{h^{\ell}}\ )
\end{aligned}
$$

$n \times n$

Spatial filter



Spectral filter



$$
\hat{w}(\Lambda) = \begin{bmatrix} \hat{w}(\lambda_1) & & 0 \\ & \ddots & \\ 0 & & \hat{w}(\lambda_n) \end{bmatrix}
$$

- First spectral technique for ConvNets
- Limitations :
  - No guarantee of spatial localization of filters
  - O(n) parameters to learn per layer
  - O(n^2) learning complexity (Fourier transform with full matrix ϕ)

[1] Bruna, Zaremba, Szlam, LeCun, Spectral Networks and Locally Connected Networks on Graphs, 2014

SplineGCNs[1,2]

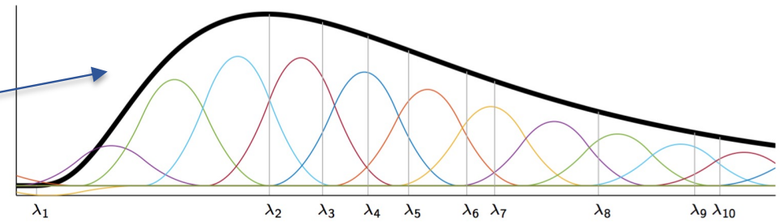
- Graph spectral convolutional layer :

$$
\begin{aligned}
h^{\ell+1}_{n\times d} &= \eta(\ w^\ell * h^\ell\ ) \\
&= \eta(\ \Phi \hat{w}^\ell(\Lambda)\Phi^T h^\ell\ ) \\
\hat{w}^\ell(\Lambda) &= \mathrm{diag}(Bw^\ell) \\
n\times n & \qquad\qquad K\times 1 \\
& \qquad\quad n\times K \\
& \qquad \underbrace{\qquad\qquad}_{n\times n}
\end{aligned}
$$

The K coefficients w^l are learned by backpropagation

Smooth spectral filters/ Linear combination of K smooth kernels B (splines)

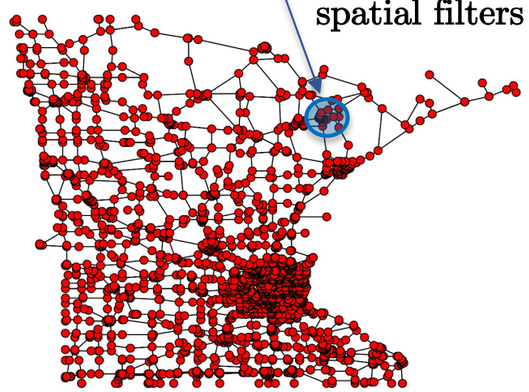
Smooth spectral filters



Parseval's Identity
Localization in space ⇔
Smoothness in frequency domain
(Heisenberg's uncertainty principle)

$$\int |x|^{2k}|w(x)|^2 dx = \int |\frac{\partial^k \hat{w}(\lambda)}{\partial \lambda^k}|^2 d\lambda$$

Localized spatial filters



- Localized filters in space (fast-decaying)
- O(*1*) parameters to learn per layer
- O(n^2) learning complexity (Fourier transform with full matrix ϕ)

[1] Bruna, Zaremba, Szlam, LeCun, Spectral Networks and Locally Connected Networks on Graphs, 2014
[2] Henaff, Bruna, LeCun, Deep Convolutional Networks on Graph-Structured Data, 2015

LapGCNs[1]

- How to learn in linear time O(n) (w.r.t. graph size n) ?
  - O(n^2) complexity comes from the direct use of Laplacian eigenvectors :

$$\underset{n \times d}{O(w * h)} = \underset{n \times n}{O(\Phi} \underset{n \times n}{\hat{w}^{\ell}(\Lambda)} \underset{n \times d}{\Phi^T h)} = O(n^2)$$

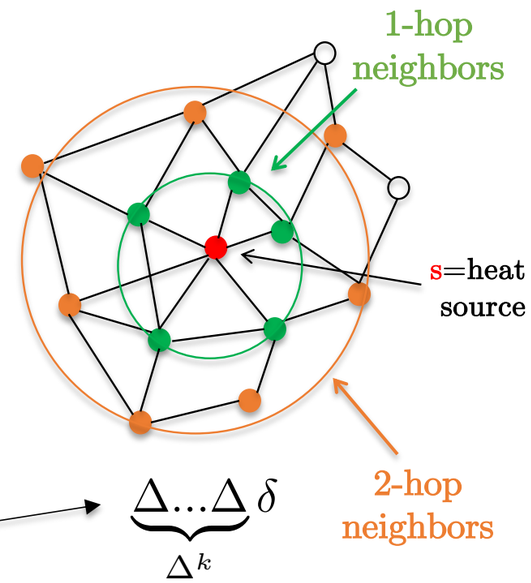
Full matrix

  - How to avoid the eigen-decomposition ?
    - Learn directly functions of the Laplacian !

$$w * h = \hat{w}(\Delta)h$$

$$\underset{n \times n}{\hat{w}(\Delta)} = \sum_{k=0}^{K-1} w_k \underset{n \times n}{\Delta^k}$$

Coefficients w_k are learned by backpropagation.



Filters are exactly localized in k-hop supports.
(each Laplacian operation increases the support of a function by 1 hop)

[1] Defferrard, Bresson, Vandergheynst, Convolutional neural networks on graphs with fast localized spectral filtering, 2016

LapGCNs

- **Learning complexity :**

$$
\begin{aligned}
w * h &= \hat{w}(\Delta)h \\
&= \sum_{k=0}^{K-1} w_k \Delta^k h \\
&= \sum_{k=0}^{K-1} w_k X_k, \text{ with } \underset{n \times n}{X_k} = \underset{n \times n}{\Delta} \underset{n \times d}{X_{k-1}} \text{ and } \underset{n \times d}{X_0} = \underset{n \times d}{h}
\end{aligned}
$$

Recursive equation

- Sequence $\{X_k\}$ is generated by multiplying a matrix Δ and a vector X_{k-1} ⇒ Complexity is O(E.K)=O(n) for sparse (real-world) graphs.
- No eigen-decomposition of Laplacian (ϕ,Λ) was required.
  - The name spectral GCNs can be misguided as the Lap eigen-decomposition is not used (computations are done in the spatial domain, not the spectral domain).
- Graph convolutional layers are (sparse) linear operations, thus GPU friendly (but not yet optimized).

LapGCNs

- Implementation :

$$\underset{n \times d}{h^{\ell+1}} = \eta\Big(\sum_{k=0}^{K-1} \underset{n \times n}{w_k^\ell} \underset{n \times d}{\Delta^k h^\ell} \Big)$$

$$= \eta\Big(\sum_{k=0}^{K-1} w_k^\ell \underset{n \times d}{X_k} \Big)$$

$$= \eta\Big(\underbrace{(w^\ell)^T \bar{X}}_{1 \times nd} \Big)$$

reshape
$n \times d$

$$\text{with } \underset{K \times nd}{\bar{X}} = \begin{bmatrix} - & \bar{X}_0 & - \\ & \vdots & \\ - & \bar{X}_{K-1} & - \end{bmatrix}$$

$$\underset{1 \times nd}{\bar{X}_k} = \text{reshape}(\underset{n \times d}{X_k})$$

$$\underset{K \times 1}{w^\ell} = \begin{bmatrix} w_0^\ell \\ \vdots \\ w_{K-1}^\ell \end{bmatrix}$$

- Filters are exactly localized in K-hop support
- O(1) parameters to learn per layer
- O(n) learning complexity
- Monomials basis are unstable under coefficients perturbation (hard to optimize)

$$1, x, x^2, x^3, ... \quad \rightarrow \quad \Delta^0, \Delta^1, \Delta^2, \Delta^3, ...$$

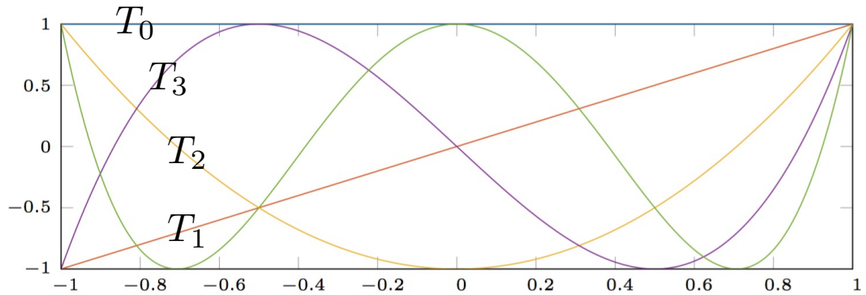
Chebyshev Polynomials

- **Graph spectral convolution with Chebyshev polynomials :**

$$
\begin{aligned}
w * h &= \hat{w}(\Delta)h \\
&= \sum_{k=0}^{K-1} w_k T_k(\Delta)h \\
&= \sum_{k=0}^{K-1} w_k X_k, \text{ with } X_k = 2\tilde{\Delta}X_{k-1} - X_{k-2}, X_0 = h, X_1 = \tilde{\Delta}h \text{ and } \tilde{\Delta} = 2\lambda_n^{-1}\Delta - \mathrm{I}
\end{aligned}
$$

Recursive equation

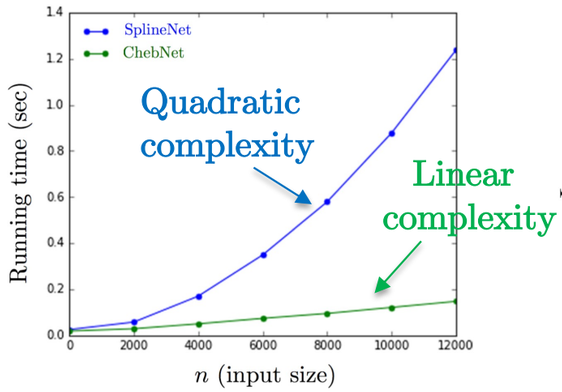
- Filters are exactly localized in K-hop support
- O(1) parameters to learn per layer
- O(n) learning complexity
- Stable under coefficients perturbation



