Point Cloud Processing II

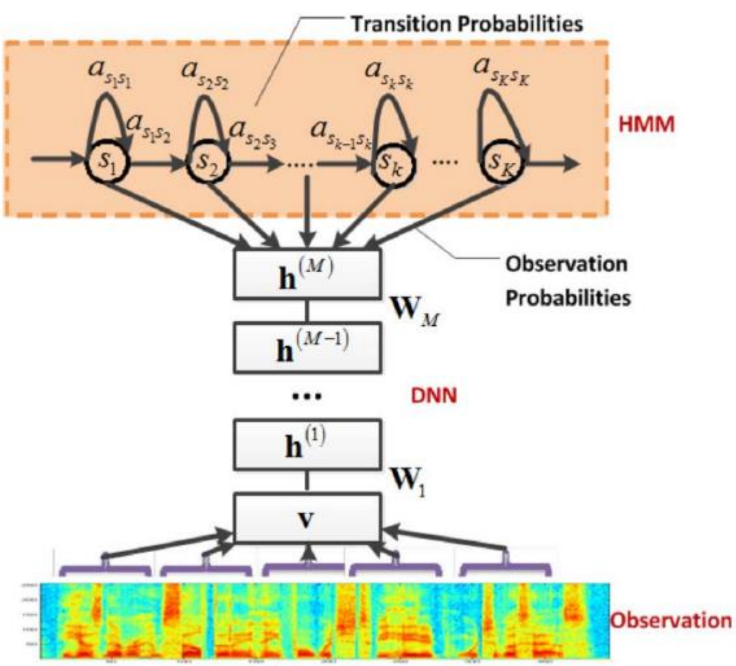
Deep Learning methods

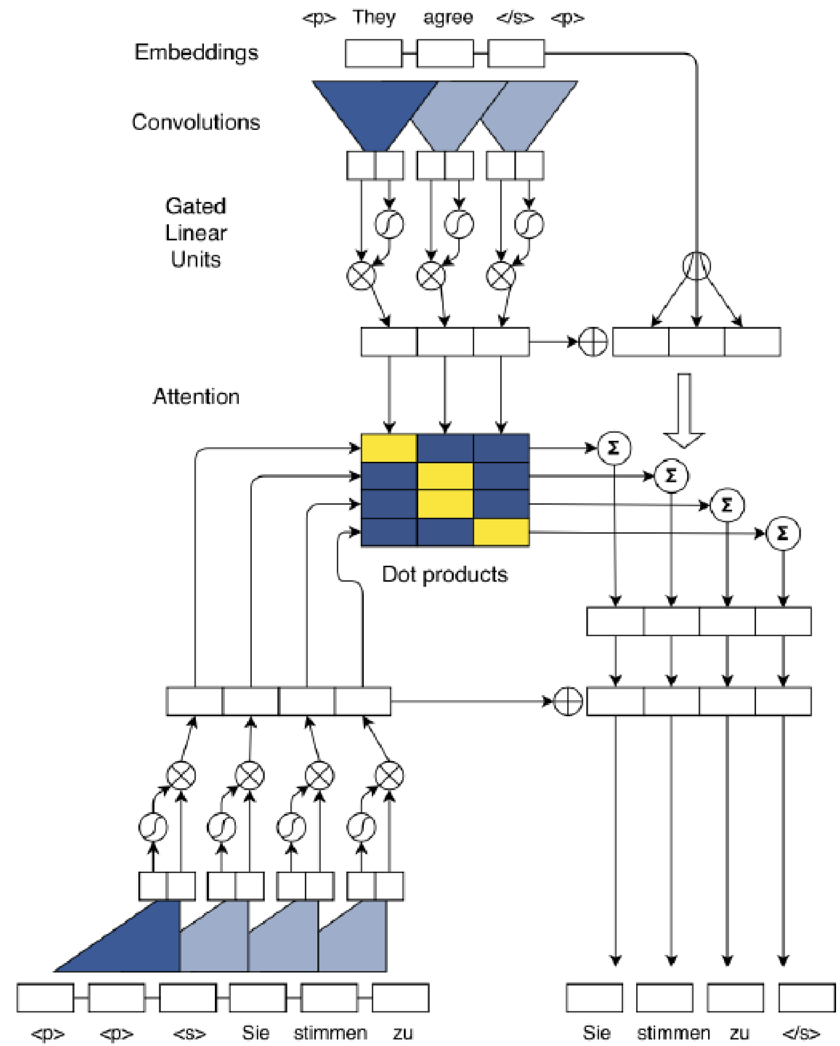
Why Deep Learning ?

- Deep learning has helped to boost performance in multiple fields
  - Speech recognition
  - Language translation
  - Image processing
  - …
- In most cases,
  - Data were structured in regular grids
  - Parameter sharing was advantageous
- How can we use DL on point clouds?
  - More generally, on graphs?

Speech recognition & Language translation

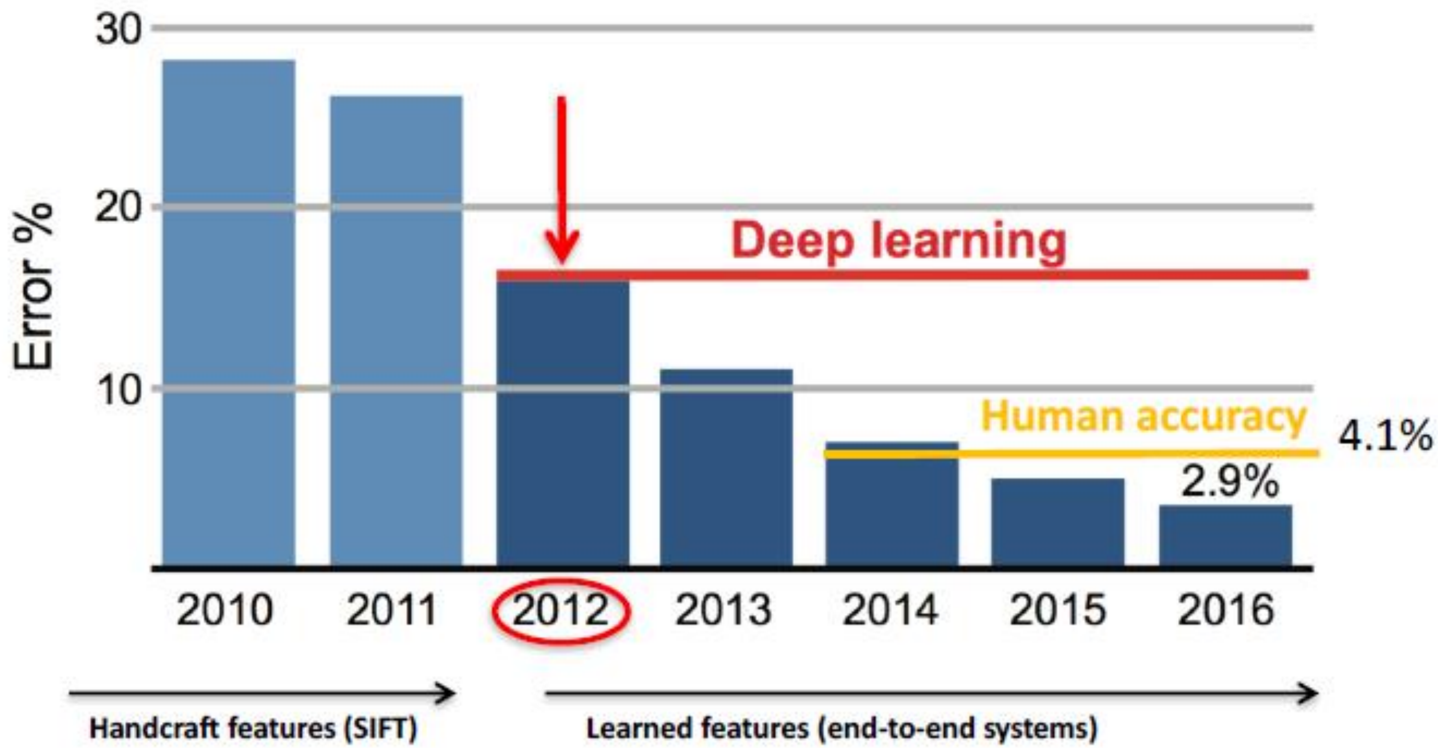
- Recurrent Neural Networks (RNNs)



