Convolutional Neural Networks on Graphs with Fast Localized Spectral Filtering

by M. Defferrard, X. Bresson, P. Vandergheynst, 2016

Paper presentation

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July 8th, 2020

Table of Contents

- **Convolutional neural networks (CNNs)**, introduced in 1989 by Yann LeCun [1], are able to learn **local stationary structures** which are composed into **multi-scale patterns**. They led to **breakthroughs in image, video and sound recognition tasks**.
- Defferard and colleagues [2] introduced a **generalization of CNNs to graphs**, which encode **complex data structures** lying on irregular or non-euclidean domains.

Introduction

- **Convolutional neural networks (CNNs)**, introduced in 1989 by Yann LeCun [1], are able to learn **local stationary structures** which are composed into **multi-scale patterns**. They led to **breakthroughs in image, video and sound recognition tasks**.
- Defferard and colleagues [2] introduced a **generalization of CNNs to graphs**, which encode **complex data structures** lying on irregular or non-euclidean domains.
- Main challenges:
  - Construct a **convolution operator on irregular grids**;
  - Design **strictly localized filters**, as in standard CNNs;
  - Compute forward- and backward-propagation with a **linear complexity** w.r.t. the filter support's size and the number of edges;
  - Design an **efficient pooling operator** (which yields smaller graphs by grouping vertices together);
  - Obtain **high experimental performance** on both standard image and more complex data recognition tasks.

Section 2

Background on CNNs

Description of a convolutional layer

Forward-propagation:

$$\mathbf{X}_s \xrightarrow{\text{Conv}(\mathbf{W})} \mathbf{Y}_s \xrightarrow{\text{ReLu}} \mathbf{A}_s \xrightarrow{\text{Pool}} \mathbf{Z}_s$$

with:

- $\mathbf{X}_s \in \mathbb{R}^{C\times M\times M}$, $\mathbf{Y}_s, \mathbf{A}_s \in \mathbb{R}^{D\times M\times M}$ and $\mathbf{Z}_s \in \mathbb{R}^{D\times N\times N}$ (feature maps for the s-th training sample);
- $\mathbf{W} \in \mathbb{R}^{D\times C\times \mu\times \mu}$ (convolution kernels – **trainable parameters**);
- $C, D > 0$ (number of input and output feature maps);
- $M, N > 0$ such that $N < M$ (sizes of the input and output feature maps);
- $\mu \ll M$ (size of the convolution kernels).

- Conv: convolutional layer (see slide 7);
- ReLu: rectified linear unit (non-linear pointwise operation);
- Pool: pooling operator (e.g. max pooling).

Illustration of a convolutional layer

Computation of the d-th output feature map, for $d \in [0\,..\,D-1]$:

$$\mathbf{Y}_{s,d} = b_d + \sum_{c=0}^{C-1} (\mathbf{W}_{d,c} \star \mathbf{X}_{s,c})$$

where $\star$ denotes the **cross-correlation** operator (slid sum-product).

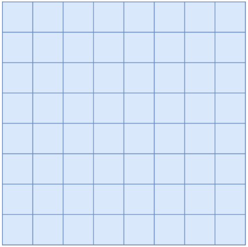

Figure: c-th input feature map $\mathbf{X}_{s,c} \in \mathbb{R}^{M \times M}$, for a given $c \in [0\,..\,C-1]$

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0	0	0	0	0	0	0	0	0	0
0									0
0									0
0									0
0									0
0									0
0									0
0									0
0									0
0	0	0	0	0	0	0	0	0	0

Figure: c-th input feature map, extended with zeros (padding)

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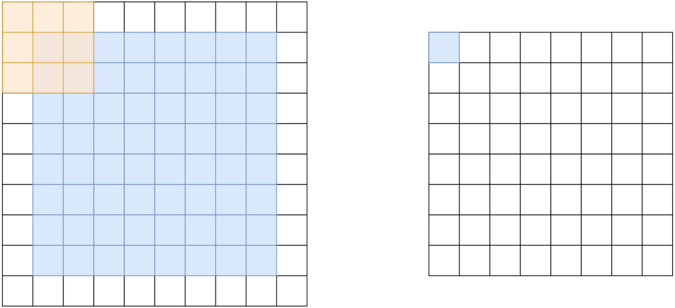

Figure: Cross-correlation mapping the c-th input $\mathbf{X}_{s,c}$ (left, in blue) to the d-th output, using the kernel $\mathbf{W}_{d,c} \in \mathbb{R}^{\mu \times \mu}$ (left, in orange). Right: $(\mathbf{W}_{d,c} \star \mathbf{X}_{s,c})$.