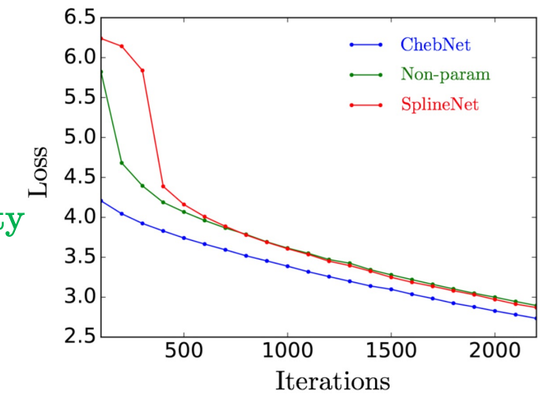
Orthonormal basis

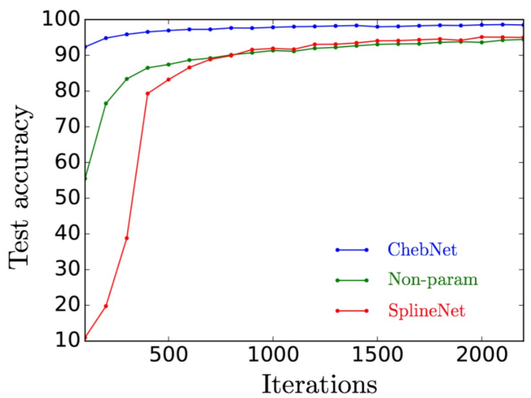
MNIST Numerical Experiment[1]

Running time



Optimization





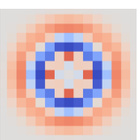
Accuracy

Model	Order	Accuracy
LeNet5	-	99.33%
SplineNet	25	97.75%
ChebNet	25	99.14%

- ChebNets :
  - ConvNets for arbitrary graph domains
  - Same O(n) learning complexity (but larger complexity constant)
  - Limitation : Isotropic model

- Isotropy vs anisotropy
  - Standard ConvNets produce anisotropic filters because Euclidean grids have directional structures (up, down, left, right).

  - Spectral ConvNets like ChebNets compute isotropic filters because there is no notion of directions on arbitrary graphs.



[1] Defferrard, Bresson, Vandergheynst, Convolutional neural networks on graphs with fast localized spectral filtering, 2016

ChebNets for Multiple Graphs

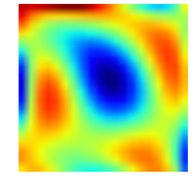
- **Multi-graph spectral convolution**[1] :

$$\underset{n_1 \times n_2 \times d}{h^{\ell+1}} = \eta(\ \hat{w}(\Delta_1, \Delta_2) * h^{\ell}\ )$$

$$h^{\ell+1} = \eta\Big(\ \sum_{k_1=0}^{K_1-1} \sum_{k_2=0}^{K_2-1} \underset{K_1 \times K_2}{w_{k_1,k_2}} \underset{n_1 \times n_1}{T_{k_1}(\Delta_1)} \underset{n_2 \times n_2}{T_{k_2}(\Delta_2)} h^{\ell}\ \Big)$$

$$\underset{n_1 \times n_2}{\hat{w}(\lambda_1, \lambda_2)} = \sum_{k_1=0}^{K_1-1} \sum_{k_2=0}^{K_2-1} w_{k_1,k_2} T_{k_1}(\Lambda_1) T_{k_2}(\Lambda_2)$$

2D Spectral filter



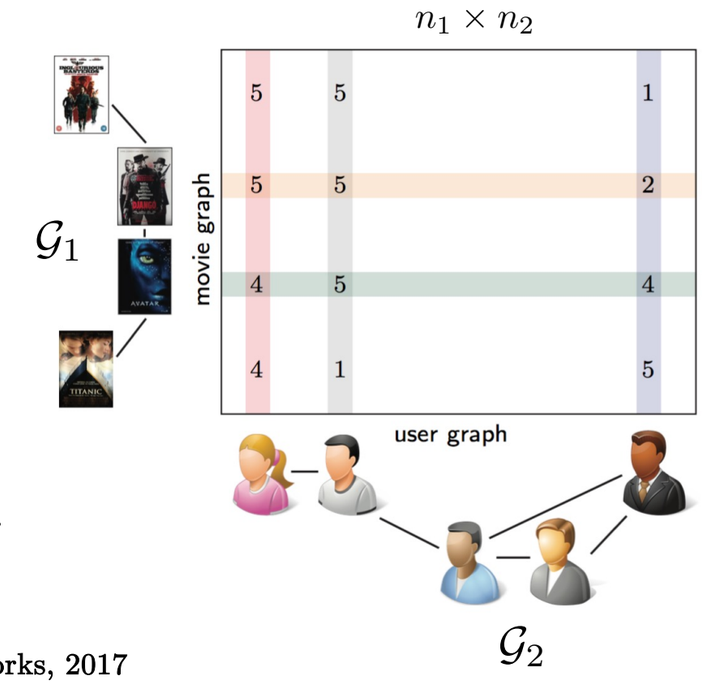
$\hat{w}(\lambda_1, \lambda_2)$

The $K_1.K_2$ coefficients $w_{k1,k2}$ are learned by backpropagation.

- **Recommendation task (Netflix)**
  - **Matrix Completion with Multiple Graphs**[2] :

$$\min_{h \in \mathbb{R}^{n_1 \times n_2}} \quad \|h\|_* + \mu \|\Omega \circ (h - r)\|_{\mathrm{F}}^2$$

$$+ \mu_1 \underbrace{\mathrm{tr}(h \Delta_1 h^\top)}_{\|h\|_{\mathcal{G}_1}^2} + \mu_2 \underbrace{\mathrm{tr}(h^\top \Delta_2 h)}_{\|h\|_{\mathcal{G}_2}^2}$$



[1] F Monti, M Bronstein, X Bresson, Geometric matrix completion with recurrent multi-graph neural networks, 2017
[2] V Kalofolias, X Bresson, M Bronstein, P Vandergheynst, Matrix completion on graphs, 2014

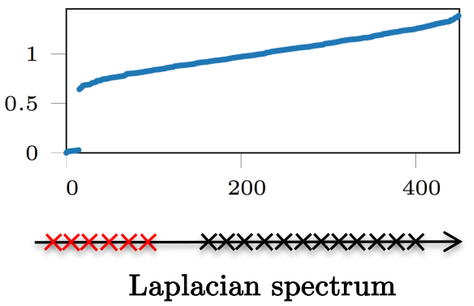
CayleyNets[1]

- ChebGCNs are unstable to produce filters with frequency bands of interest (graph communities).
- Cayley rationals can :

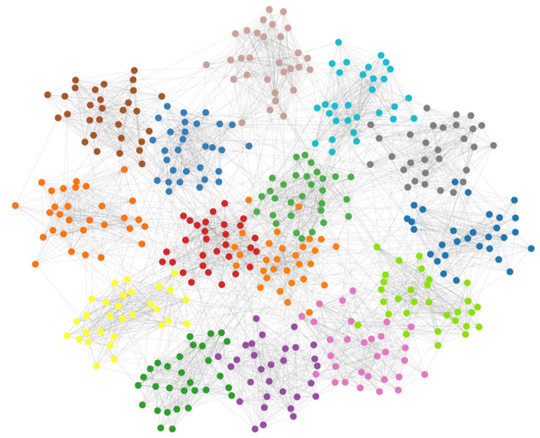
Spectral zoom z focuses on frequency bands.

$$\hat{w}(\Delta) = w_0 + 2\mathrm{Re}\{\sum_{k=0}^{K-1} w_k \frac{(z\Delta - i)^k}{(z\Delta + i)^k}\}$$

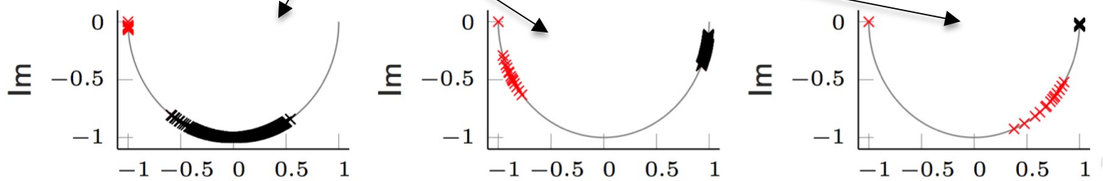
The K coefficients w_k are learned by backpropagation.