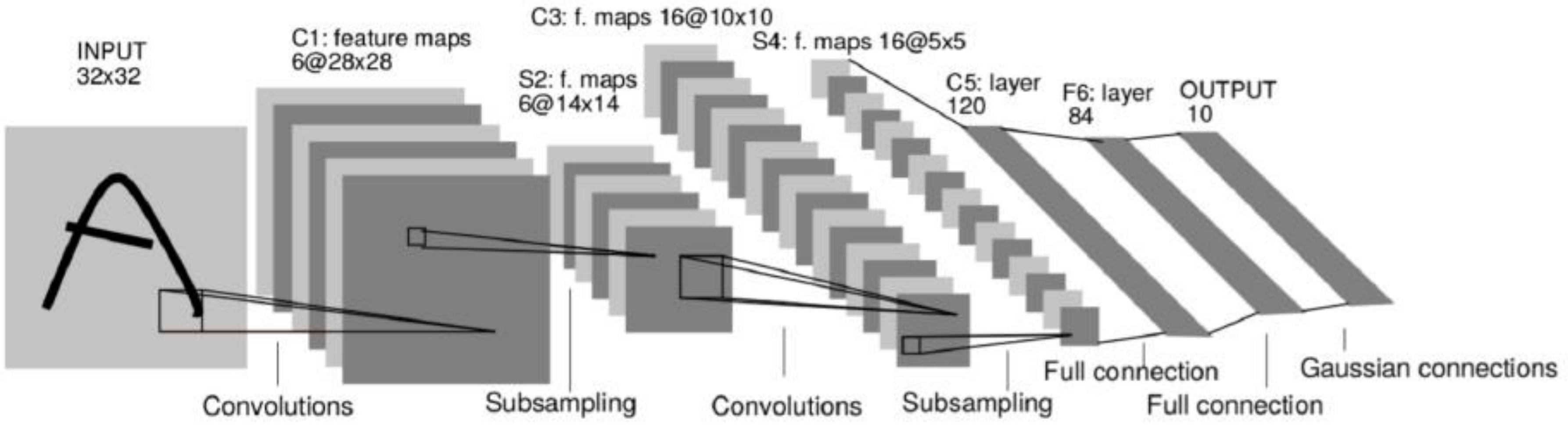


Deep learning w/images

- Convolutional Neural Networks (CNNs)



Convolutional Neural Networks (CNN)



- Coarse of dimensionality
  - Images of ~ 10^6 pixels
    - Very small ratio samples / dimension
  - CNNs useful for high-dimensional problems
    - Locality / Parameter sharing

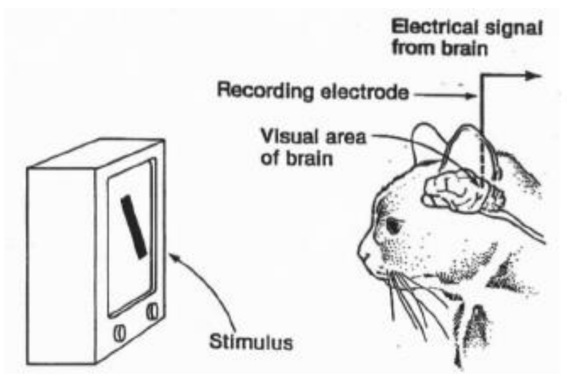
Compositional assumption

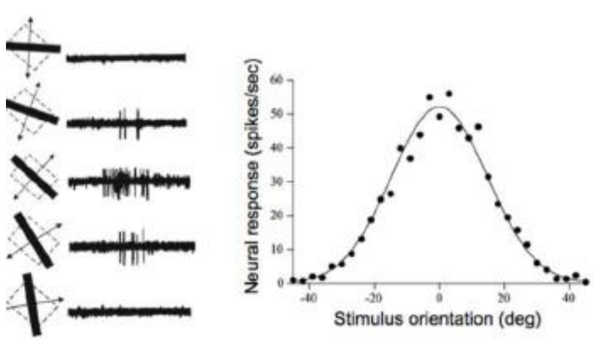
- Data (images, videos, sounds) are compositional
  - They are formed of patterns that are
    - Local
    - Stationary
    - Multi-scale (hierarchical)
- Convolutional neural networks
  - Leverage the compositionality structure of data
  - They extract compositional features

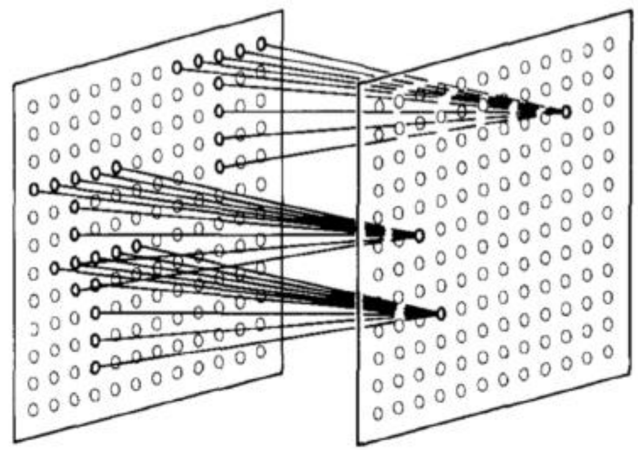
Locality

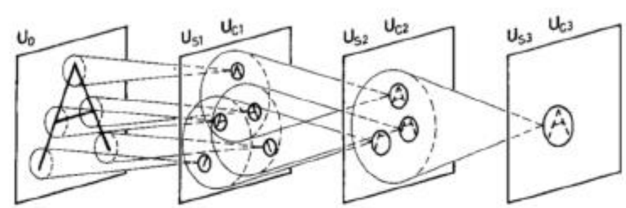
- Local
- Stationary
- Multi-scale (hierarchical)

- Inspired in the visual cortex
- Local receptive fields
  - Activate in the presence of local features





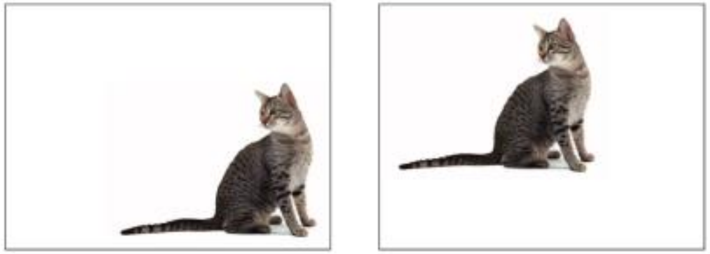




- Local
- Stationary
- Multi-scale (hierarchical)

Stationarity

- Global stationarity
  - Translation invariance

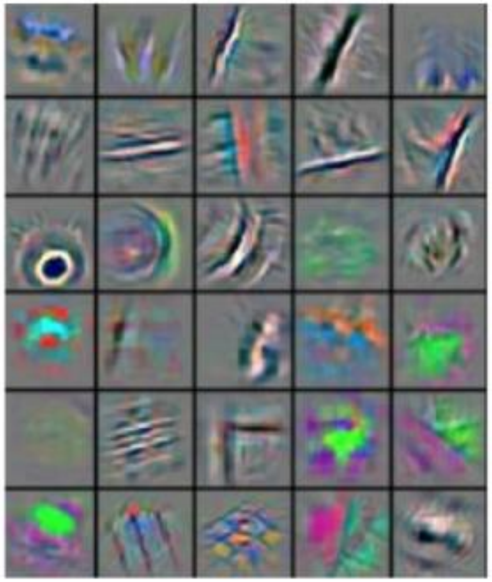
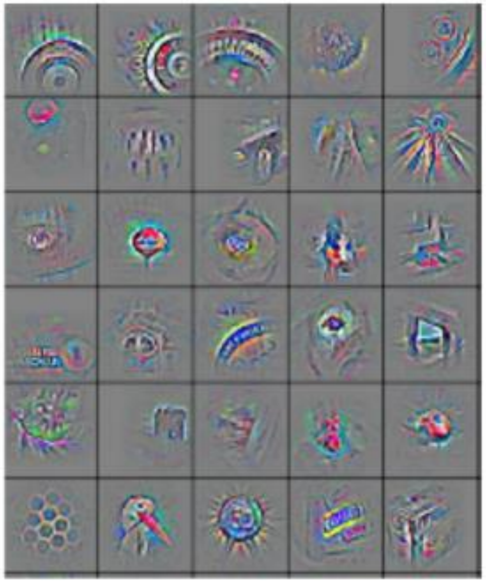


- Local stationarity
  - Similar patches are shared across the data domain
  - Local invariance
  - Good for intra-class variation

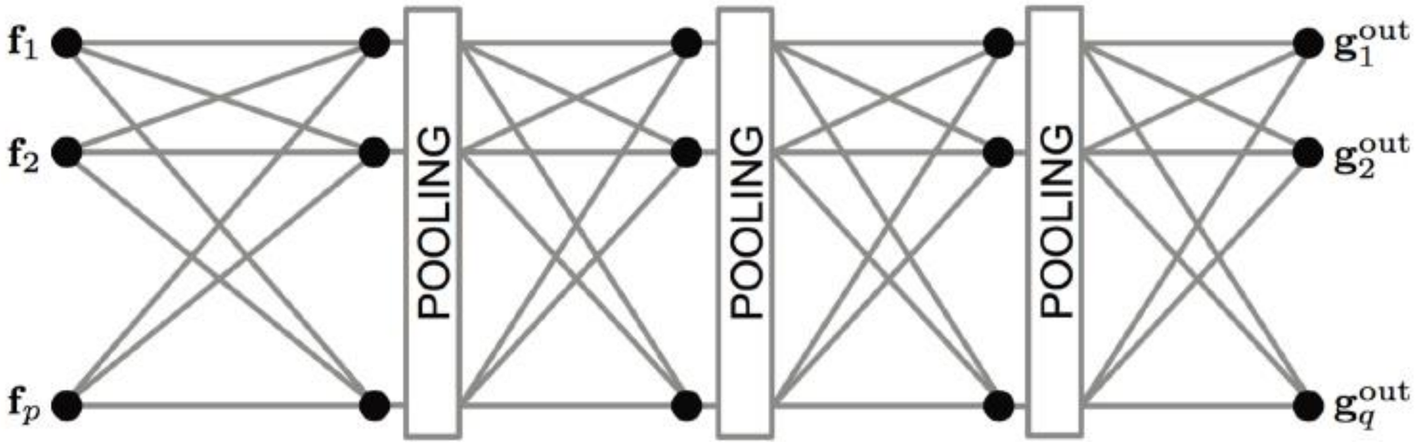
- Local
- Stationary
- Multi-scale (hierarchical)