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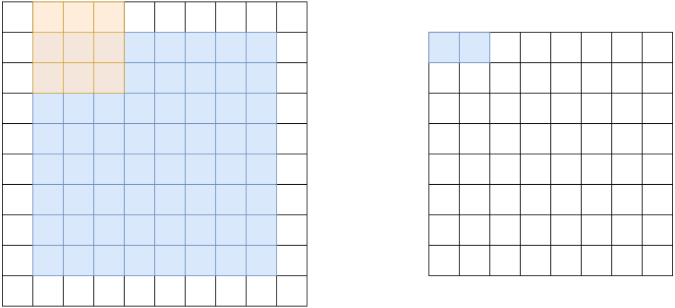

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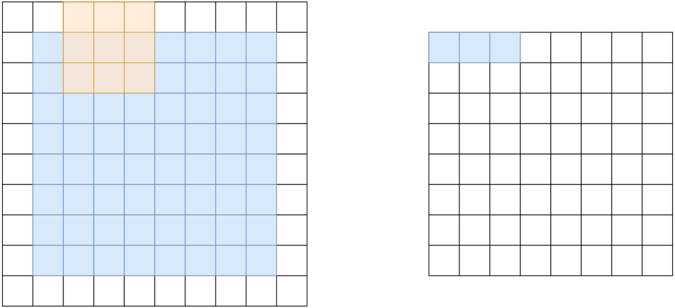

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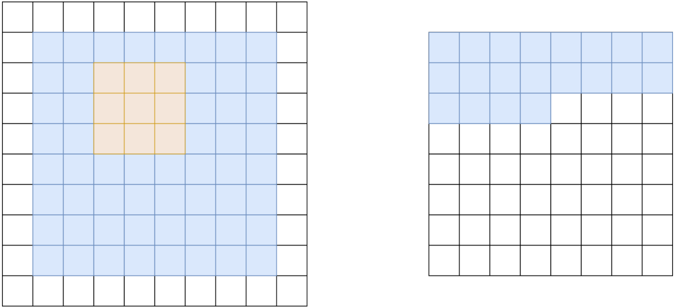

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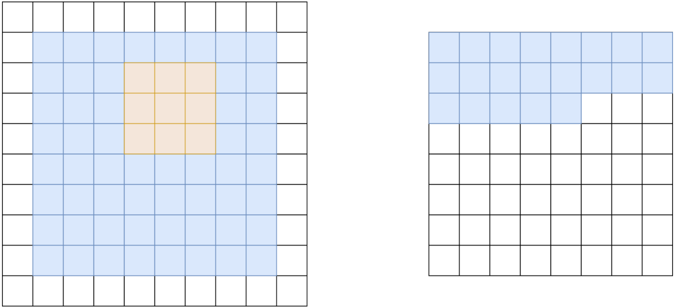

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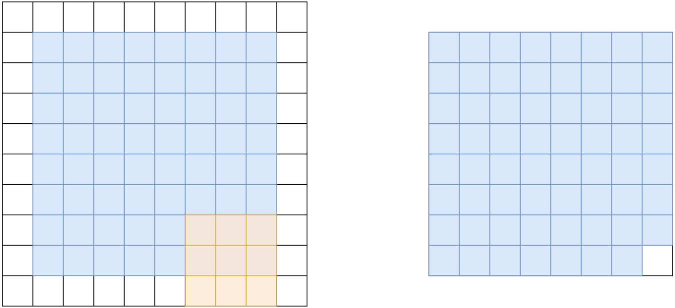

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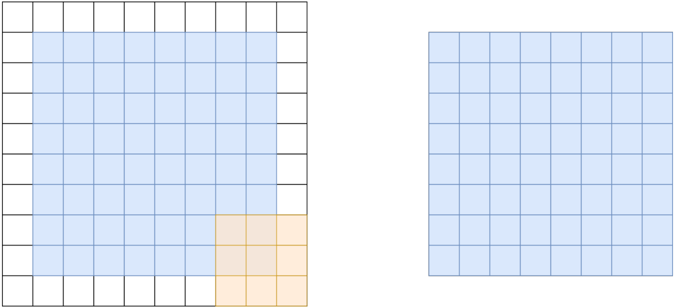

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Convolution versus cross-correlation

- Matrix convolution product:

$$(\mathbf{U} * \mathbf{V})[m,n] = \sum_{i\in\mathbb{Z}} \sum_{j\in\mathbb{Z}} \mathbf{U}[i,j] \cdot \mathbf{V}[m-i, n-j]$$

- Cross-correlation:

$$(\mathbf{U} \star \mathbf{V})[m,n] = \sum_{i\in\mathbb{Z}} \sum_{j\in\mathbb{Z}} \mathbf{U}[i,j] \cdot \mathbf{V}[m+i, n+j]$$

Proposition 2.1

$$\mathbf{U} \star \mathbf{V} = \overline{\mathbf{U}} * \mathbf{V}$$

where $\overline{\mathbf{U}}[m,n] = \mathbf{U}[-m,-n]$.