Laplacian spectrum



Spectral zoom



- CayleyNets
  - Same properties as ChebNets
  - Localized in frequency (with spectral zoom)
  - Richer class of filters for the same order K
  - Isotropic model

[1] R Levie, F Monti, X Bresson, MM Bronstein, CayleyNets: Graph convolutional neural networks with complex rational spectral filters, 2018

Outline

- Part 1 : Traditional ConvNets
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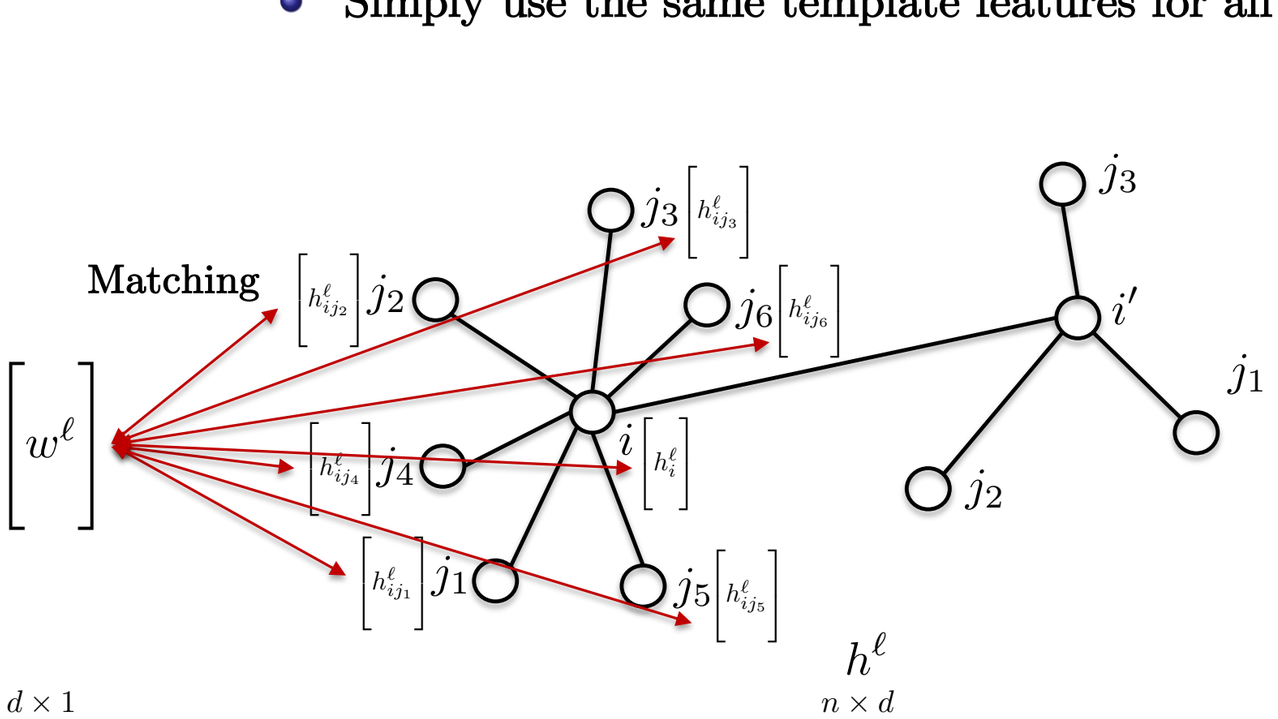
- Part 2: Spectral Graph ConvNets
  - Spectral Convolution
  - Spectral GCNs
- **Part 3 : Spatial Graph ConvNets**
  - **Template Matching**
  - Isotropic GCNs
  - Anisotropic GCNs
  - DGL : Implemented layers and lab demo
- Conclusion

Template Matching

- How to define template matching for graphs ?
  - Main issue is the absence of node ordering/positioning.
    - Node indices are arbitrary and do not match the same information.
  - How to design template matching invariant to node re-parametrization ?
    - Simply use the same template features for all neighbors !



$$\underset{\text{scalar}}{h_i^{\ell+1}} = \eta\Big(\sum_{j \in \mathcal{N}_i} \underbrace{\langle \overset{d \times 1}{w^\ell}, \overset{d \times 1}{h_{ij}^\ell} \rangle}_{(h_{ij}^\ell)^T w^\ell} \Big)$$

One feature

$$\underset{d \times 1}{h_i^{\ell+1}} = \eta\Big(\sum_{j \in \mathcal{N}_i} \overset{d \times d}{W^\ell} \overset{d \times 1}{h_{ij}^\ell} \Big)$$

d features

$$\underset{n \times d}{h^{\ell+1}} = \eta\Big(\underset{n \times n}{A} \underset{n \times d}{h^\ell} \overset{d \times d}{W^\ell} \Big)$$

Vectorial representation

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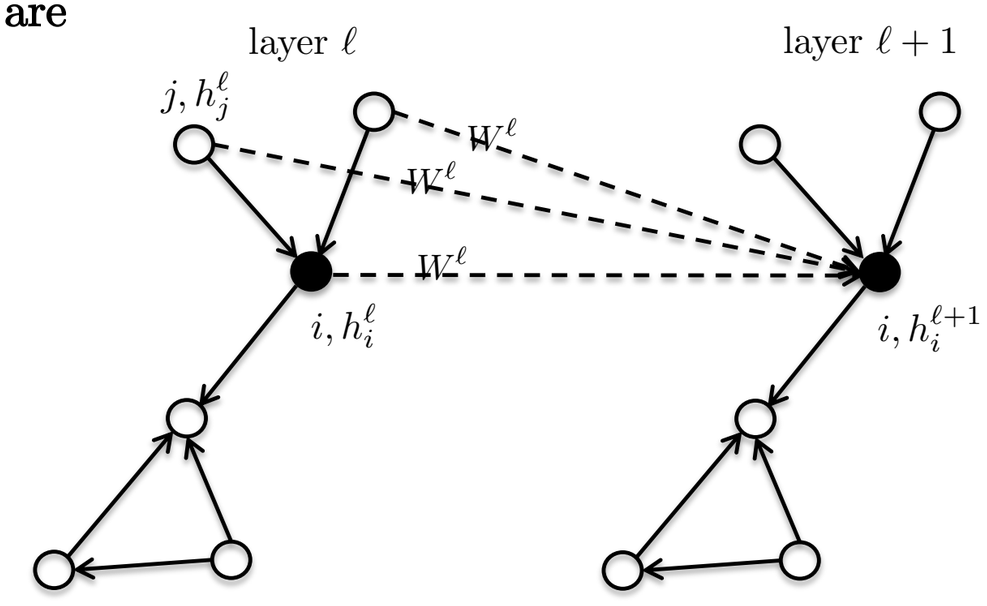
Vanilla GCNs[1,2,3]

- Simplest formulation of spatial GCNs
  - Handle the absence of node ordering
    - Invariant by node re-parametrization
  - Deal with different neighborhood sizes
  - Local reception field by design (only neighbors are considered)
  - Weight sharing (convolution property)
  - Independent of graph size
  - Limited to isotropic capability

$$\underset{n \times d}{h^{\ell+1}} = \eta(\overset{n \times n}{D^{-1}} \underset{n \times n}{A} \underset{n \times d}{h^{\ell}} \underset{d \times d}{W^{\ell}}) \quad \text{Matrix representation}$$

$$\underset{d \times 1}{h_i^{\ell+1}} = \eta(\underbrace{\frac{1}{d_i}}_{\text{scalar}} \sum_{j \in \mathcal{N}_i} \underset{d \times d}{A_{ij}} \underset{d \times d}{W^{\ell}} \underset{d \times 1}{h_j^{\ell}}) \quad \text{Vectorial representation}$$

Mean



$$h_i^{\ell+1} = f_{\text{GCN}}(h_i^\ell, \{h_j^\ell : j \to i\})$$

[1] Scarselli, Gori, Tsoi, Hagenbuchner, Monfardini, The Graph Neural Network Model, 2009
[2] Kipf, Welling, Semi-supervised classification with graph convolutional networks, 2016
[3] Sukhbaatar, Szlam, Fergus, Learning multiagent communication with backpropagation, 2016

ChebNets[1] and Vanilla GCNs[2,3]

- Vanilla GCNs is a simplification of ChebNets.
  - Truncated expansion of Chebyshev spectral convolution :

$$
\begin{aligned}
h^{\ell+1} &= \eta(\ w^{\ell} * h^{\ell}\ ) \\
&= \eta(\ \hat{w}^{\ell}(\Delta) h^{\ell}\ ) \\
&= \eta(\ \sum_{k=0}^{K-1} w_k^{\ell} T_k(\Delta) h^{\ell}\ )
\end{aligned}
$$

Suppose $K = 2,\ w_0^{\ell} = w^{\ell},\ w_1^{\ell} = -w^{\ell},\ \lambda_n = 2,$

$$
\begin{aligned}
h^{\ell+1} &= \eta(\ w^{\ell}(T_0(\Delta) - T_1(\Delta)) h^{\ell}\ ) \\
&= \eta(\ w^{\ell}(\mathrm{I} + D^{-1/2} A D^{-1/2}) h^{\ell}\ )
\end{aligned}
$$

Operator with largest eigenvalue in [0,2] may cause divergence.

Add self-loop to graphs $\hat{A} = A + \mathrm{I}$

$$
\begin{aligned}
h^{\ell+1} &= \eta(\ w^{\ell} \hat{D}^{-1/2} \hat{A} \hat{D}^{-1/2} h^{\ell}\ ) \quad \text{(single feature)} \\
&= \eta(\ \hat{D}^{-1/2} \hat{A} \hat{D}^{-1/2} h^{\ell} W^{\ell}\ ) \quad (d \text{ features}) \\
h_i^{\ell+1} &= \eta(\ \frac{1}{\hat{d}_i^{-1/2}} \sum_{j \in \mathcal{N}_i} \frac{1}{\hat{d}_j^{-1/2}} \hat{A}_{ij} W^{\ell} h_j^{\ell}\ )
\end{aligned}
$$

with

$$
\begin{cases}
T_0 = I \\
T_1 = \tilde{\Delta} = \dfrac{2}{\lambda_n} \Delta - \mathrm{I} \overset{\lambda_n = 2}{=} \Delta - I \\
\Delta = \mathrm{I} - D^{-1/2} A D^{-1/2}
\end{cases}
$$

[1] Defferrard, Bresson, Vandergheynst, Convolutional neural networks on graphs with fast localized spectral filtering, 2016
[2] Kipf, Welling, Semi-supervised classification with graph convolutional networks, 2016
[3] Sukhbaatar, Szlam, Fergus, Learning multiagent communication with backpropagation, 2016

GraphSage[1]

- Vanilla GCNs (supposing $A_{ij} = 1$) : $h_i^{\ell+1} = \eta(\frac{1}{d_i} \sum_{j \in \mathcal{N}_i} W^\ell h_j^\ell)$
- GraphSage :
  - Differentiate template weights W^l between neighbors h_j and central node h_i.
  - Isotropic GCNs

