Лекция 5. Графови невронни мрежи.

DSCM023 „Прогнозиране чрез анализ на данни - III“

ИНСТИТУТ *за* СЪВРЕМЕННИ ФИЗИЧЕСКИ ИЗСЛЕДВАНИЯ

НОВ БЪЛГАРСКИ УНИВЕРСИТЕТ

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https://facebook.com/nbudatascience

План

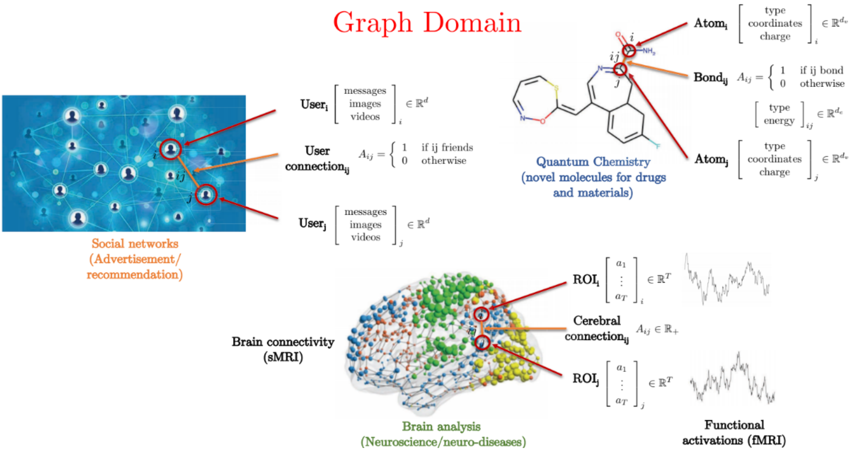
Графи и въпроси върху операцията конволюция

Спекрална теория на графи

Конволюция на графи in inverse space

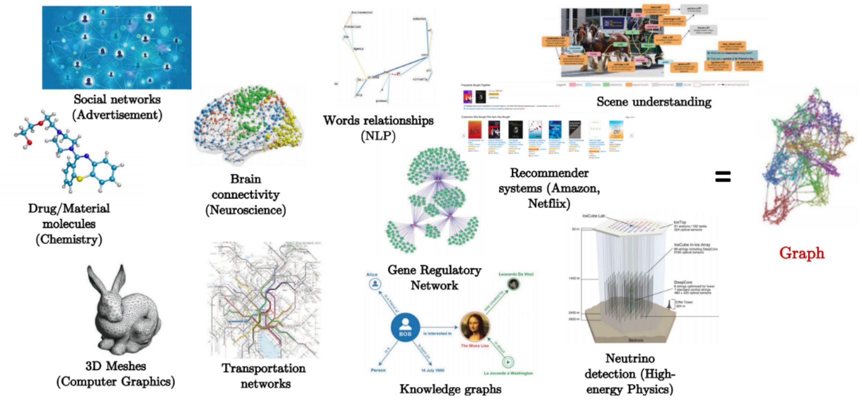
Графи и въпроси върху операцията конволюция

https://youtu.be/Iiv9R6BjxHM



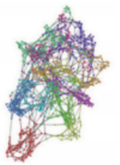
Graph Domain
User$_i$ $\begin{bmatrix} \text{messages} \\ \text{images} \\ \text{videos} \end{bmatrix}_i \in \mathbb{R}^d$
User connection$_{ij}$ $A_{ij} = \begin{cases} 1 & \text{if ij friends} \\ 0 & \text{otherwise} \end{cases}$
User$_j$ $\begin{bmatrix} \text{messages} \\ \text{images} \\ \text{videos} \end{bmatrix}_j \in \mathbb{R}^d$
i
ij
j
Social networks (Advertisement/ recommendation)
Atom$_i$ $\begin{bmatrix} \text{type} \\ \text{coordinates} \\ \text{charge} \end{bmatrix}_i \in \mathbb{R}^{d_v}$
Bond$_{ij}$ $A_{ij} = \begin{cases} 1 & \text{if ij bond} \\ 0 & \text{otherwise} \end{cases}$
$\begin{bmatrix} \text{type} \\ \text{energy} \end{bmatrix}_{ij} \in \mathbb{R}^{d_e}$
Atom$_j$ $\begin{bmatrix} \text{type} \\ \text{coordinates} \\ \text{charge} \end{bmatrix}_j \in \mathbb{R}^{d_v}$
Quantum Chemistry (novel molecules for drugs and materials)
ROI$_i$ $\begin{bmatrix} a_1 \\ \vdots \\ a_T \end{bmatrix}_i \in \mathbb{R}^T$
Cerebral connection$_{ij}$ $A_{ij} \in \mathbb{R}_+$
ROI$_j$ $\begin{bmatrix} a_1 \\ \vdots \\ a_T \end{bmatrix}_j \in \mathbb{R}^T$
Brain connectivity (sMRI)
Brain analysis (Neuroscience/neuro-diseases)
Functional activations (fMRI)