Let's assume the following values have already been computed:

- E: loss computed over a minibatch of S samples;
- $\left\{\nabla_{(\mathbf{Y}_{s,d})}E \middle| s \in [0\mathinner{..}S-1]\,, d \in [0\mathinner{..}D-1]\right\}$: gradients w.r.t. the outputs;

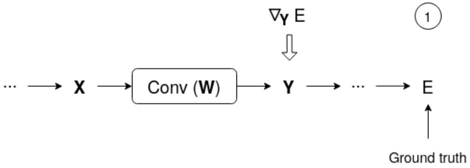
Then, backpropagates the gradient in $\mathcal{O}(SCD \cdot \mu^2 N^2)$:

$$\nabla_{(\mathbf{W}_{d,c})}E = \sum_{s=1}^{S} \left(\nabla_{(\mathbf{Y}_{s,d})}E\right) \star \mathbf{X}_{s,c}$$

$$\nabla_{(\mathbf{X}_{s,c})}E = \sum_{d=1}^{D} \left(\nabla_{(\mathbf{Y}_{s,d})}E\right) * \mathbf{W}_{d,c}$$

Finally, update the weights using stochastic gradient descent:

$$\mathbf{W}_{d,c} \leftarrow \left(\mathbf{W}_{d,c} - \eta \cdot \nabla_{(\mathbf{W}_{d,c})}E\right)$$



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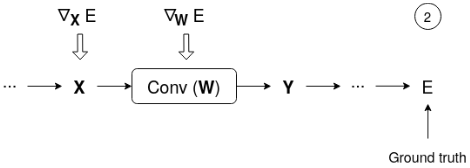

For any sample s and any output d:

$$\mathbf{Z}_{s,d}[m,n] = \max_{i,j \in \{0,1\}} \Big(\mathbf{Y}_{s,d}[2m+i,\, 2n+j] \Big)$$

with $\mathbf{Y}_{s,d} \in \mathbb{R}^{N \times N}$ and $\mathbf{Z}_{s,d} \in \mathbb{R}^{(N/2)\times(N/2)}$.

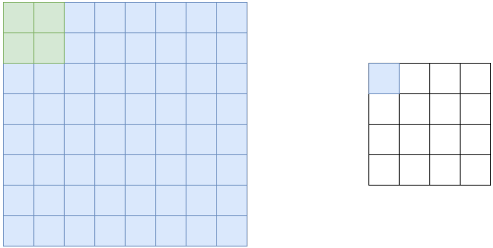

Illustration of a pooling layer
Example of max pooling with size 2 × 2

For any sample s and any output d:

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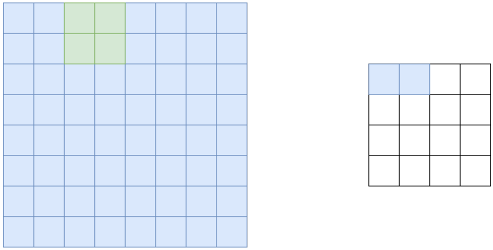

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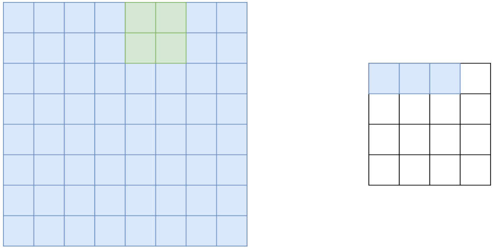

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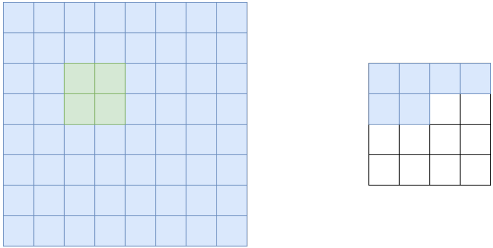

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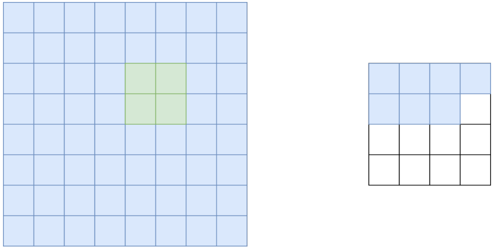

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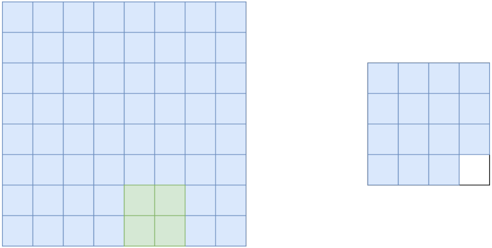