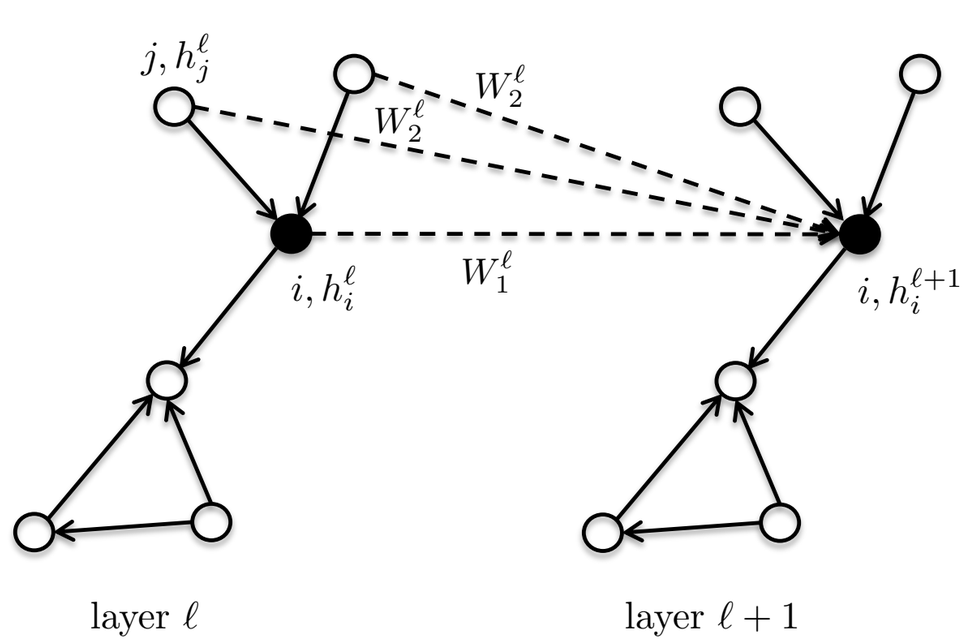
$$\underset{d \times 1}{h_i^{\ell+1}} = \eta(\underset{d \times d}{W_1^\ell} \underset{d \times 1}{h_i^\ell} + \underbrace{\frac{1}{d_i} \sum_{j \in \mathcal{N}_i} \underset{d \times d}{W_2^\ell} \underset{d \times 1}{h_j^\ell}}_{})$$

$\text{Mean}_{j \in \mathcal{N}_i} \ W_2^\ell h_j^\ell$

Or alternatively,

$\text{Max}_{j \in \mathcal{N}_i} \ W_2^\ell h_j^\ell$

$\text{LSTM}^\ell(h_j^\ell)$



[1] Hamilton, Ying, Leskovec, Inductive representation learning on large graphs, 2017

Graph Isomorphism Networks[1] (GIN)

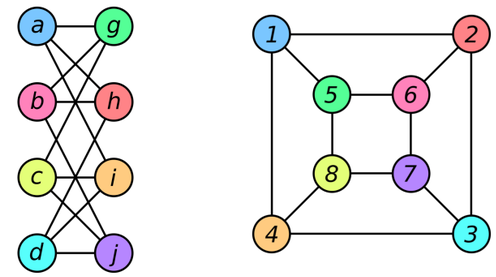
- Architecture that can differentiate graphs that are not isomorphic.
  - Graph isomorphism is an equivalent relation for similar graph structures.

- Isotropic GCNs

$$h_i^{\ell+1}_{d\times 1} = \mathrm{ReLU}(\underset{d\times d}{W_2^\ell}\ \mathrm{ReLU}(\ \mathrm{BN}(\underset{d\times d}{W_1^\ell}\hat{h}_i^{\ell+1}\ )\ )\ )$$

Batch normalization

$$\hat{h}_i^{\ell+1}_{d\times 1} = (1+\epsilon)\, h_i^\ell + \sum_{j\in\mathcal{N}_i} h_j^\ell$$



Example of two isomorphic graphs

[1] Xu, Hu, Leskovec, Jegelka, How powerful are graph neural networks?, 2018

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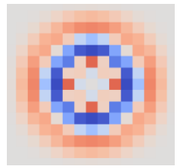
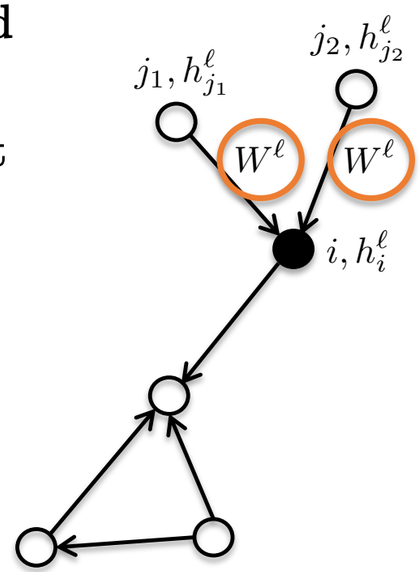
Anisotropic GCNs

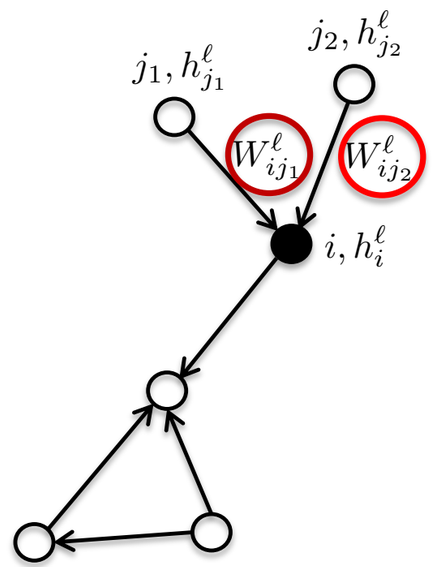
- Reminder :
  - Standard ConvNets produce anisotropic filters because Euclidean grids have directional structures (up, down, left, right).
  - GCNs such as ChebNets, CayleyNets, Vanilla GCNs, GraphSage, GIN compute isotropic filters as there is no notion of directions on arbitrary graphs.



- How to get anisotropy back in GNNs ?
  - Natural edge features[1,2] if available (e.g. different bond connections between atoms).
  - We need an anisotropic mechanism that is independent of the node parametrization.
  - Edge degrees[3]/Edge gates[4]/Attention mechanism[5] : MoNets[3], GAT[5], GatedGCNs[4] can treat neighbors differently.



Isotropic weights



Anisotropic weights

[1] Gilmer, Schoenholz, Riley, Vinyals, Dahl, Neural message passing for quantum chemistry, 2017
[2] Bresson, Laurent, A Two-Step Graph Convolutional Decoder for Molecule Generation, 2019
[3] Monti, Boscaini, Masci, Rodolà, J. Svoboda, M. Bronstein, Geometric deep learning on graphs and manifolds using mixture model CNNs, 2016
[4] Bresson, Laurent, Residual gated graph convnets, 2017
[5] Velickovic, Cucurull, Casanova, Romero, Lio, Bengio, Graph Attention Networks, 2018

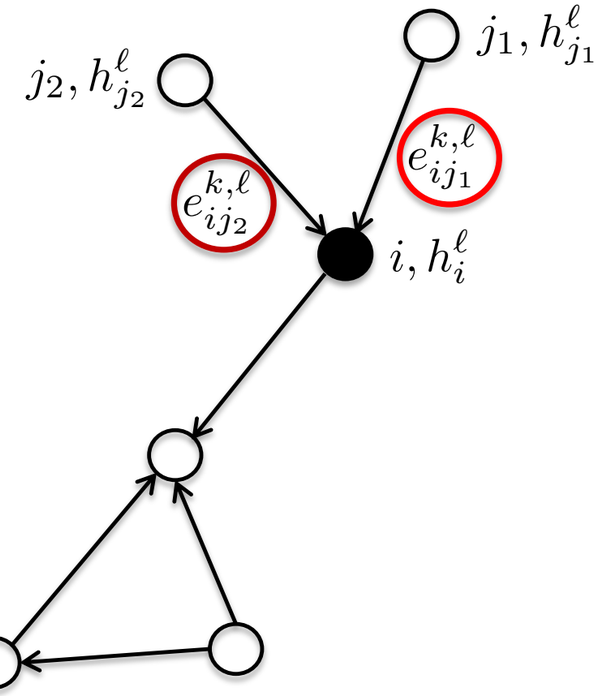
MoNets[1]

- MoNets[1] leverage the Bayesian Gaussian Mixture Model (GMM)[2].

$$h_i^{\ell+1}_{d\times 1} = \mathrm{ReLU}\Big(\sum_{k=1}^{K}\sum_{j\in\mathcal{N}_i}\underbrace{e_{ij}^{k,\ell}}_{\text{scalar}}\underbrace{W_1^{k,\ell}}_{d\times d}\underbrace{h_j^{\ell}}_{d\times 1}\Big)$$

$$\underset{\text{scalar}}{e_{ij}^{k,\ell}} = \exp\Big(-\frac{1}{2}\underbrace{(u_{ij}^{\ell}-\mu_k^{\ell})^T}_{1\times 2}\underbrace{(\Sigma_k^{\ell})^{-1}}_{2\times 2}\underbrace{(u_{ij}^{\ell}-\mu_k^{\ell})}_{2\times 1}\Big)$$

$$\underset{2\times 1}{u_{ij}^{\ell}} = \mathrm{Tanh}\Big(\underbrace{A^{\ell}}_{2\times 2}\ \underbrace{(\deg_i^{-1/2},\deg_j^{-1/2})}_{2\times 1}+\underbrace{a^{\ell}}_{2\times 1}\Big)$$



[1] Monti, Boscaini, Masci, Rodolà, J. Svoboda, M. Bronstein, Geometric deep learning on graphs and manifolds using mixture model CNNs, 2016
[2] Dempster, Laird, Rubin, Maximum Likelihood from Incomplete Data Via the EM Algorithm, 1977