Multi-scale

- Simple structures can be combined
  - To compose more abstract features
    - Those can be re-combined again in a similar fashion
  - Inspired by the brain
    - Visual primary cortex

Compositional layers



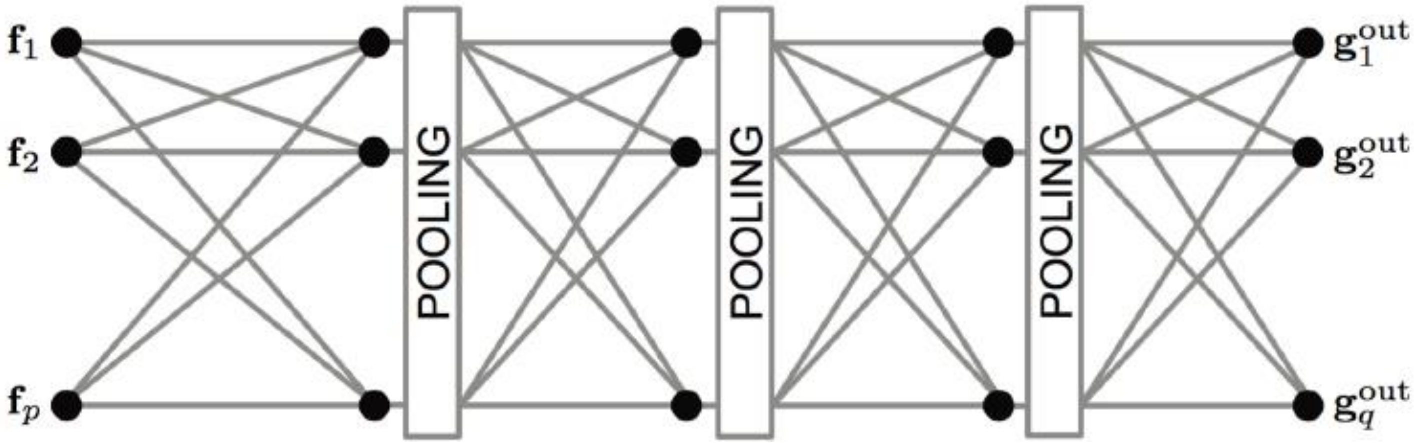
$$\begin{aligned} \mathbf{f}_l &= l\text{-th image feature (R,G,B channels), } \dim(\mathbf{f}_l) = n \times 1 \\ \mathbf{g}_l^{(k)} &= l\text{-th feature map, } \dim(\mathbf{g}_l^{(k)}) = n_l^{(k)} \times 1 \end{aligned}$$

Convolutional layer $\mathbf{g}_l^{(k)} = \xi\left(\sum_{l'=1}^{q_{k-1}} \mathbf{W}_{l,l'}^{(k)} \star \xi\left(\sum_{l'=1}^{q_{k-2}} \mathbf{W}_{l,l'}^{(k-1)} \star \xi\left(\cdots \mathbf{f}_{l'}\right)\right)\right)$

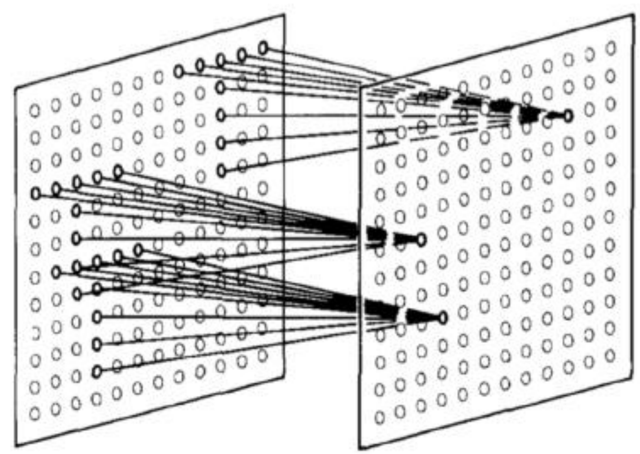
Activation, e.g. $\xi(x) = \max\{x, 0\}$ rectified linear unit (ReLU)

Pooling $\mathbf{g}_l^{(k)}(x) = \|\mathbf{g}_l^{(k-1)}(x') : x' \in \mathcal{N}(x)\|_p \quad p = 1, 2, \text{ or } \infty$

Compositional layers

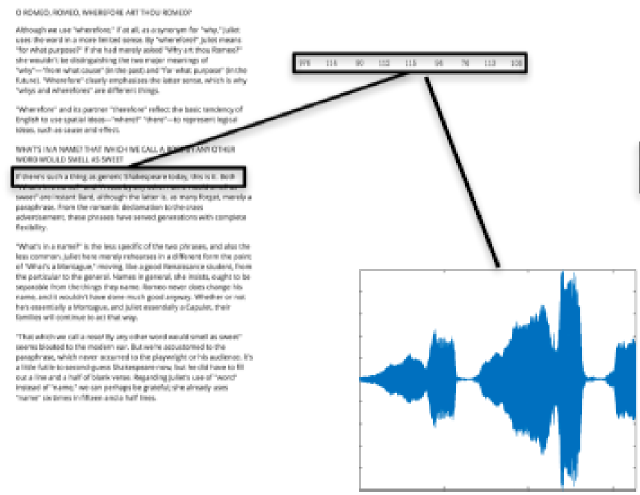


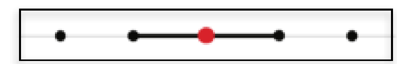
- Convolutional layers
  - Parameters are shared across different "neurons"
  - Huge reduction in computational complexity
    - With respect to Fully-Connected (FC) layers



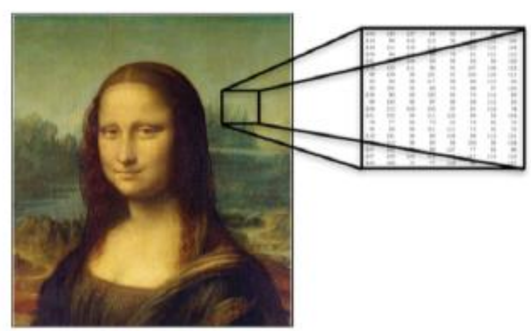
Data domain for CNNs

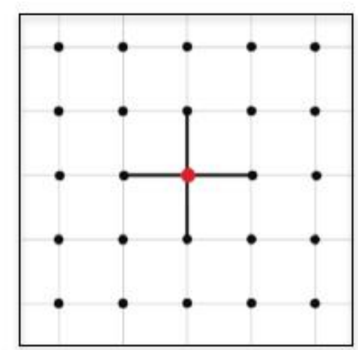
- Domains with regular sampling structures
- 1-D Euclidean domain
  - Sentences, words
  - Sound
- 2-D Euclidean domain
  - Images
- 3-D Euclidean domain
  - Video
  - Volumes