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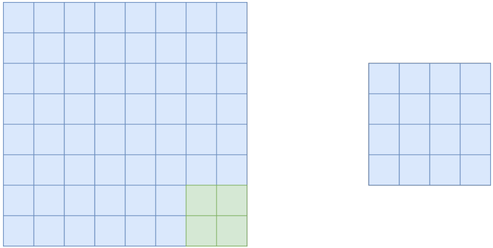


Section 3

Convolution layers on graphs

Notations

- Graph $\mathcal{G} = (\mathcal{V}, \mathcal{E}, \mathbf{A})$, with:
  - $|\mathcal{V}| = N$;
  - $\mathbf{A} \in \mathbb{R}^{N \times N}$ such that $\mathbf{A}_{ij} \neq 0 \implies (i, j) \in \mathcal{E}$.
- $\mathbf{L} \in \mathbb{R}^{N \times N}$: positive semidefinite reference matrix for $\mathcal{G}$;
- $\mathbf{U}, \mathbf{\Lambda} \in \mathbb{R}^{N \times N}$, with:
  - $\mathbf{U} = [\mathbf{u}_0, \dots, \mathbf{u}_{N-1}]$: eigenvectors of $\mathbf{L}$ (graph Fourier modes);
  - $\mathbf{\Lambda} = \mathrm{diag}(\lambda_0, \dots, \lambda_{N-1})$: eigenvalues of $\mathbf{L}$ (graph frequencies);

  such that $\mathbf{L} = \mathbf{U}\mathbf{\Lambda}\mathbf{U}^\top$;
- Input signal $\mathbf{x} \in \mathbb{R}^N$, defined on the nodes of $\mathcal{G}$;
- $\hat{\mathbf{x}}$: graph Fourier transform of $\mathbf{x}$, such that $\hat{\mathbf{x}} = \mathbf{U}^\top \mathbf{x}$.

From classical to graph convolutions

Forward-propagation for any sample s and any output d:

Classical CNN:

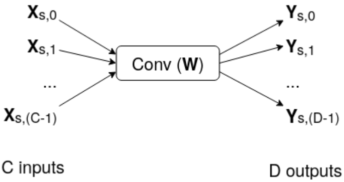
$$\mathbf{Y}_{s,d} = \sum_{c=0}^{C-1} (\mathbf{W}_{d,c} \star \mathbf{X}_{s,c}) = \sum_{c=0}^{C-1} \left(\overline{\mathbf{W}_{d,c}} * \mathbf{X}_{s,c}\right)$$

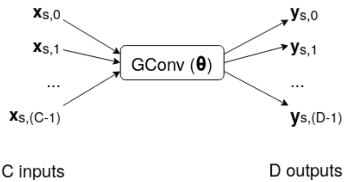
according to proposition 2.1.

Graph CNN:

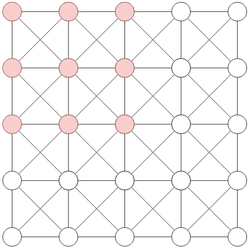
$$\mathbf{y}_{s,d} = \sum_{c=0}^{C-1} (\overline{\boldsymbol{\theta}_{d,c}} *_{(\mathcal{G})} \mathbf{x}_{s,c})$$

where $*_{(\mathcal{G})}$ has to be defined.





Issue with spatial convolution: **no unique definition of translation** on graphs.



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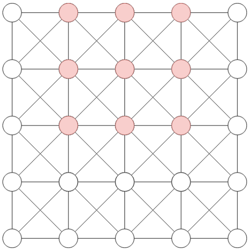

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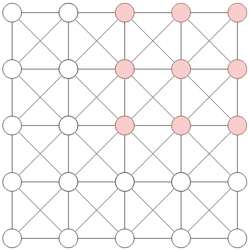

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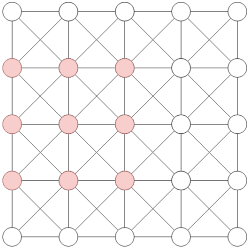

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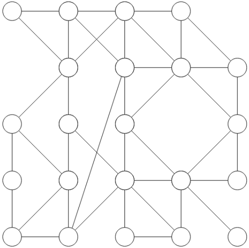