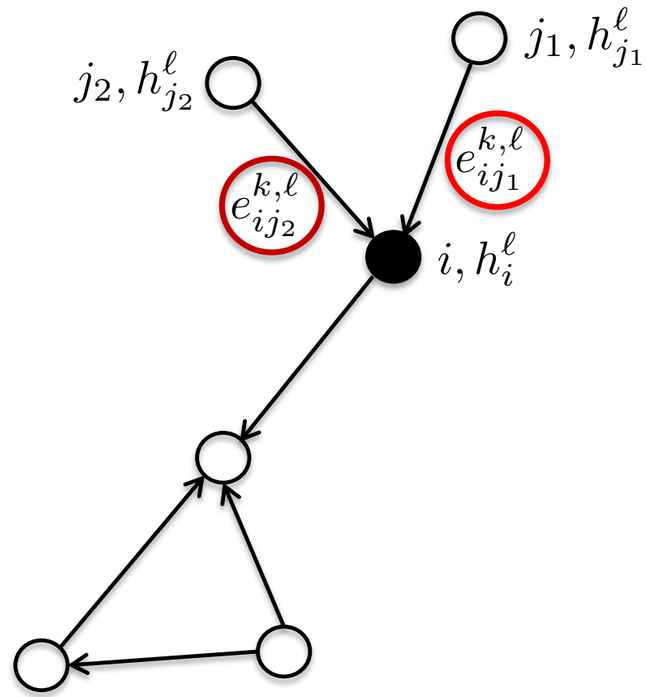
Graph Attention Networks[1] (GAT)

- GAT uses the attention mechanism[2] to introduce anisotropy in the neighborhood aggregation function.
- The network employs a multi-headed architecture to increase the learning capacity, similar to Transformers[3].

$$\underset{d \times 1}{h_i^{\ell+1}} = \text{Concat}_{k=1}^{K} \Big(\text{ELU} \Big(\sum_{j \in \mathcal{N}_i} \underset{\text{scalar}}{e_{ij}^{k,\ell}} \underset{\frac{d}{K} \times d}{W_1^{k,\ell}} h_j^{\ell} \Big) \Big)^{d \times 1}$$

$$\underset{\text{scalar}}{e_{ij}^{k,\ell}} = \text{Softmax}_{\mathcal{N}_i}(\hat{e}_{ij}^{k,\ell}) = \frac{\exp(\hat{e}_{ij}^{k,\ell})}{\sum_{j' \in \mathcal{N}_i} \exp(\hat{e}_{ij'}^{k,\ell})}$$

$$\hat{e}_{ij}^{k,\ell} = \text{LeakyReLU} \Big(\underset{1 \times \frac{2d}{K}}{W_2^{k,\ell}} \underbrace{\text{Concat}\big(W_1^{k,\ell} h_i^{\ell},\ W_1^{k,\ell} h_j^{\ell}\big)}_{\frac{2d}{K} \times 1} \Big)$$



[1] Velickovic, Cucurull, Casanova, Romero, Lio, Bengio, Graph Attention Networks, 2018
[2] Bahdanau, Cho, Bengio, Neural machine translation by jointly learning to align and translate, 2014
[3] Vaswani, Shazeer, Parmar, Uszkoreit, Jones, Gomez, Kaiser, Polosukhin, Attention is all you need, 2017

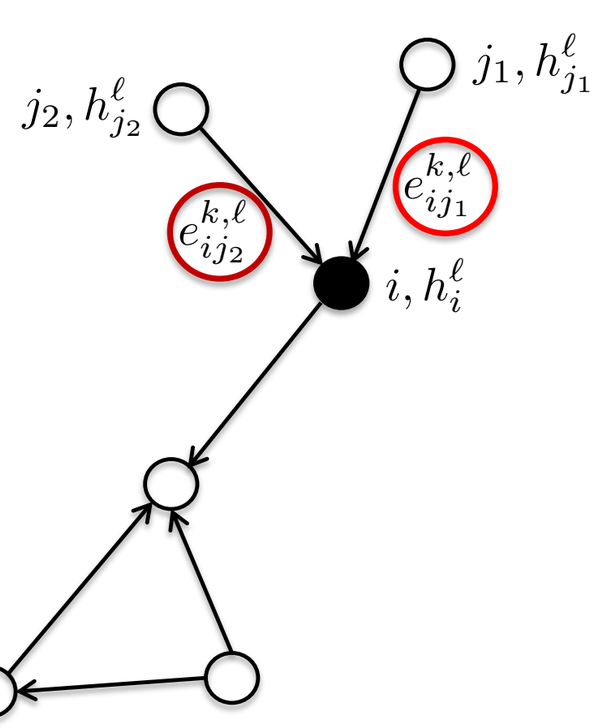
Gated Graph ConvNets[1]

- GatedGCNs use edge gates to design an anisotropic variant of GCNs.
  - Edge gates can be regarded as a soft attention process, related to the standard sparse attention mechanism[2].
  - Edge features are explicit (important for edge prediction tasks).
- Residual connections and batch normalization enhance learning speed and generalization.

$$h_i^{\ell+1}_{d\times 1} = h_i^{\ell} + \mathrm{ReLU}\Big(\mathrm{BN}\Big(\underset{d\times d}{W_1^{\ell}}\underset{d\times 1}{h_i^{\ell}} + \sum_{j\in\mathcal{N}_i}\underset{d\times 1}{e_{ij}^{\ell}} \odot \underset{d\times d}{W_2^{\ell}}\underset{d\times 1}{h_j^{\ell}}\Big)\Big)$$

$$e_{ij}^{\ell}{}_{d\times 1} = \frac{\sigma(\hat{e}_{ij}^{\ell})}{\sum_{j'\in\mathcal{N}_i}\sigma(\hat{e}_{ij'}^{\ell}) + \varepsilon}$$

$$\hat{e}_{ij}^{\ell}{}_{d\times 1} = \hat{e}_{ij}^{\ell-1} + \mathrm{ReLU}\Big(\mathrm{BN}\big(\underset{d\times d}{V_1^{\ell}}h_i^{\ell-1} + \underset{d\times d}{V_2^{\ell}}h_j^{\ell-1} + \underset{d\times d}{V_3^{\ell}}\hat{e}_{ij}^{\ell-1}\big)\Big)$$



[1] Bresson, Laurent, Residual gated graph convnets, 2017
[2] Bahdanau, Cho, Bengio, Neural machine translation by jointly learning to align and translate, 2014

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DGL Library (Amazon)

- Website : https://www.dgl.ai, https://docs.dgl.ai
- DGL 1.0 : https://www.dgl.ai/release/2023/02/20/release.html

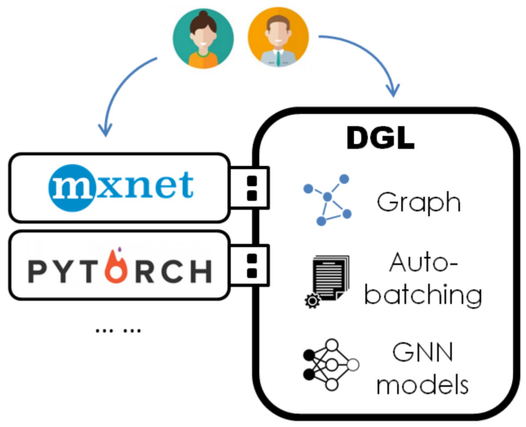
DeepGraphLibrary
@DGLGraph

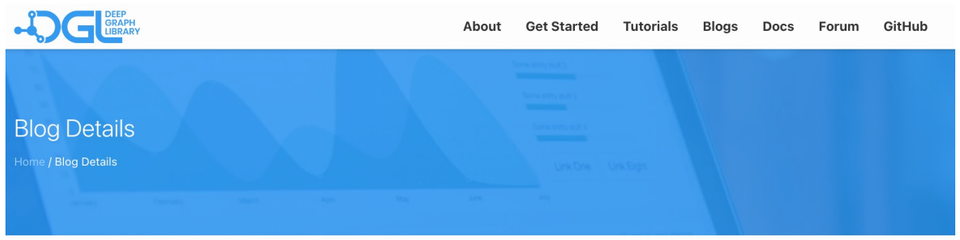
DGL 1.0 has arrived! Huge milestone of the past 3+ years of development.

👉Check out the blog for the release summary and the highlight of the brand new DGL-Sparse package dgl.ai/release/2023/0...

#DGL #GML

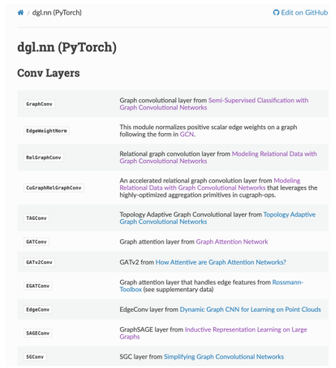
11:52 PM · Feb 23, 2023 · **56.2K** Views





DGL 1.0: Empowering Graph Machine Learning For Everyone

DGL-implemented GCNs


dgl.nn (PyTorch)

Edit on GitHub

dgl.nn (PyTorch)