1D grid

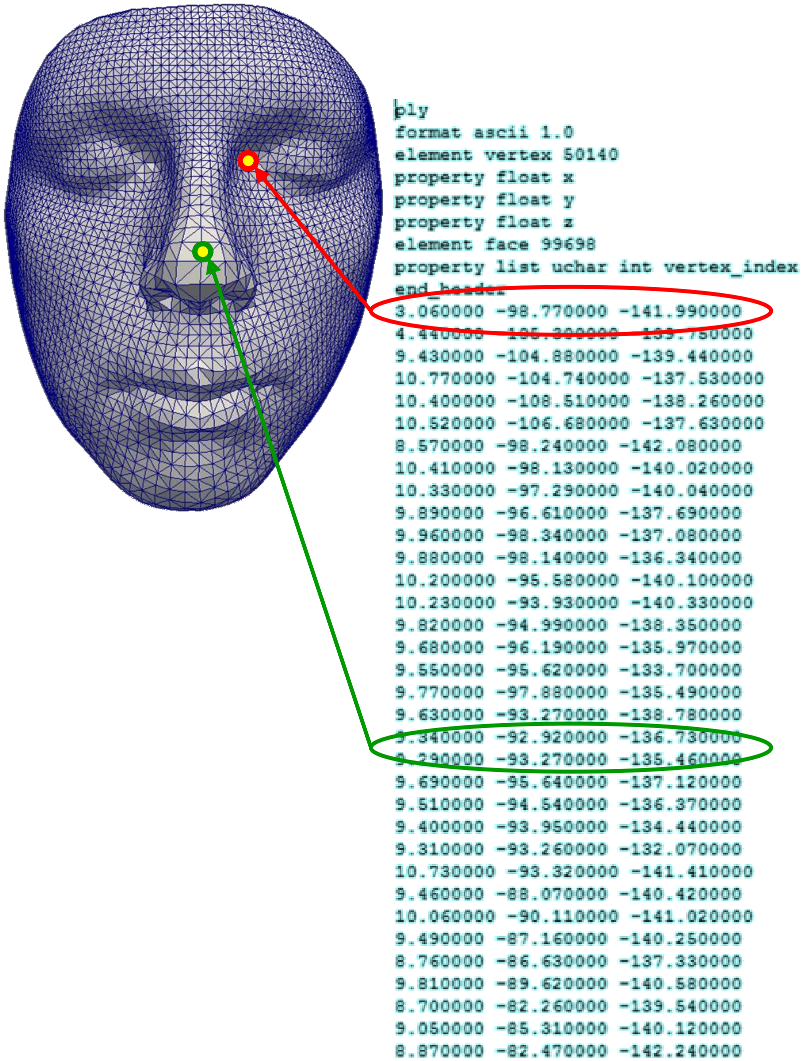


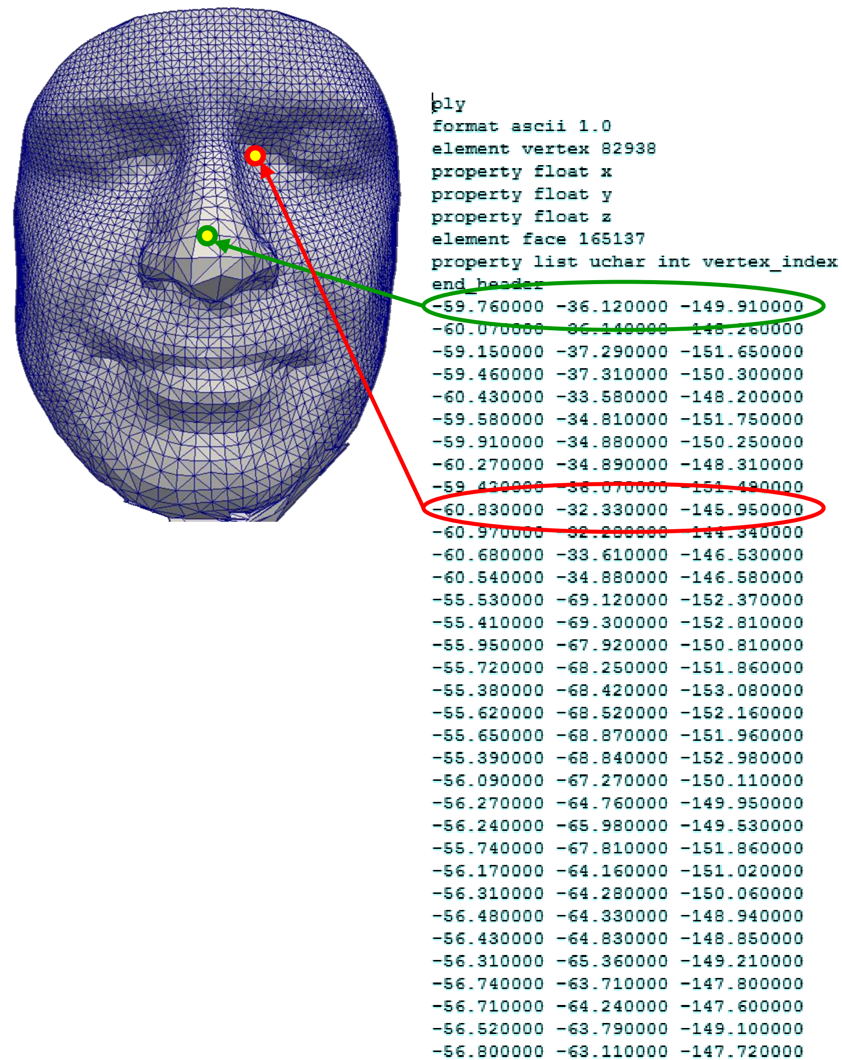


2D grids

How about point clouds?

Input points are inherently not ordered





How about point clouds?

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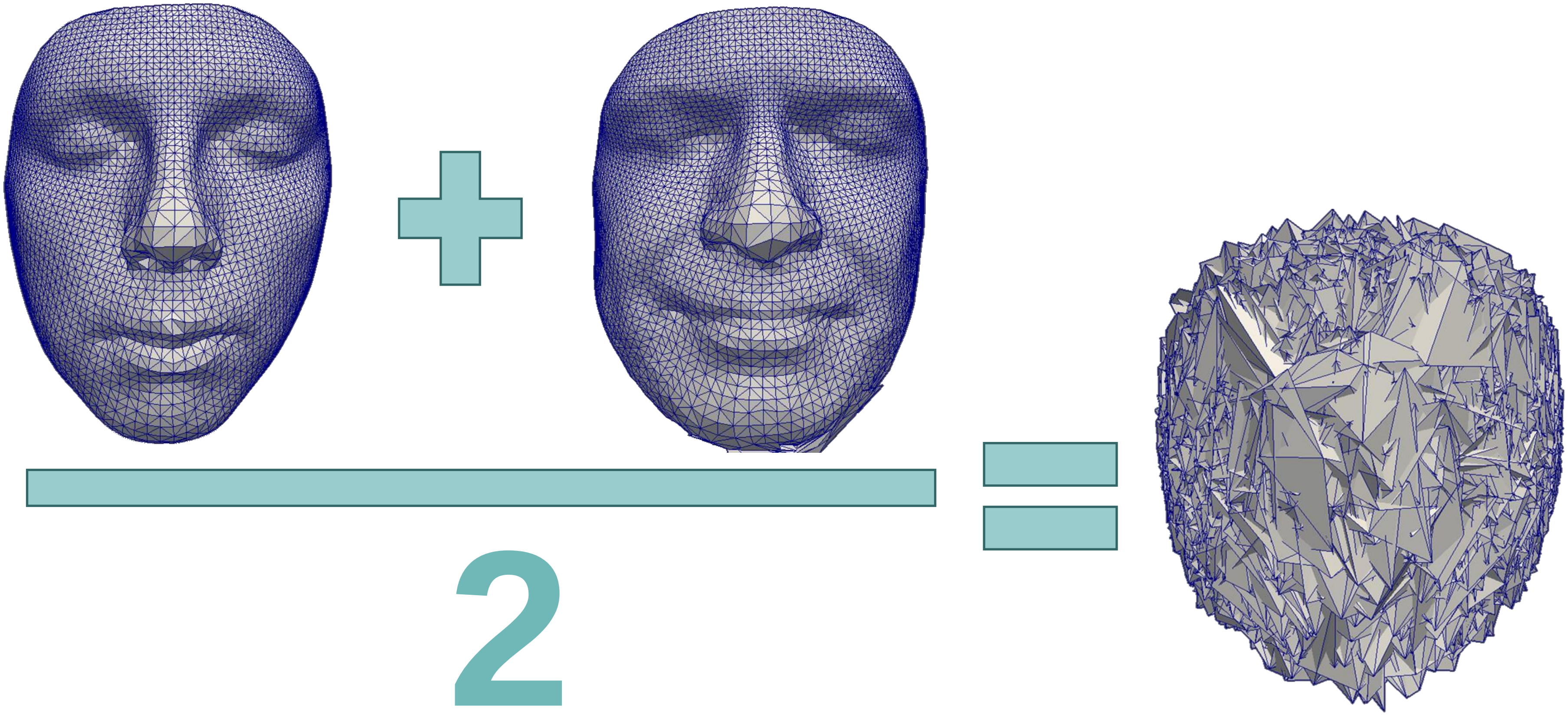


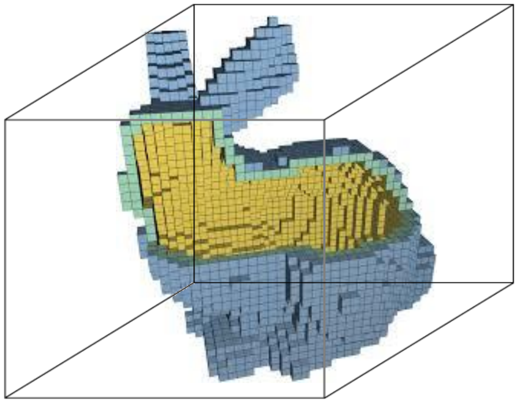
This does not work because surface points are not in correspondence

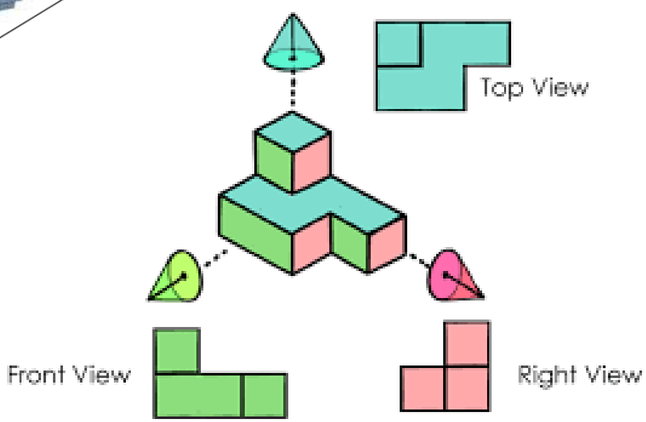
How can we apply DL to point clouds?