Graph convolution via Fourier transform

Instead, use convolution properties **in the Fourier domain**:

$$\mathbf{G}^{(d)}(\mathbf{x}_s) = \mathbf{y}_{s,d} = \sum_{c=0}^{C-1} (\overline{\boldsymbol{\theta}_{d,c}} *_{(\mathcal{G})} \mathbf{x}_{s,c})$$

$$= \underbrace{\sum_{c=0}^{C-1} \underbrace{\mathbf{U} \cdot \underbrace{g^{(d,c)}(\boldsymbol{\Lambda}) \cdot \overbrace{\mathbf{U}^\top \mathbf{x}_{s,c}}^{\widehat{\mathbf{x}_{s,c}}}}_{\text{filtering}}}_{\text{inverse Fourier transform}}}_{\text{sum over all inputs}}$$

with $g^{(d,c)} : \mathbb{R}_+ \to \mathbb{R}$ and $g^{(d,c)}(\boldsymbol{\Lambda}) = \text{diag}\left(g^{(d,c)}(\lambda_0), \dots, g^{(d,c)}(\lambda_{N-1})\right)$.

$\Longrightarrow$ For any input c and output d, $g^{(d,c)}$ only needs to be defined on the graph frequencies $\lambda_0, \dots, \lambda_{N-1}$, giving a weight to the corresponding eigenspaces.

Parametrization of graph filters

First approach: non-parametric filters

Let $\boldsymbol{\theta}_{d,c} \in \mathbb{R}^N$ such that $g^{(d,c)}(\lambda_n) = \boldsymbol{\theta}_{d,c}[n]$ for any $n \in [0 \mathinner{.\,.} N-1]$.

- ✗ Not localized in space;
- ✗ N trainable parameters ($\ll N$ for standard CNNs);
- ✗ Filtering operation: $\mathcal{O}(N^2)$ (linear complexity for standard CNNs).

Let $\boldsymbol{\theta}_{d,c} \in \mathbb{R}^K$ $(K \ll N)$ such that for any $n \in [0\,..\,N-1]$:

$$g^{(d,c)}(\lambda_n) = \sum_{k=0}^{K-1} \boldsymbol{\theta}_{d,c}[k] \cdot \lambda_n^k$$

- ✓ K-**localized filters**: for any $i, j \in [0\,..\,N-1]$, $\mathbf{y}_{s,d}[j]$ is influenced by $\mathbf{x}_{s,c}[i]$ only if $d_{\mathcal{G}}(i,j) \leq (K-1)$, where $d_{\mathcal{G}}$ denotes the minimum number of edges connecting vertices i and j;
- ✓ K **trainable parameters**, which is equal to the filter spatial extension (similarly to standard 1D CNNs);
- ✗ Filtering operation: $\mathcal{O}(N^2)$ (linear complexity for standard CNNs).

Let $\boldsymbol{\theta}_{d,c} \in \mathbb{R}^K$ $(K \ll N)$ such that for any $n \in [0\,..\,N-1]$:

$$g^{(d,c)}(\lambda_n) = \sum_{k=0}^{K-1} \boldsymbol{\theta}_{d,c}[k] \cdot T_k(\tilde{\lambda}_n)$$

with $\tilde{\lambda} = 2\lambda/\lambda_{\max} - 1$ and $T_k \in \mathcal{P}_k(\mathbb{R})$ (Chebyshev polynomials) such that:

$$\begin{cases} T_0(u) = 1 \\ T_1(u) = u \\ T_k(u) = 2uT_{k-1}(u) - T_{k-2}(u) \quad \text{for any } k \geq 2 \end{cases}$$

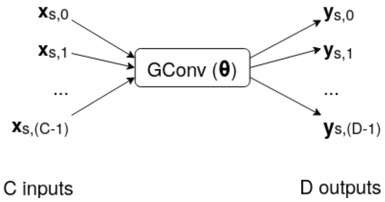
- ✓ K-**localized filters**: for any $i, j \in [0\,..\,N-1]$, $\mathbf{y}_{s,d}[j]$ is influenced by $\mathbf{x}_{s,c}[i]$ only if $d_{\mathcal{G}}(i,j) \leq (K-1)$, where $d_{\mathcal{G}}$ denotes the minimum number of edges connecting vertices i and j;
- ✓ K **trainable parameters**, which is equal to the filter spatial extension (similarly to standard 1D CNNs);
- ✓ **Fast filtering operation** with complexity $\mathcal{O}(K|\mathcal{E}|) \ll \mathcal{O}(N^2)$ (takes advantage of the sparsity of $\mathbf{L}$).