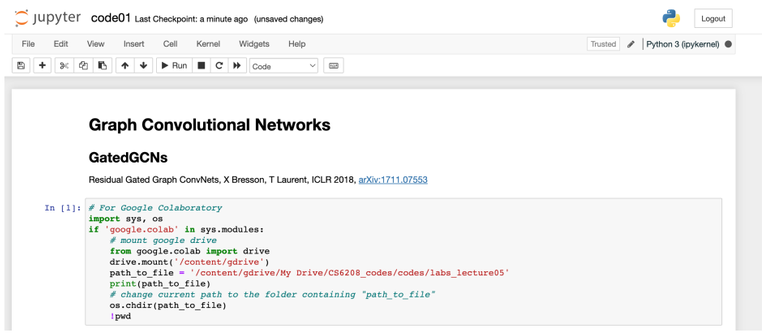
Conv Layers

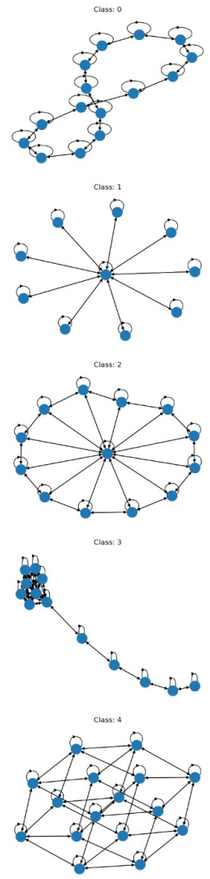
GraphConv	Graph convolutional layer from Semi-Supervised Classification with Graph Convolutional Networks
EdgeWeightNorm	This module normalizes positive scalar edge weights on a graph following the form in GCN.
RelGraphConv	Relational graph convolution layer from Modeling Relational Data with Graph Convolutional Networks
CuGraphRelGraphConv	An accelerated relational graph convolution layer from Modeling Relational Data with Graph Convolutional Networks that leverages the highly-optimized aggregation primitives in cugraph-ops.
TAGConv	Topology Adaptive Graph Convolutional layer from Topology Adaptive Graph Convolutional Networks
GATConv	Graph attention layer from Graph Attention Network
GATv2Conv	GATv2 from How Attentive are Graph Attention Networks?
EGATConv	Graph attention layer that handles edge features from Rossmann-Toolbox (see supplementary data)
EdgeConv	EdgeConv layer from Dynamic Graph CNN for Learning on Point Clouds
SAGEConv	GraphSAGE layer from Inductive Representation Learning on Large Graphs
SGConv	SGC layer from Simplifying Graph Convolutional Networks

- Implemented layers in DGL : https://docs.dgl.ai/api/python/nn-pytorch.html
- Graph convolutional layers
  - ChebNet : https://docs.dgl.ai/generated/dgl.nn.pytorch.conv.ChebConv.html?highlight=chebnet
  - GCN : https://docs.dgl.ai/generated/dgl.nn.pytorch.conv.GraphConv.html#dgl.nn.pytorch.conv.GraphConv
  - GraphSage : https://docs.dgl.ai/generated/dgl.nn.pytorch.conv.SAGEConv.html#dgl.nn.pytorch.conv.SAGEConv
  - GIN : https://docs.dgl.ai/generated/dgl.nn.pytorch.conv.GINConv.html#dgl.nn.pytorch.conv.GINConv
- Attention layers
  - GAT : https://docs.dgl.ai/generated/dgl.nn.pytorch.conv.GATConv.html#dgl.nn.pytorch.conv.GATConv
  - GraphTransformer : https://doc-build.dgl.ai/notebooks/sparse/graph_transformer.html

Lab 1: GatedGCNs[1]

- Run code01.ipynb





Train GNN

```
In [9]:
# datasets
train_loader = DataLoader(trainset, batch_size=50, shuffle=True, collate_fn=collate)
test_loader = DataLoader(testset, batch_size=50, shuffle=False, collate_fn=collate)
val_loader = DataLoader(valset, batch_size=50, shuffle=False, drop_last=False, collate_fn=collate)

# Create model
net_parameters = {}
net_parameters['input_dim'] = 1
net_parameters['hidden_dim'] = 100
net_parameters['output_dim'] = 8 # nb of classes
net_parameters['L'] = 4
net = GatedGCN_Net(net_parameters)

optimizer = torch.optim.Adam(net.parameters(), lr=0.0001)

epoch_train_losses = []
epoch_test_losses = []
epoch_val_losses = []
epoch_train_accs = []
epoch_test_accs = []
epoch_val_accs = []
for epoch in range(50):

    start = time.time()
    epoch_train_loss, epoch_train_acc = train_one_epoch(net, train_loader)
    epoch_test_loss, epoch_test_acc = evaluate_network(net, test_loader)
    epoch_val_loss, epoch_val_acc = evaluate_network(net, val_loader)

    print('Epoch {}, time {:.4f}, train_loss: {:.4f}, test_loss: {:.4f}, val_loss: {:.4f} \n                    train_
```

```
Epoch 0, time 1.6418, train_loss: 2.0092, test_loss: 2.0319, val_loss: 2.0319
                  train_acc: 0.2343, test_acc: 0.1200, val_acc: 0.1200
Epoch 1, time 1.6794, train_loss: 1.9021, test_loss: 1.9863, val_loss: 1.9863
                  train_acc: 0.3943, test_acc: 0.1200, val_acc: 0.1200
Epoch 2, time 1.7416, train_loss: 1.8032, test_loss: 1.9217, val_loss: 1.9217
                  train_acc: 0.3771, test_acc: 0.2600, val_acc: 0.2600
Epoch 3, time 1.7690, train_loss: 1.7355, test_loss: 1.8438, val_loss: 1.8438
                  train_acc: 0.3771, test_acc: 0.3500, val_acc: 0.3500
Epoch 4, time 1.7733, train_loss: 1.6713, test_loss: 1.7568, val_loss: 1.7568
                  train_acc: 0.4314, test_acc: 0.3600, val_acc: 0.3600
Epoch 5, time 1.4200, train_loss: 1.6167, test_loss: 1.6712, val_loss: 1.6712
                  train_acc: 0.5029, test_acc: 0.3700, val_acc: 0.3700
Epoch 6, time 1.7266, train_loss: 1.5380, test_loss: 1.5942, val_loss: 1.5942
                  train_acc: 0.5171, test_acc: 0.4600, val_acc: 0.4600
Epoch 7, time 1.5330, train_loss: 1.4817, test_loss: 1.5212, val_loss: 1.5212
                  train_acc: 0.5886, test_acc: 0.4900, val_acc: 0.4900
Epoch 8, time 1.4076, train_loss: 1.4333, test_loss: 1.4440, val_loss: 1.4440
                  train_acc: 0.6000, test_acc: 0.5800, val_acc: 0.5800
Epoch 9, time 1.6103, train_loss: 1.3739, test_loss: 1.3811, val_loss: 1.3811
                  train_acc: 0.6371, test_acc: 0.5800, val_acc: 0.5800
```

[1] Bresson, Laurent, Residual gated graph convnets, 2017

Lab 1: GatedGCNs

DGL creates a batch of graphs

```python
# collate function
def collate(samples):
    graphs, labels = map(list, zip(*samples)) # samples is a list of pairs (graph, label).
    labels = torch.tensor(labels)
    tab_sizes_n = [ graphs[i].number_of_nodes() for i in range(len(graphs))] # graph sizes
    tab_snorm_n = [ torch.FloatTensor(size,1).fill_(1./float(size)) for size in tab_sizes_n ]
    snorm_n = torch.cat(tab_snorm_n).sqrt() # normalization constant for better optimization
    tab_sizes_e = [ graphs[i].number_of_edges() for i in range(len(graphs))] # nb of edges
    tab_snorm_e = [ torch.FloatTensor(size,1).fill_(1./float(size)) for size in tab_sizes_e ]
    snorm_e = torch.cat(tab_snorm_e).sqrt() # normalization constant for better optimization
    batched_graph = dgl.batch(graphs) # batch graphs
    return batched_graph, labels, snorm_n, snorm_e


# create artifical data feature (= in degree) for each node
def create_artificial_features(dataset):
    for (graph,_) in dataset:
        graph.ndata['feat'] = graph.in_degrees().view(-1, 1).float()
        graph.edata['feat'] = torch.ones(graph.number_of_edges(),1)
    return dataset


# use artifical graph dataset of DGL
trainset = MiniGCDataset(8, 10, 20)
trainset = create_artificial_features(trainset)
print(trainset[0])
```

```
    (DGLGraph(num_nodes=13, num_edges=39,
              ndata_schemes={'feat': Scheme(shape=(1,), dtype=torch.float32)}
              edata_schemes={'feat': Scheme(shape=(1,), dtype=torch.float32)}), 0)
```

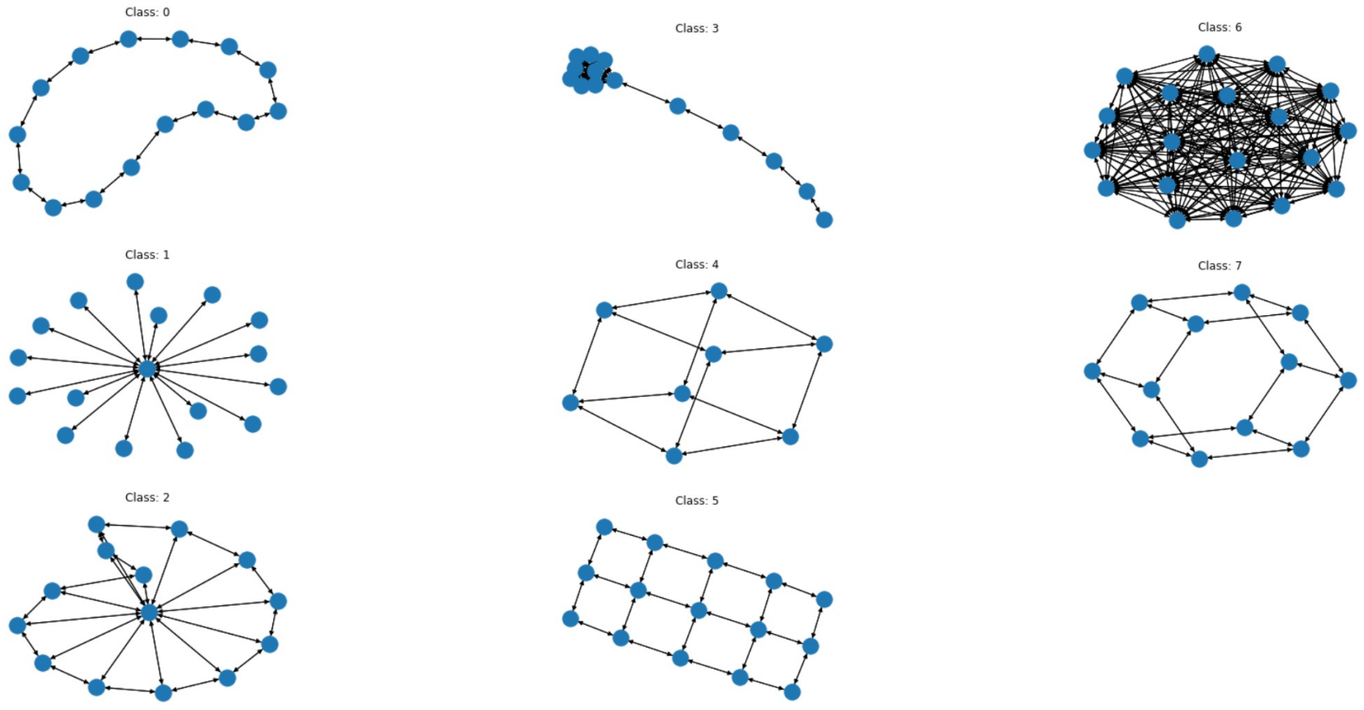
$$\frac{1}{\sqrt{V_k}}, \frac{1}{\sqrt{E_k}}$$