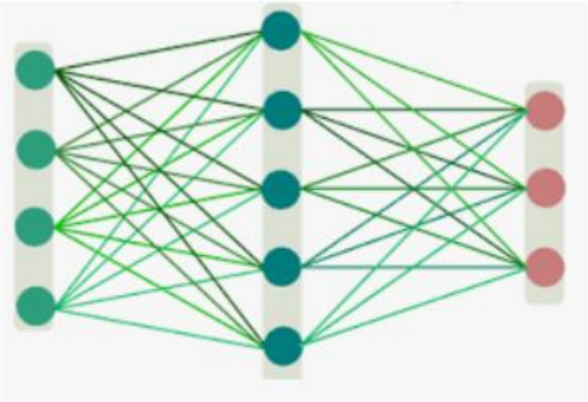
- Transform the representation
  - Voxelization
    - 3D-CNN
  - Projection / rendering
    - 2D-CNN
  - Feature extraction
    - Fully-connected networks
- Networks specifically designed for point clouds
  - PointNet / PointNet++
- Graph Neural Netowkrs
  - Generalization to non-Euclidean sampling grids

DL on point-clouds
Transformed Representations

- Voxelization
  - 3D-CNN
- Projection / rendering
  - 2D-CNN
- Feature extraction
  - Fully-connected networks

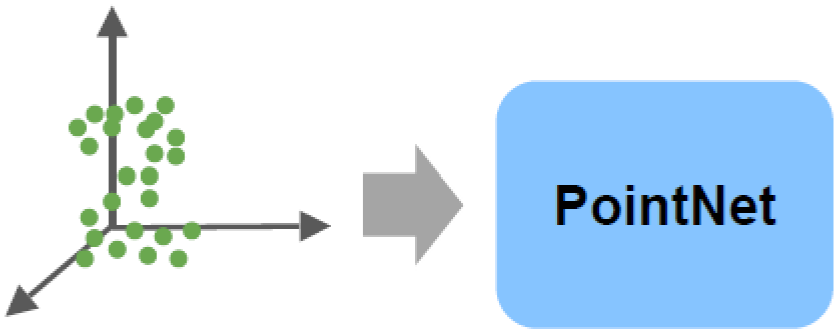


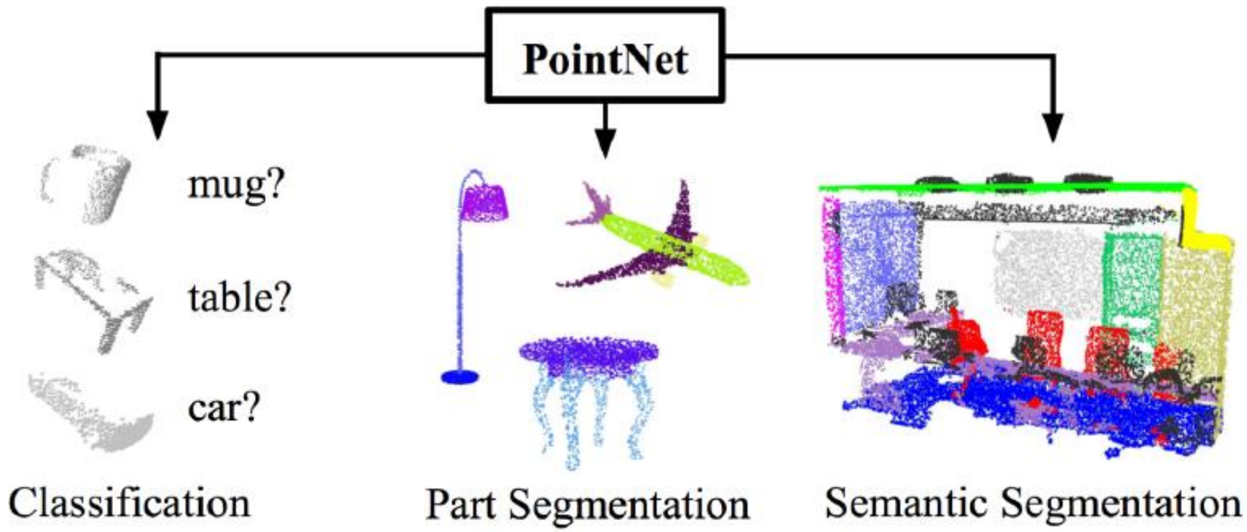




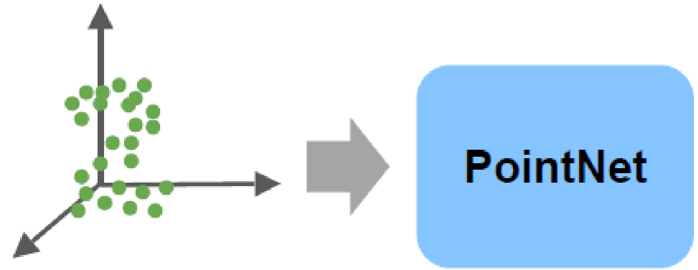
DL on point-clouds: PointNet

- End-to-end learning for point data
  - Scattered
  - Unordered
- Unified framework for various tasks

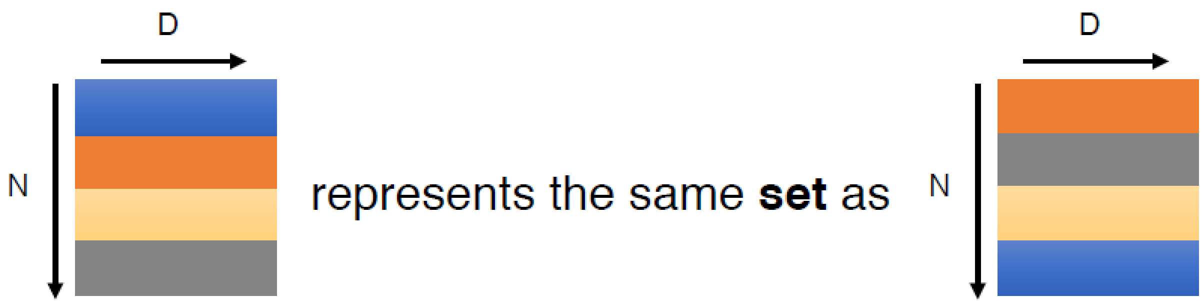




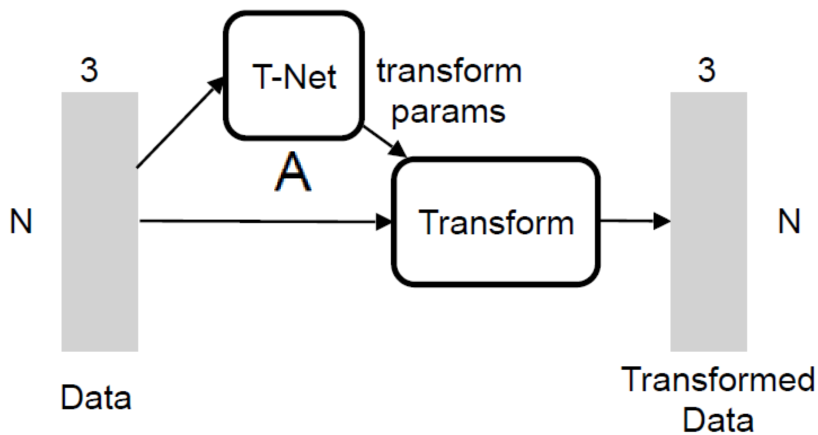
PointNet



- Unordered point set as input
  - The model should be invariant to permutations



- Invariance to rigid transformations

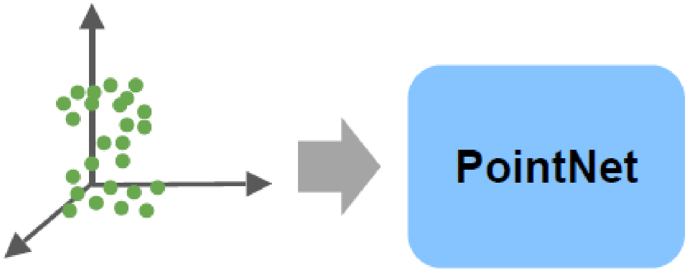


Regularization:

Transform matrix A close to orthogonal:

$$L_{reg} = \|I - AA^T\|_F^2$$

PointNet



- The model should be invariant to permutations

$$f(x_1, x_2, \ldots, x_n) \equiv f(x_{\pi_1}, x_{\pi_2}, \ldots, x_{\pi_n}), \quad x_i \in \mathbb{R}^D$$