Graph Domain



Graph Domain

- Graphs G are defined by :
  - Vertices V
  - Edges E
  - Adjacency matrix A
- Graph features :
  - Node features : $h_i,\ h_j$ (atom type)
  - Edge features : e_{ij} (bond type)
  - Graph features : g (molecule energy)



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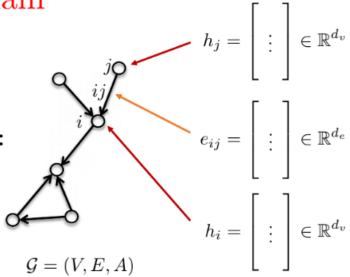
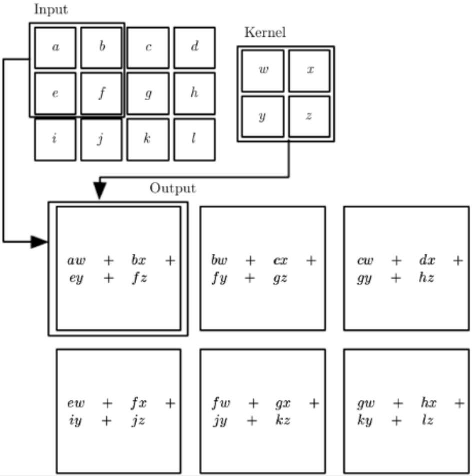


$$\underbrace{\begin{gathered}\mathcal{G} = (V, E, A) \\ V = \{1, .., n\}\end{gathered}}$$

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

Операцията „конволюция“



- Convolutional layer (for grids) :

$$\underset{n_1 \times n_2 \times d}{h^{\ell+1}} = \underset{3 \times 3 \times d}{w^{\ell}} * \underset{n_1 \times n_2 \times d}{h^{\ell}}$$

$*$

$=$

h^{ℓ}

Image/Hidden features

w^{ℓ}

Pattern/kernel (learned by backpropagation)

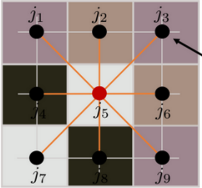
$h^{\ell+1}$

Convolution

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

$$3 \times 3 \times d \qquad n_1 \times n_2 \times d$$

$$
\begin{aligned}
h_i^{\ell+1} &= w^\ell * h_i^\ell \\
&= \sum_{\underbrace{j \in \Omega}_{j \in \mathcal{N}_i}} \langle w_j^\ell, \underbrace{h_{i-j}^\ell}_{h_{i+j}^\ell = h_{ij}^\ell} \rangle \\
&= \sum_{j \in \mathcal{N}_i} \langle w_j^\ell, h_{ij}^\ell \rangle \\
&= \sum_{j \in \mathcal{N}_i} \langle \begin{bmatrix} \\ w_j^\ell \\ \\ \end{bmatrix}, \begin{bmatrix} \\ h_{ij}^\ell \\ \\ \end{bmatrix} \rangle
\end{aligned}
$$



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

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

Template features at j_3

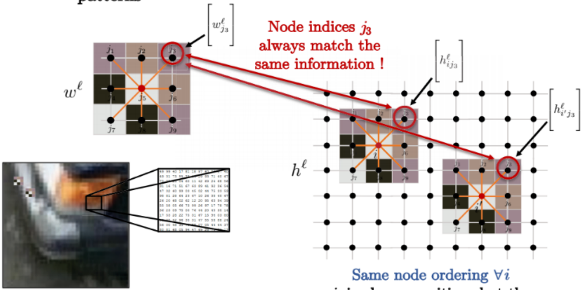
All nodes of the template w^l are always ordered/positioned the same way !