Graph normalization constants

Create artificial node feature (input degree) and edge feature (value 1)

Lab 1: GatedGCNs

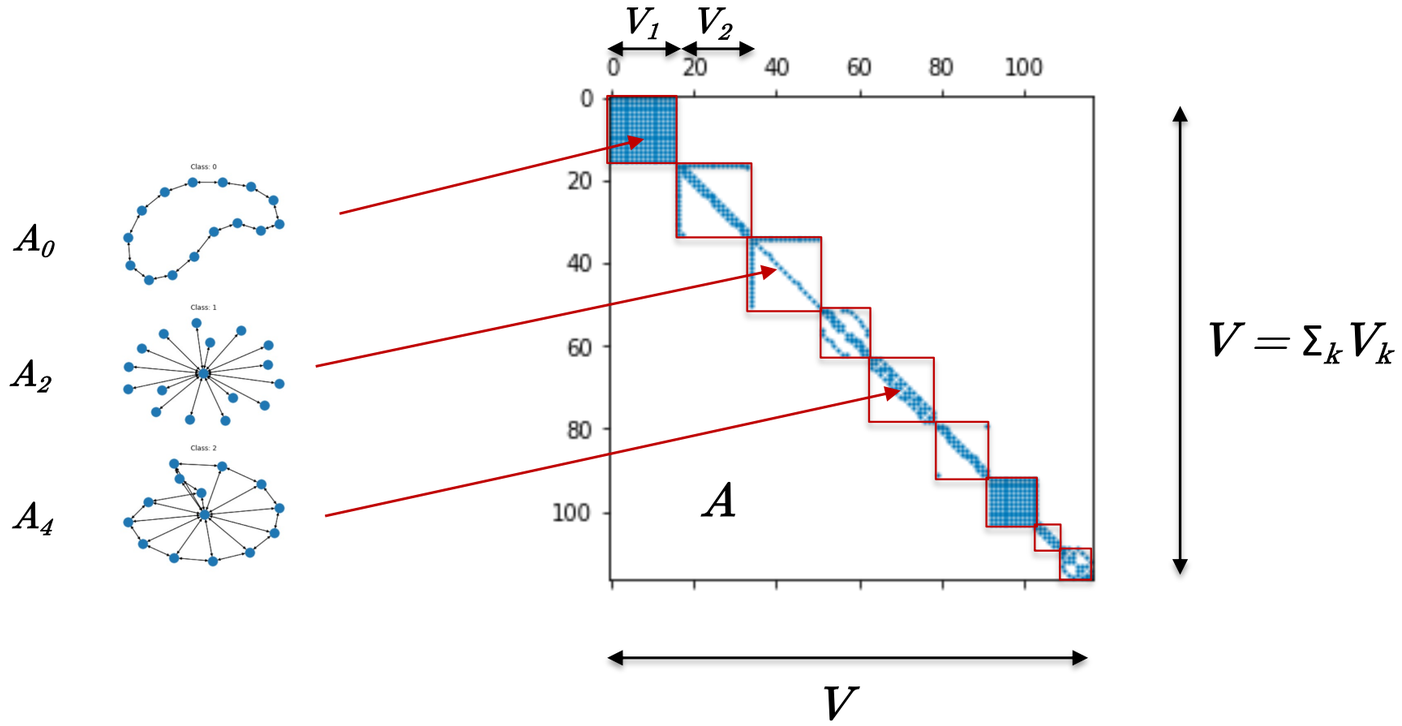
```
# use artifical graph dataset of DGL
trainset = MiniGCDataset(8, 10, 20)
```



Lab 1: GatedGCNs

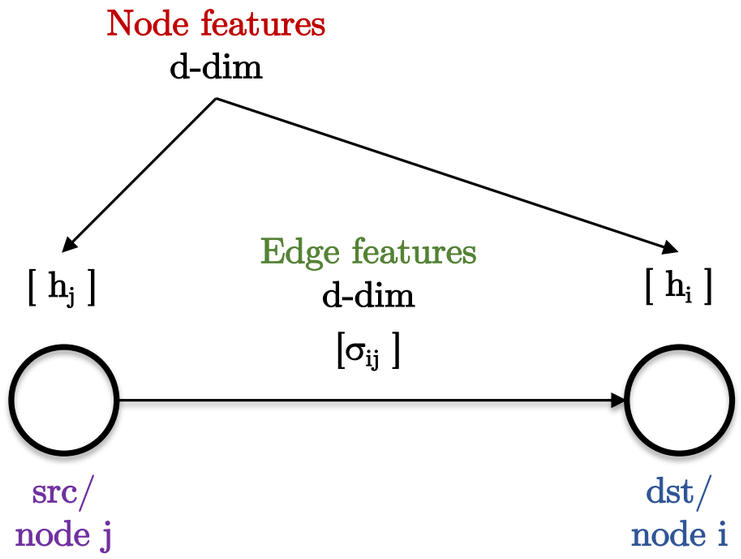
- Understanding DGL :
  - How to process K graphs of different sizes ?

    Form a (big) sparse block diagonal matrix A with K adjacency matrices A_k.



Lab 1: GatedGCNs

- Basic structure of an edge in DGL :

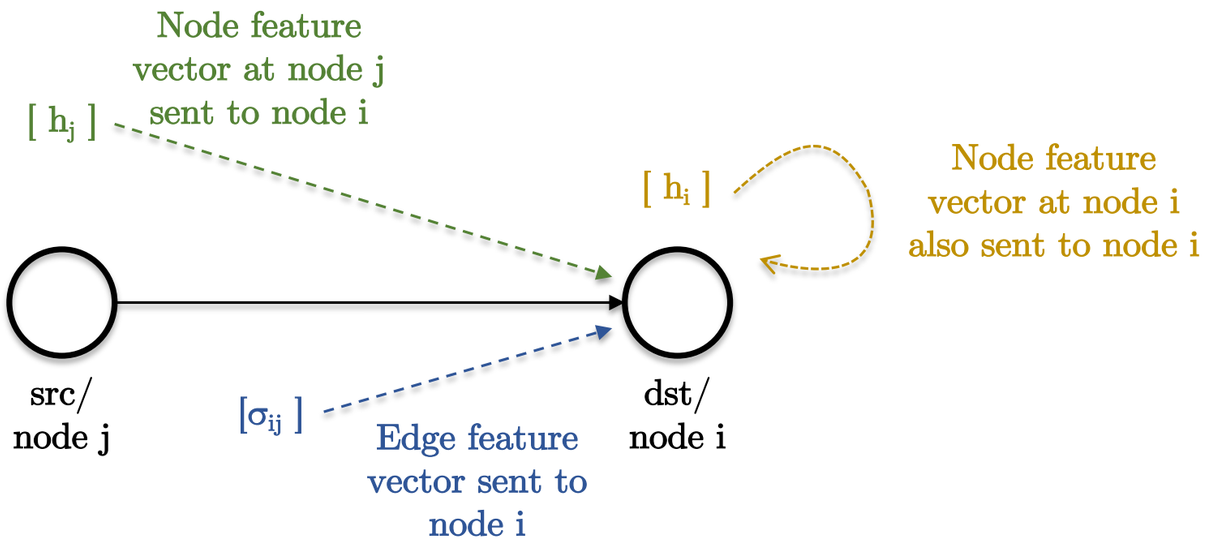


- Goal is to compute efficiently expressions of the form :

$$f_i = h_i + \Sigma_{j \to i}\, \sigma_{ij} \circ h_j$$

Lab 1: GatedGCNs

- Step 1 : Message passing function defined on edges
  - Node feature and edge feature are passed along all edges connecting a node.



h_j : edges.src['h'] . size() = E x d

h_i : edges.dst['h'] . size() = E x d

σ_{ij} : edges.data['σ'] . size() = E x d

#edges

All message passing operations can be done in parallel !

Lab 1: GatedGCNs

- Step 2 : Reduce function defined on nodes
  - Reduce functions of the form : $f_i = h_i + \Sigma_{j \to i} \sigma_{ij} \circ h_j$
  - Reduce function collects all messages passed in Step 1.
  - Code : f = h_i + torch.sum (h_j x σ_{ij} , dim=1) . size() = V x d

#nodes

Sum over neighbors

- GPU acceleration :
  - DGL batches the nodes with the same number of neighbors.