Forward-propagation in $\mathcal{O}(SCD \cdot K|\mathcal{E}|)$:

$$\begin{aligned}\mathbf{y}_{s,d} &= \sum_{c=0}^{C-1} (\overline{\boldsymbol{\theta}_{d,c}} *_{(\mathcal{G})} \mathbf{x}_{s,c}) \\ &= \sum_{c=0}^{C-1} (\mathcal{T}_{\mathbf{L}}(\mathbf{x}_{s,c}) \cdot \boldsymbol{\theta}_{d,c})\end{aligned}$$

with:

- $\boldsymbol{\theta}_{d,c} \in \mathbb{R}^K$ vector of Chebyshev coefficients;
- $\mathcal{T}_{\mathbf{L}} : \mathbb{R}^N \to \mathbb{R}^{N \times K}$, computed in $\mathcal{O}(K|\mathcal{E}|)$ with K recursive computations.

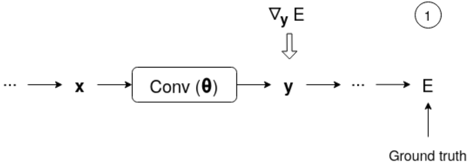


Gradient backpropagation in $\mathcal{O}(SCD \cdot K|\mathcal{E}|)$ (assuming $|\mathcal{E}| \sim N$):

$$\nabla_{(\boldsymbol{\theta}_{d,c})} E = \sum_{s=0}^{S-1} \left[\mathcal{T}_{\mathbf{L}}(\mathbf{x}_{s,c})^\top \cdot \nabla_{(\mathbf{y}_{s,d})} E \right]$$

$$\nabla_{(\mathbf{x}_{s,c})} E = \sum_{d=0}^{D-1} \left[\mathcal{T}_{\mathbf{L}} \left(\nabla_{(\mathbf{y}_{s,d})} E \right) \cdot \boldsymbol{\theta}_{d,c} \right]$$

where the loss E is computed over a minibatch of S samples.



Stochastic gradient descent: $\boldsymbol{\theta}_{d,c} \leftarrow \left(\boldsymbol{\theta}_{d,c} - \eta \cdot \nabla_{(\boldsymbol{\theta}_{d,c})} E \right)$

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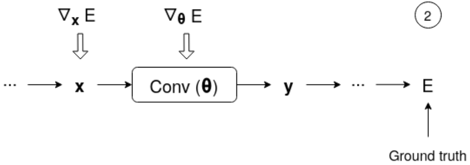

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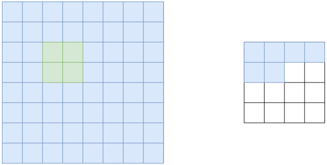
Section 4

Pooling layers on graphs

Forward-propagation for any sample s and any output d:

Classical CNN:

$$\mathbf{Z}_{s,d}[\boldsymbol{n}] = \max_{\boldsymbol{i}\in\{0,1\}^2} \left(\mathbf{Y}_{s,d}[2\boldsymbol{n}+\boldsymbol{i}]\right)$$



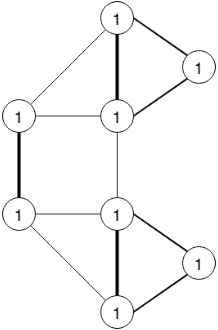
Graph CNN:

$$\mathbf{z}_{s,d}[n] = \max_{m\in\pi_n} \left(\mathbf{y}_{s,d}[m]\right)$$

where $\pi_n \subset [0\,..\,N-1]$ denotes the set of neighboring nodes that are reduced into one in the output graph.

Goal: find a graph structure $\mathcal{G}' = (\mathcal{V}', \mathcal{E}', \mathbf{W}')$ with $|\mathcal{V}'| = N' = \lceil N/2 \rceil$ and a grouping $\{\pi_n\}_{n\in[0..N'-1]}$, such that local geometric structures are preserved.

- Graph clustering is **NP-hard**.
- Approximation with a **greedy algorithm**: Graclus multilevel clustering.



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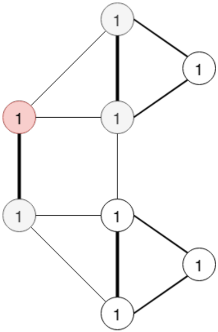

Graph coarsening using Graclus multilevel clustering algorithm

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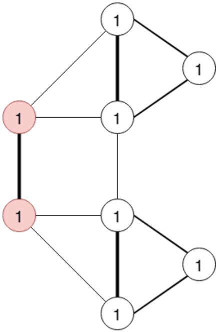

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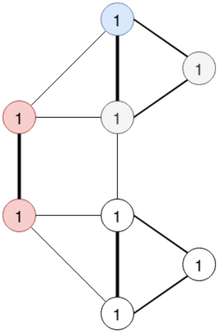

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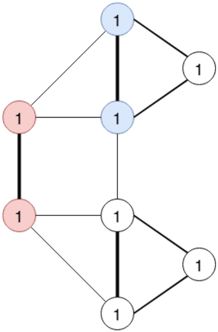