ℓ

Convolution

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

$$
\begin{aligned}
h_i^{\ell+1} &= w^\ell * h_i^\ell \\
&= \sum_{j \in \mathcal{N}_i} \langle w_j^\ell, h_{ij}^\ell \rangle \\
&= \sum_{j \in \mathcal{N}_i} \left\langle \begin{bmatrix} w_j^\ell \end{bmatrix}, \begin{bmatrix} h_{ij}^\ell \end{bmatrix} \right\rangle
\end{aligned}
$$



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

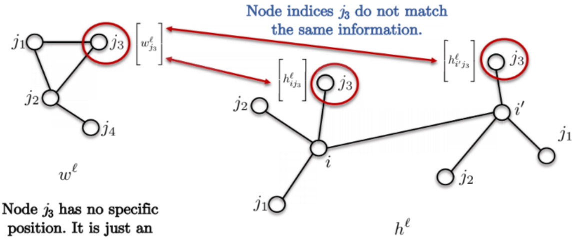
$$\left\langle \begin{bmatrix} w_{j_3}^\ell \end{bmatrix}, \begin{bmatrix} h_{ij_3}^\ell \end{bmatrix} \right\rangle$$

$$\left\langle \begin{bmatrix} w_{j_3}^\ell \end{bmatrix}, \begin{bmatrix} h_{i'j_3}^\ell \end{bmatrix} \right\rangle$$

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) ?



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

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

$$\langle \left[w^\ell_{j_3} \right], \left[h^\ell_{ij_3} \right] \rangle$$

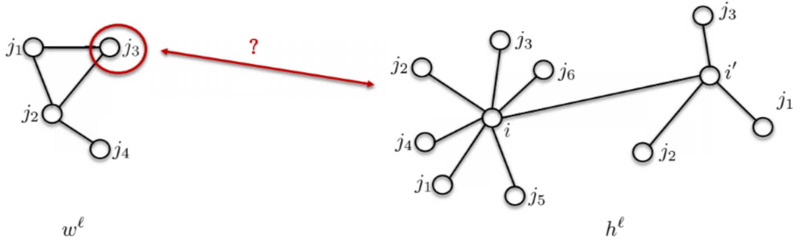
$$\langle \left[w^\ell_{j_3} \right], \left[h^\ell_{i'j_3} \right] \rangle$$

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

$$h_i^{\ell+1} = w^\ell *_{\mathcal{G}} h_i^\ell$$
$n \times d$
$$= \cancel{\sum_{j \in \mathcal{N}_i} \langle w_j^\ell, h_{ij}^\ell \rangle}$$

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 $\mathrm{O}(n^2)$ complexity, but if the domain is a grid then complexity can be reduced to $\mathrm{O}(n\log n)$ 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 $\mathrm{O}(n)$ 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

Трансформация на Фурие (напомняне).

Права и обратна трансформация:

$$H(f) = \int_{-\infty}^{\infty} h(t) e^{2\pi i f t} dt, \qquad h(t) = \int_{-\infty}^{\infty} H(f) e^{-2\pi i f t} df$$

If ...	then ...
$h(t)$ is real	$H(-f) = [H(f)]^*$
$h(t)$ is imaginary	$H(-f) = -[H(f)]^*$
$h(t)$ is even	$H(-f) = H(f)$ [i.e., $H(f)$ is even]
$h(t)$ is odd	$H(-f) = -H(f)$ [i.e., $H(f)$ is odd]
$h(t)$ is real and even	$H(f)$ is real and even
$h(t)$ is real and odd	$H(f)$ is imaginary and odd
$h(t)$ is imaginary and even	$H(f)$ is imaginary and even
$h(t)$ is imaginary and odd	$H(f)$ is real and odd

$$F(g * f) = F(g).F(f), \qquad g * f = F^{-1}(F(g).F(f))$$

Права и обратна трансформация:

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$h(t)$ is real and even	$H(f)$ is real and even
$h(t)$ is real and odd	$H(f)$ is imaginary and odd
$h(t)$ is imaginary and even	$H(f)$ is imaginary and even
$h(t)$ is imaginary and odd	$H(f)$ is real and odd

$$F(g * f) = F(g).F(f), \qquad g * f = F^{-1}(F(g).F(f))$$

За дискретни данни h_k:

$$H_n = \sum_{k=0}^{N-1} h_k e^{2\pi i k n/N}, h_k = \frac{1}{N} \sum_{n=0}^{N-1} H_n e^{-2\pi i k n/N}, \sum_{k=0}^{N-1} |h_k|^2 = \frac{1}{N} \sum_{n=0}^{N-1} |H_n|^2$$

Колко опрации са нужни за дискретното преобразуване на Фурие $H_n = \sum_{k=0}^{N-1} W^{nk} h_k$, където $W \equiv e^{2\pi i/N}$? Може би $\sim N^2$...