#nodes in $batch_1$

$$h_j = \text{nodes.mailbox}[\text{`}h_j\text{'}] = \begin{pmatrix} batch_1 .size() = 11 \text{ x } 12 \text{ x d} \\ \vdots \\ batch_{34} .size() = 14 \text{ x } 9 \text{ x d} \end{pmatrix}$$

#neighbors

$$\sigma_{ij} = \text{nodes.mailbox}[\text{`}\sigma_{ij}\text{'}] = \quad \text{same structure than } h_j$$

$$h_i = \text{nodes.data}[\text{`h'}] \text{ . size()} = \text{V x d}$$

Lab 1: GatedGCNs

GatedGCN layer :

$$h_i^{\ell+1} = h_i^\ell + \mathrm{ReLU}\Big(\mathrm{BN}\Big(A^\ell h_i^\ell + \sum_{j\sim i} \eta(e_{ij}^\ell) \odot B^\ell h_j^\ell\Big)\Big)/\sqrt{V_k},$$

$$\eta(e_{ij}^\ell) = \frac{\sigma(e_{ij}^\ell)}{\sum_{j'\sim i}\sigma(e_{ij'}^\ell) + \varepsilon},$$

$$e_{ij}^{\ell+1} = e_{ij}^\ell + \mathrm{ReLU}\Big(\mathrm{BN}\Big(C^\ell e_{ij}^\ell + D^\ell h_i^{\ell+1} + E^\ell h_j^{\ell+1}\Big)\Big)/\sqrt{E_k}.$$

```python
class GatedGCN_layer(nn.Module):

    def __init__(self, input_dim, output_dim):
        super(GatedGCN_layer, self).__init__()
        self.A = nn.Linear(input_dim, output_dim, bias=True)
        self.B = nn.Linear(input_dim, output_dim, bias=True)
        self.C = nn.Linear(input_dim, output_dim, bias=True)
        self.D = nn.Linear(input_dim, output_dim, bias=True)
        self.E = nn.Linear(input_dim, output_dim, bias=True)
        self.bn_node_h = nn.BatchNorm1d(output_dim)
        self.bn_node_e = nn.BatchNorm1d(output_dim)

    def message_func(self, edges):
        Bh_j = edges.src['Bh']
        e_ij = edges.data['Ce'] +  edges.src['Dh'] + edges.dst['Eh'] # e_ij = Ce_ij + Dhi + Ehj
        edges.data['e'] = e_ij
        return {'Bh_j' : Bh_j, 'e_ij' : e_ij}

    def reduce_func(self, nodes):
        Ah_i = nodes.data['Ah']
        Bh_j = nodes.mailbox['Bh_j']
        e = nodes.mailbox['e_ij']
        sigma_ij = torch.sigmoid(e) # sigma_ij = sigmoid(e_ij)
        h = Ah_i + torch.sum( sigma_ij * Bh_j, dim=1 ) / torch.sum( sigma_ij, dim=1 )  # hi = Ahi + sum_j eta_ij * Bhj
        return {'h' : h}

    def forward(self, g, h, e, snorm_n, snorm_e):

        h_in = h # residual connection
        e_in = e # residual connection

        g.ndata['h']  = h
        g.ndata['Ah'] = self.A(h)
        g.ndata['Bh'] = self.B(h)
        g.ndata['Dh'] = self.D(h)
        g.ndata['Eh'] = self.E(h)
        g.edata['e']  = e
        g.edata['Ce'] = self.C(e)
        g.update_all(self.message_func,self.reduce_func)
        h = g.ndata['h'] # result of graph convolution
        e = g.edata['e'] # result of graph convolution

        h = h* snorm_n # normalize activation w.r.t. graph node size
        e = e* snorm_e # normalize activation w.r.t. graph edge size

        h = self.bn_node_h(h) # batch normalization
        e = self.bn_node_e(e) # batch normalization

        h = F.relu(h) # non-linear activation
        e = F.relu(e) # non-linear activation

        h = h_in + h # residual connection
        e = e_in + e # residual connection

        return h, e
```

Lab 1: GatedGCNs

MLP classifier layer

```python
class MLP_layer(nn.Module):

    def __init__(self, input_dim, output_dim, L=2): # L = nb of hidden layers
        super(MLP_layer, self).__init__()
        list_FC_layers = [ nn.Linear( input_dim, input_dim, bias=True ) for l in range(L) ]
        list_FC_layers.append(nn.Linear( input_dim, output_dim , bias=True ))
        self.FC_layers = nn.ModuleList(list_FC_layers)
        self.L = L

    def forward(self, x):
        y = x
        for l in range(self.L):
            y = self.FC_layers[l](y)
            y = F.relu(y)
        y = self.FC_layers[self.L](y)
        return y
```

GatedGCN Network

```python
class GatedGCN_Net(nn.Module):

    def __init__(self, net_parameters):
        super(GatedGCN_Net, self).__init__()
        input_dim = net_parameters['input_dim']
        hidden_dim = net_parameters['hidden_dim']
        output_dim = net_parameters['output_dim']
        L = net_parameters['L']
        self.embedding_h = nn.Linear(input_dim, hidden_dim)
        self.embedding_e = nn.Linear(1, hidden_dim)
        self.GatedGCN_layers = nn.ModuleList([ GatedGCN_layer(hidden_dim, hidden_dim) for _ in range(L) ])
        self.MLP_layer = MLP_layer(hidden_dim, output_dim)

    def forward(self, g, h, e, snorm_n, snorm_e):

        # input embedding
        h = self.embedding_h(h)
        e = self.embedding_e(e)

        # graph convnet layers
        for GGCN_layer in self.GatedGCN_layers:
            h,e = GGCN_layer(g,h,e,snorm_n,snorm_e)

        # MLP classifier
        g.ndata['h'] = h
        y = dgl.mean_nodes(g,'h')
        y = self.MLP_layer(y)

        return y
```

Node input embedding

Edge input embedding

Run graphNN layers

Compute graph vectorial representation by a (simple) average of all node features with DGL.

Use MLP classifier

Lab 1: GatedGCNs

```python
def train_one_epoch(net, data_loader):
    """
    train one epoch
    """
    net.train()
    epoch_loss = 0
    epoch_train_acc = 0
    nb_data = 0
    gpu_mem = 0
    for iter, (batch_graphs, batch_labels, batch_snorm_n, batch_snorm_e) in enumerate(data_loader):
        batch_x = batch_graphs.ndata['feat'].to(device)
        batch_e = batch_graphs.edata['feat'].to(device)
        batch_snorm_n = batch_snorm_n.to(device)
        batch_snorm_e = batch_snorm_e.to(device)
        batch_labels = batch_labels.to(device)
        batch_scores = net.forward(batch_graphs, batch_x, batch_e, batch_snorm_n, batch_snorm_e)
        gpu_mem = net.gpu_memory(gpu_mem)
        loss = net.loss(batch_scores, batch_labels)
        optimizer.zero_grad()
        loss.backward()
        optimizer.step()
        epoch_loss += loss.detach().item()
        epoch_train_acc += net.accuracy(batch_scores,batch_labels)
        nb_data += batch_labels.size(0)
    epoch_loss /= (iter + 1)
    epoch_train_acc /= nb_data
    return epoch_loss, epoch_train_acc, gpu_mem
```

Train function

```python
# datasets
train_loader = DataLoader(trainset, batch_size=50, shuffle=True, collate_fn=collate)
test_loader = DataLoader(testset, batch_size=50, shuffle=False, collate_fn=collate)
val_loader = DataLoader(valset, batch_size=50, shuffle=False, drop_last=False, collate_fn=collate)

# Create model
net_parameters = {}
net_parameters['input_dim'] = 1
net_parameters['hidden_dim'] = 100
net_parameters['output_dim'] = 8 # nb of classes
net_parameters['L'] = 4
net = GatedGCN_Net(net_parameters)
net = net.to(device)

optimizer = torch.optim.Adam(net.parameters(), lr=0.0005)

epoch_train_losses = []
epoch_test_losses = []
epoch_val_losses = []
epoch_train_accs = []
epoch_test_accs = []
epoch_val_accs = []
for epoch in range(50):

    start = time.time()
    epoch_train_loss, epoch_train_acc, gpu_mem = train_one_epoch(net, train_loader)
    epoch_test_loss, epoch_test_acc = evaluate_network(net, test_loader)
    epoch_val_loss, epoch_val_acc = evaluate_network(net, val_loader)

    print('Epoch {}, time {:.4f}, train_loss: {:.4f}, test_loss: {:.4f}, val_loss: {:.4f} \n
```

Main function

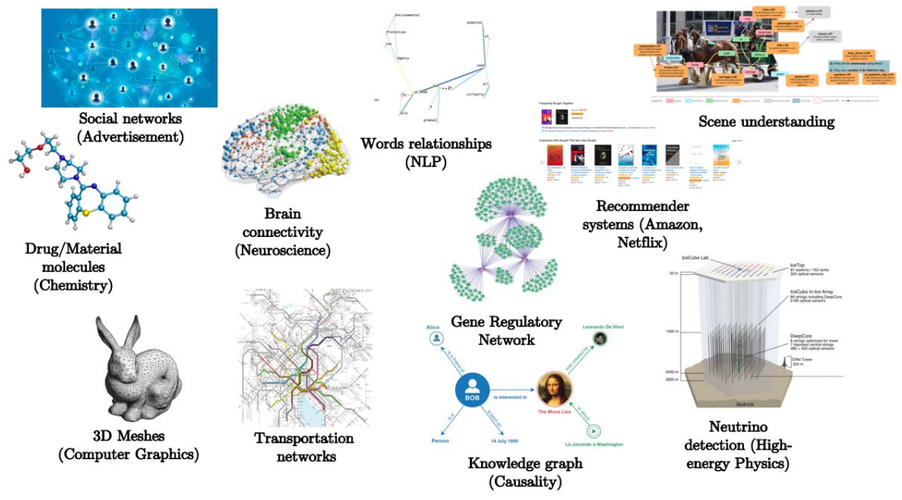
Outline

- Part 1 : Traditional ConvNets
  - Architecture
  - Graph Domain
  - Convolution
- Part 2: Spectral Graph ConvNets
  - Spectral Convolution
  - Spectral GCNs
- Part 3 : Spatial Graph ConvNets
  - Template Matching
  - Isotropic GCNs
  - Anisotropic GCNs
  - DGL : Implemented layers and lab demo
- **Conclusion**

Conclusion

- Contributions :
  - Generalization of ConvNets to data on graphs
  - Re-design convolution operator on graphs
  - Linear complexity for sparse graphs
  - GPU implementation (not yet optimized for sparse linear algebra multiplications)
  - Universal learning capacity
  - Multiple and dynamic graphs

- Applications :



"Graphs are the most important discrete models in the world!" - G. Strang (MIT)

Questions?