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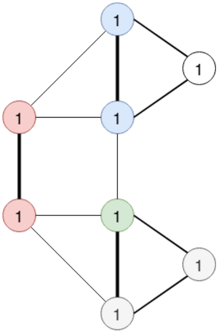

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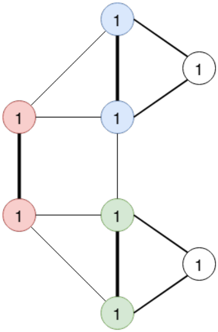

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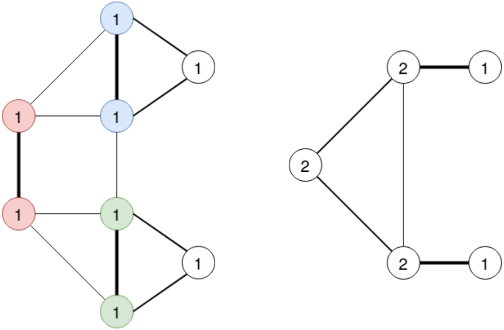

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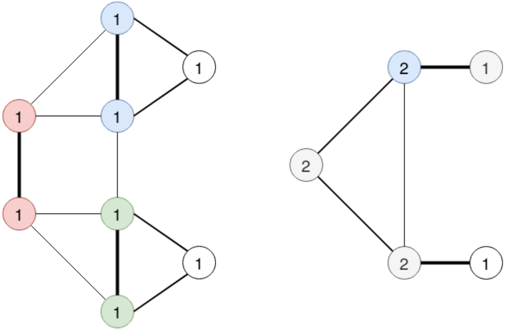

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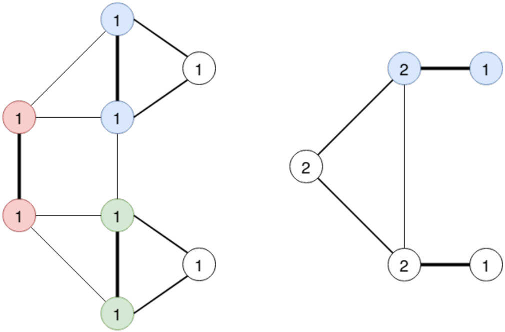

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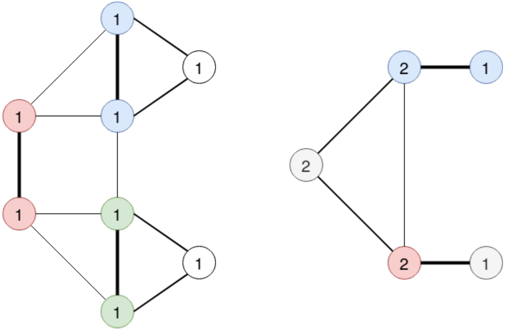

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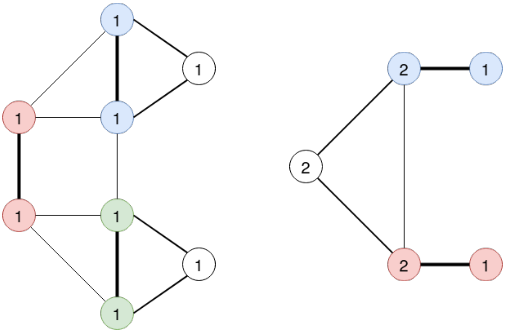

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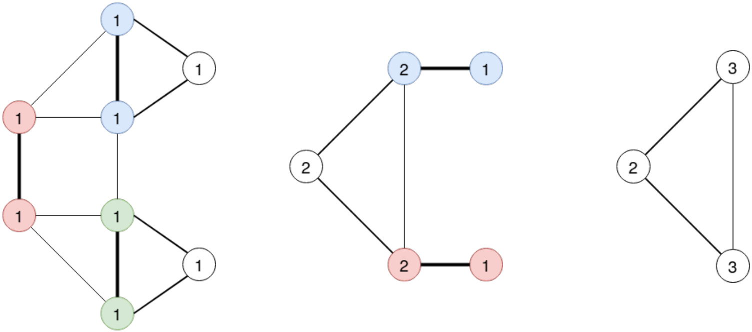

Fast pooling algorithm

Idea: rearrange vertices such that the pooling operation is computed over 2 consecutive nodes:

$$\forall n \in \left[0 \mathinner{.\,.} N' - 1\right], \pi(n) = \{2n, 2n+1\}$$

Then:

$$\mathbf{z}_{s,d}[n] = \max_{i \in \{0,1\}^2} \left(\mathbf{y}_{s,d}[2n+i]\right)$$