  - Examples

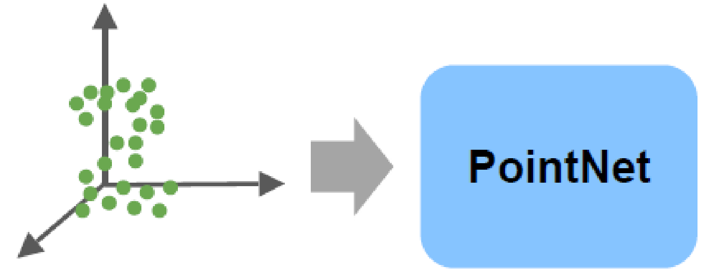
$$f(x_1, x_2, \ldots, x_n) = \max\{x_1, x_2, \ldots, x_n\}$$

$$f(x_1, x_2, \ldots, x_n) = x_1 + x_2 + \ldots + x_n$$

…

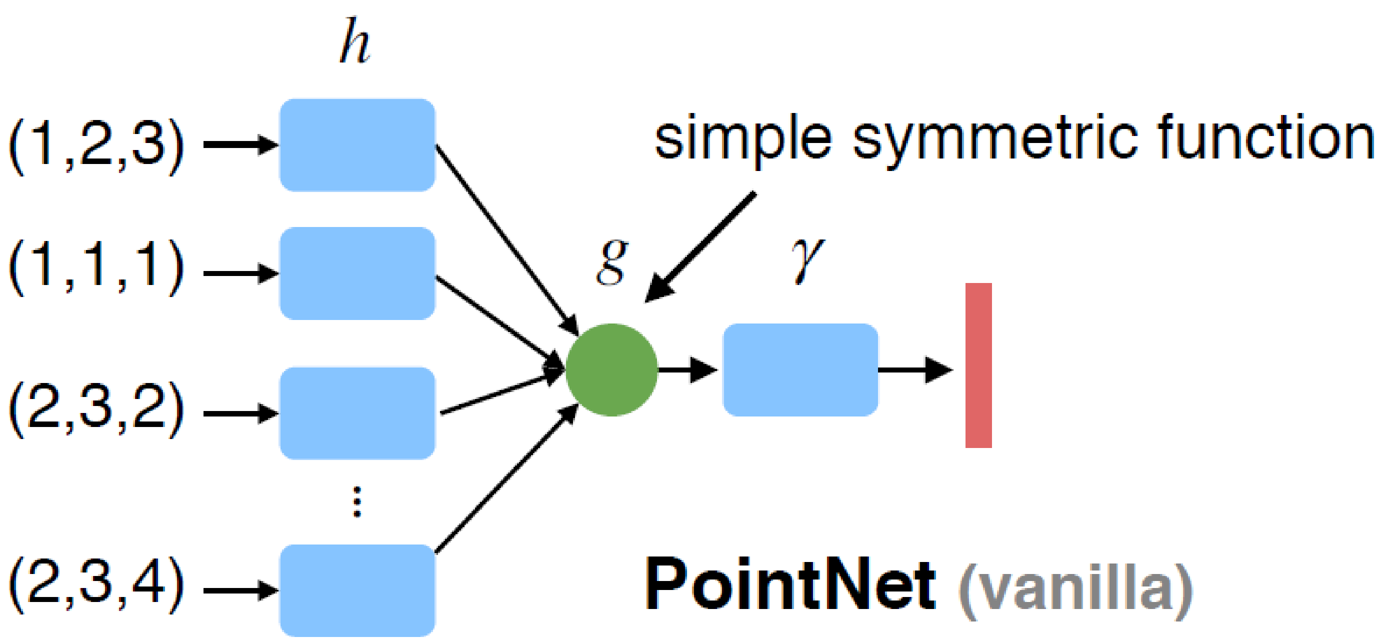
  - Then:
    - How can we construct a family of symmetric functions with neural networks?

PointNet

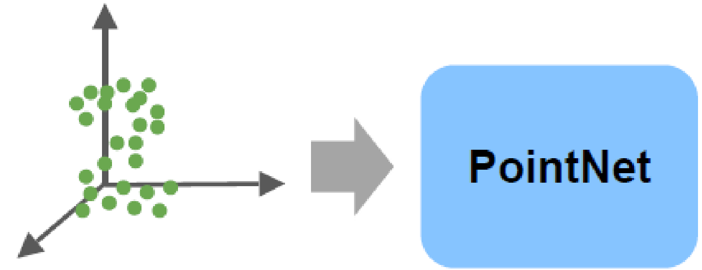


- For the function below
  - f is symmetric if g is symmetric

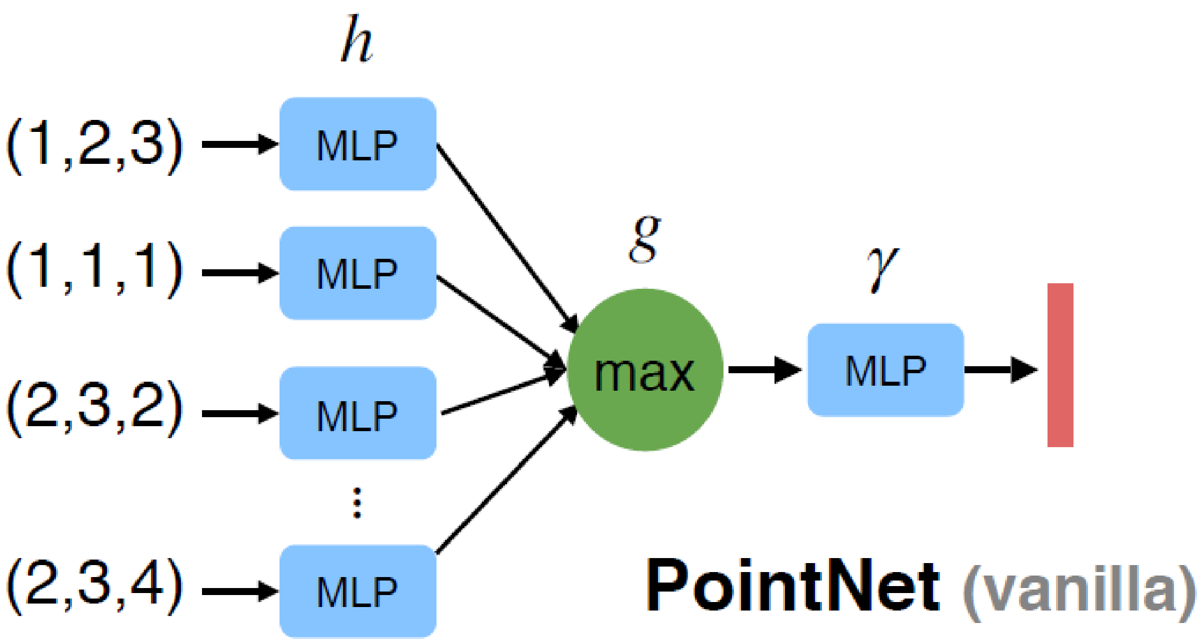
$$f(x_1, x_2, \ldots, x_n) = \gamma \circ g(h(x_1), \ldots, h(x_n))$$



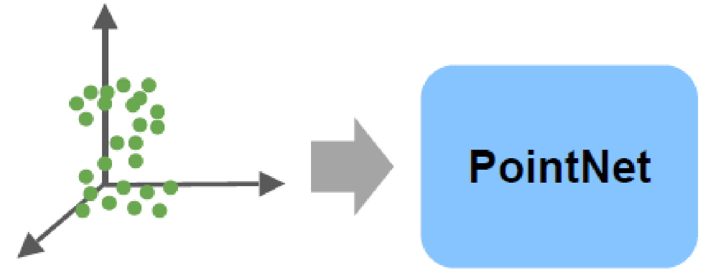
PointNet



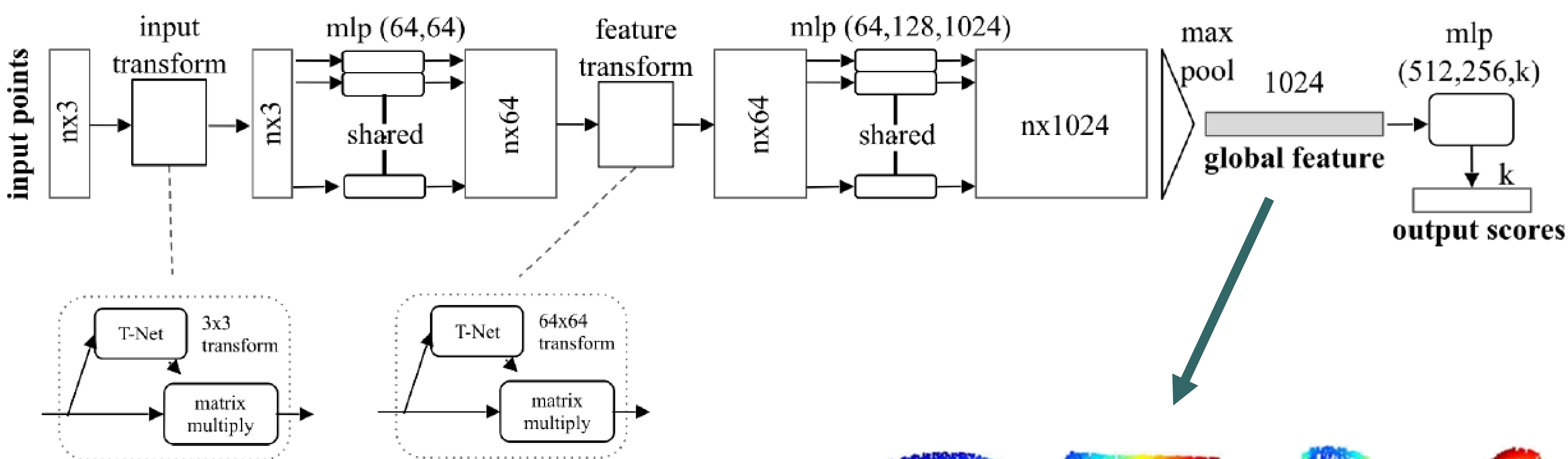
- In PointNet
  - g was chosen to be the MAX function
  - γ was chosen to be a Multi-Layer Perceptron (MLP)