Колко опрации са нужни за дискретното преобразуване на Фурие $H_n = \sum_{k=0}^{N-1} W^{nk} h_k$, където $W \equiv e^{2\pi i/N}$? Може би $\sim N^2$... Оказва се, че това може да стане с $\sim N \log_2 N$ операции. Danielson и Lanczos (1942) показват, че дискретното преобразование на Фурие с дължина N може да се запише като **сума от две** дискретни преобразования на Фурие, всяко с дължина $N/2$. Едното е преобразуванието на стойностите, който стоят на четни позиции, а другото - на нечетните:

$$F_k = \sum_{j=0}^{N-1} W^{ij} f_j = ... = F_k^e + W^k F_k^o$$

Спекрална теория на графи

ENCYCLOPEDIA OF MATHEMATICS AND ITS APPLICATIONS

Eigenspaces of graphs

D. Cvetković
University of Belgrade

P. Rowlinson
University of Stirling

S. Simić
University of Belgrade

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Spectral Graph Theory

Fan R. K. Chung

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Graph Laplacian

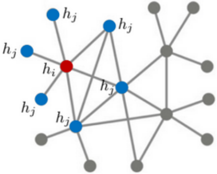
- Core operator in Spectral Graph Theory

$$\mathcal{G} = (V, E, \underset{n\times n}{A}) \quad \rightarrow \quad \underset{n\times n}{\Delta} = \mathrm{I} - D^{-1/2} A D^{-1/2} \qquad \text{Normalized Laplacian}$$

$$\text{where } \underset{n\times n}{D} = \mathrm{diag}(\sum_{j\neq i} A_{ij})$$

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

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



-

$$\Delta \equiv \nabla^2 = \sum_i \partial_{x_i}^2$$

-

$$\Delta \equiv \nabla^2 = \sum_i \partial_{x_i}^2$$

- Фурие трансформация на граф се нарича разлагането на матрицата на Лаплас за този граф по собствени вектори (създаващи, т.нар. Фурие базис на граф).

Fourier Functions

- Eigen-decomposition of graph Laplacian :

Lap Eigenvalues/
Spectrum

Lap Eigenvectors/
Fourier functions

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

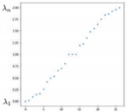
Fourier functions form an orthonormal basis

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

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

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

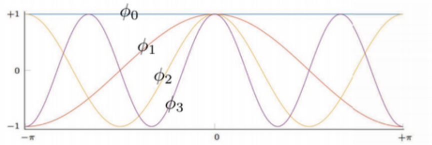
$n = 27$



Spectrum

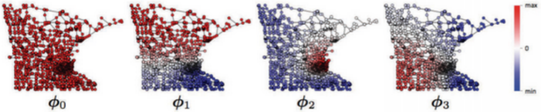
Fourier Functions

- 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] :

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

$$= \sum_{k=1}^{n} \hat{h}_k \phi_k$$

$$= \underbrace{\Phi \hat{h}}_{\mathcal{F}^{-1}(\hat{h})}$$

Fourier transforms are one line of code (linear operations)

$$\underset{n\times 1}{\mathcal{F}(h)} = \Phi^T h = \hat{h}$$

Fourier Transform/ coefficients of Fourier Series

$$\underset{n\times 1}{\mathcal{F}^{-1}(\hat{h})} = \Phi \hat{h}$$

Inverse Fourier Transform

$$= \Phi \Phi^T h = h \text{ as } \mathcal{F}^{-1} \circ \mathcal{F} = \Phi \Phi^T = \mathrm{I}$$

Orthonormal basis/ Invertible transformation

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

Конволюция на графи in inverse space

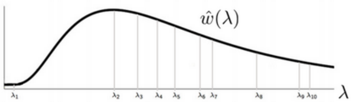
Convolution Theorem

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

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

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

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



Expensive computation $O(n^2)$
No FFT

Spectral function/filter

Notebook

`https://github.com/xbresson/spectral_graph_convnets/blob/master/02_graph_convnet_lenet5_mnist_pytorch.ipynb`