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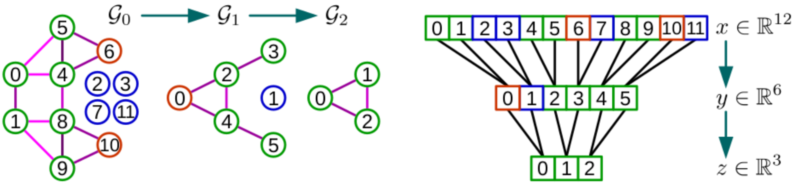


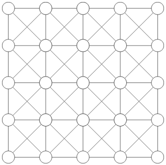
Figure: From [2]

Section 5

Numerical experiments

Applying graph CNN on image classification

- Sanity check for the model: it should at least perform well on standard image classification tasks.
- 8-NN[1] similarity graph of the 2D grid:



with weights: $\mathbf{A}[i,j] = \exp\left(-\frac{\|\mathbf{z}_j - \mathbf{z}_i\|_2^2}{\sigma^2}\right)$, where $\mathbf{z}_i \in \mathbb{R}^2$ is the coordinate of pixel i on the grid.

Model	Accuracy
Classical CNN	99.33
Proposed graph CNN	99.14

Figure: Classical vs graph CNN

		Accuracy		
Dataset	Architecture	Non-Param (2)	Spline (7) [4]	Chebyshev (4)
MNIST	GC10	95.75	97.26	97.48
MNIST	GC32-P4-GC64-P4-FC512	96.28	97.15	99.14

Figure: Different models of graph CNNs

[1] nearest neighbors

- **Text categorization** problem on the 20NEWS dataset [4].
- Using a **bag-of-words model** [5]: each document (input data) is represented as a vector $\mathbf{x} \in \mathbb{R}^N$ with $N = 10,000$ (**most common words** in the corpus). $\mathbf{x}[i]$ is the number of occurrences of word i in the document.

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- Word2vec embedding [5]: each word i is **semantically represented** as a vector $\boldsymbol{z}_i \in \mathbb{R}^d$ using (e.g. $d = 640$).
- Data structure: **16-NN graph** $\mathcal{G} = (\mathcal{V}, \mathcal{E}, \mathbf{A})$, with:
  - $|\mathcal{V}| = 10,000$;
  - $|\mathcal{E}| = 132,834$ edges (connections between the nearest neighbors, using the Euclidean distance induced by the word2vec embedding);
  - weights: $\mathbf{A}[i,j] = \exp\left(-\frac{\|\boldsymbol{z}_j - \boldsymbol{z}_i\|_2^2}{\sigma^2}\right)$.
- Model trained for 20 epochs using **Adam optimizer** [6] and initial learning rate $\eta = 0.001$.

Model	Accuracy
Linear SVM	65.90
Multinomial Naive Bayes	68.51
Softmax	66.28
FC2500	64.64
FC2500-FC500	65.76
GC32	68.26

Figure: Proposed model (GC32) is beaten by multinomial Bayes classifier but outperforms fully-connected newtorks with much less parameters.

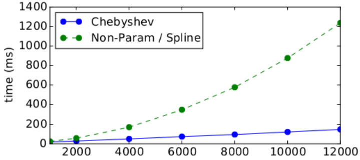

Figure: Linear complexity of the proposed model w.r.t. the data dimensionality N (vs $\mathcal{O}(N^2)$ for non-parametric CNNs or graph CNNs introduced in [7]).

Dataset	Architecture	Accuracy		
		Non-Param (2)	Spline (7) [4]	Chebyshev (4)
MNIST	GC10	95.75	97.26	97.48
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Figure: Different models of graph CNNs

Influence of graph structure on prediction accuracy

Architecture	8-NN on 2D Euclidean grid	random
GC32	97.40	96.88
GC32-P4-GC64-P4-FC512	99.14	95.39

Figure: MNIST

bag-of-words	word2vec pre-learned	word2vec learned	approximate	random
67.50	66.98	68.26	67.86	67.75

Figure: 20NEWS

- "bag-of-words": naive embedding;
- "learned": embedding learned with word2vec [5];
- "approximate": approximate nearest-neighbors algorithm used for larger datasets.

$\Longrightarrow$ The quality of the results **strongly depend on the graph structure**. It must be designed in order to fulfill **assumptions of locality and stationarity**, as in classical CNNs.

Conclusion and perspectives

Defferrard and colleagues [2] proposed a model of graph CNN able to extract local and stationary features from the data. Improvements with respect to previous graph CNNs [7] are:

- **strictly localized** convolution filters;
- **computational efficiency** which is comparable to classical CNNs;
- **higher test accuracy**.

Future work:

- Explore applications to fields where the data naturally lies on graphs, with explicit information about its structure;
- Learn optimal graph structure in parallel to CNN parameters (instead of using a pre-defined one).

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