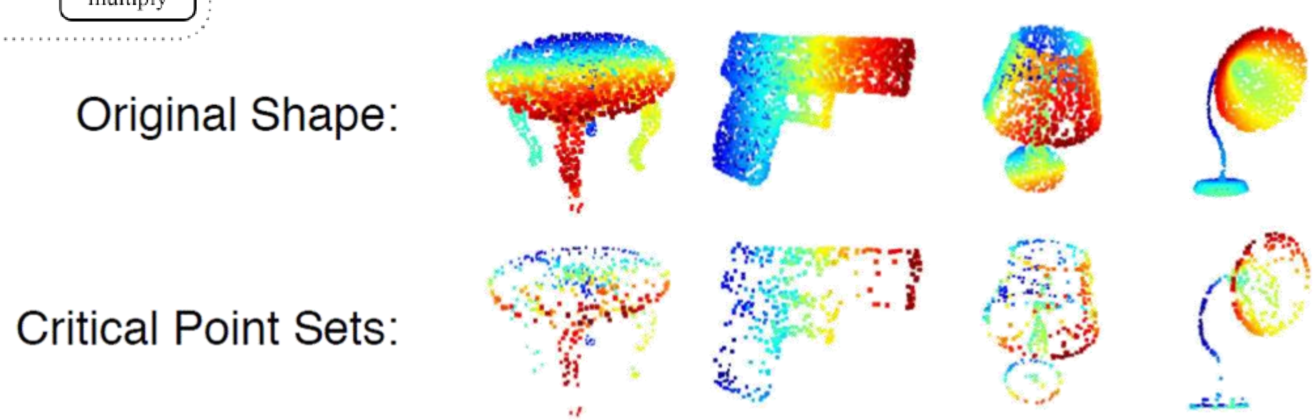


PointNet



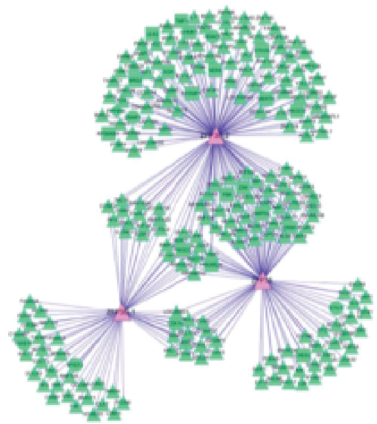
- PointNet architecture



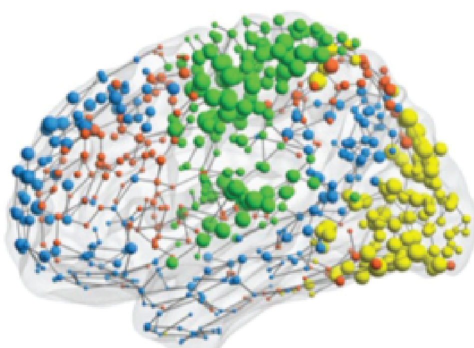


Non-Euclidean data

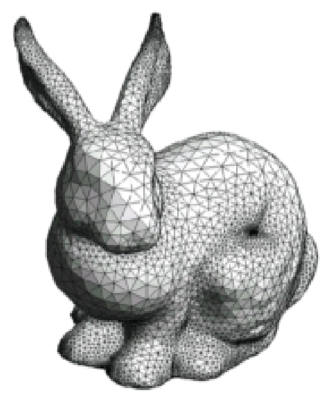
Social networks



Regulatory networks



Functional networks



3D shapes

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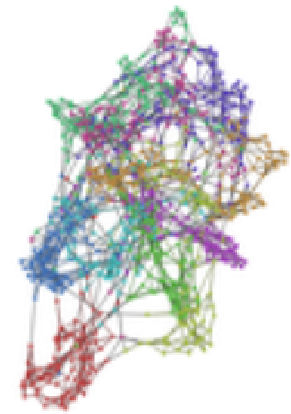
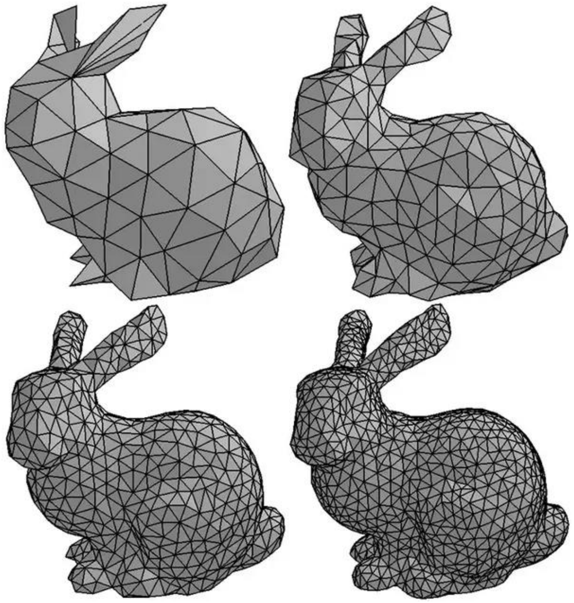


Graphs/ Networks

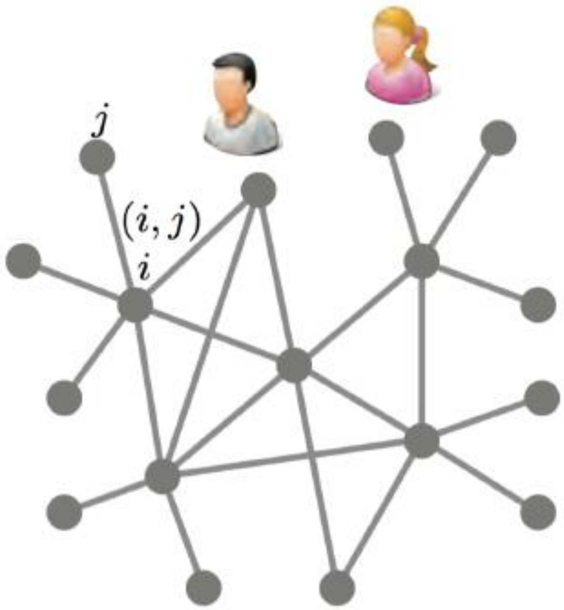
Non-Euclidean data



- Can be handled generically by using graphs

- Graph $\mathcal{G} = (\mathcal{V}, \mathcal{E})$
- Vertices $\mathcal{V} = \{1, \ldots, n\}$
- Edges $\mathcal{E} \subseteq \mathcal{V} \times \mathcal{V}$
- Vertex weights $b_i > 0$ for $i \in \mathcal{V}$
- Edge weights $a_{ij} \geq 0$ for $(i, j) \in \mathcal{E}$
- Vertex fields $L^2(\mathcal{V}) = \{f : \mathcal{V} \to \mathbb{R}^h\}$

  Represented as $\mathbf{f} = (f_1, \ldots, f_n)$

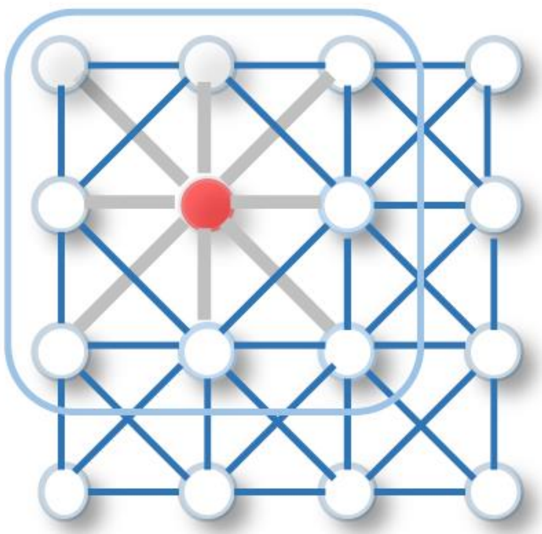


DL in Non-Euclidean data

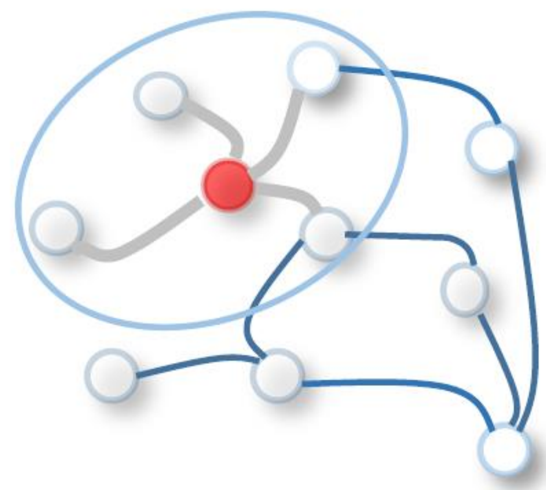
- Assumptions
  - Non-Euclidean data are
    - Locally stationary
    - Compositional
- Challenges
  - How can we extend CNNs to graph-structure data?
    - How can we extend convolutions to graphs?
  - How to define compositionality on graphs?
    - Convolution
    - Pooling
  - How can we make the above operations efficient?
    - Computation in graphs tends to be expensive

DL in Non-Euclidean data

- How about a direct extension based on neighborhoods?
  - Convolution / Pooling



Euclidean neighborhood

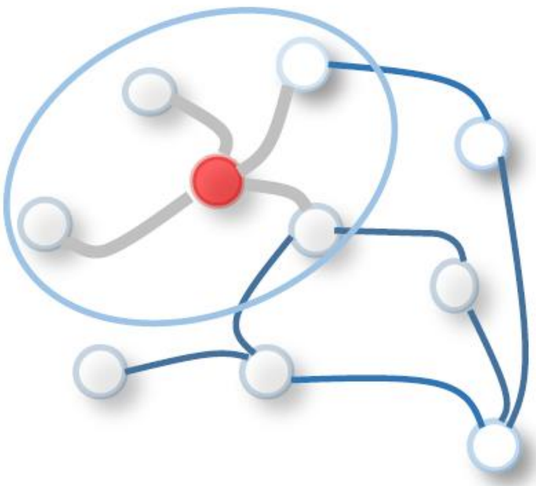


Non-Euclidean neighborhood

DL in Non-Euclidean data

- How about a direct extension based on neighborhoods?
  - Convolution / Pooling

- Numerous disadvantages
  - Non-regular neighborhoods
  - Variable sizes / cardinality
  - Cannot properly order points
  - Cannot share weights
    - Not compositional
    - Not efficient



Non-Euclidean neighborhood

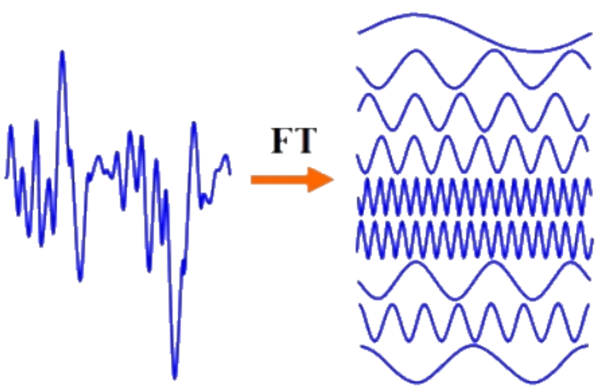
DL in Non-Euclidean data

- How about a direct extension based on neighborhoods?
  - Convolution / Pooling

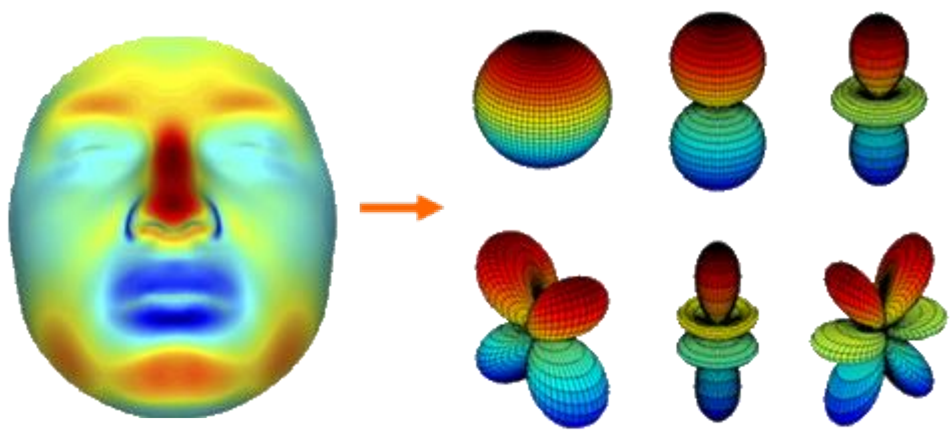
- 3 main solutions have been proposed
  - DL extensions based on RNNs
    - Message passing between neighboring nodes
  - DL extensions based on CNNs
    - Convolutions in the spectral domain
    - Convolutions directly on the graph

Spectral methods on graphs

- Relies on the decomposition of the surface geometry into its spatial frequency components,
  - Much like a Fourier transform for 1D signals



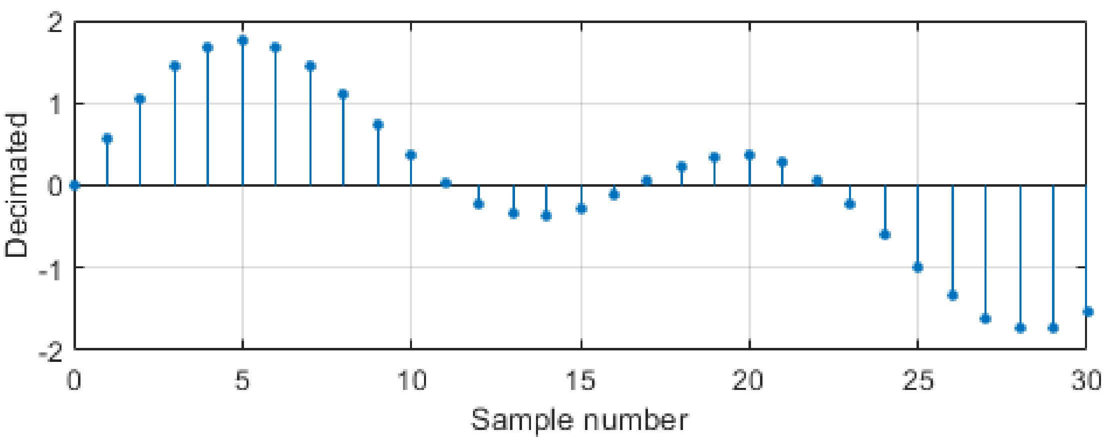
Signal in 1D



Surface in 3D

Spectral methods on graphs

- The spectrum from the Laplacian operator
  - Eigen-decomposition
    - Eigen-values are the spatial frequencies
    - Eigenvectors are the basis functions
  - Illustration from the 1-D case
    - The sampled function is defined over a uniform 1-D grid

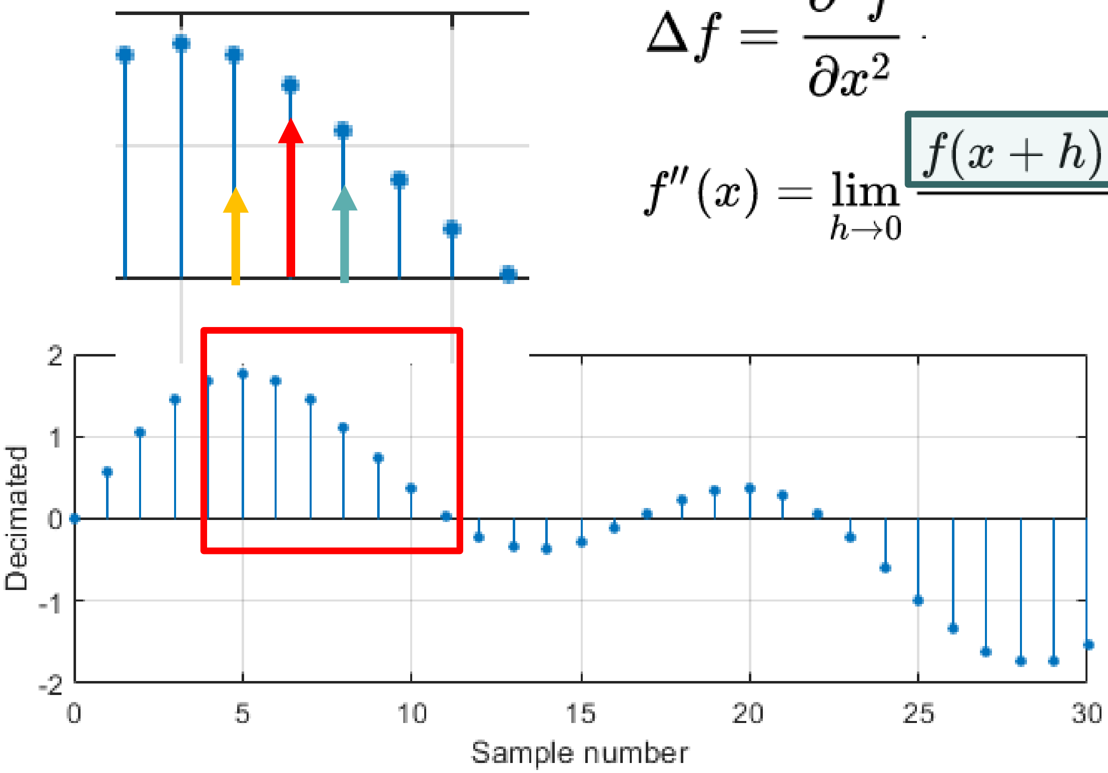


$$\Delta x = -K\,x$$

$$K = \begin{pmatrix} 2 & -1 & & & -1 \\ -1 & 2 & -1 & & \\ & \ddots & \ddots & \ddots & \\ & & -1 & 2 & -1 \\ -1 & & & -1 & 2 \end{pmatrix}$$

Spectral methods on graphs

- Illustration from the 1-D case
  - The sampled function is defined over a uniform 1-D grid



$$\Delta f = \frac{\partial^2 f}{\partial x^2}.$$

$$f''(x) = \lim_{h \to 0} \frac{\boxed{f(x+h)} - \boxed{2f(x)} + \boxed{f(x-h)}}{h^2}.$$

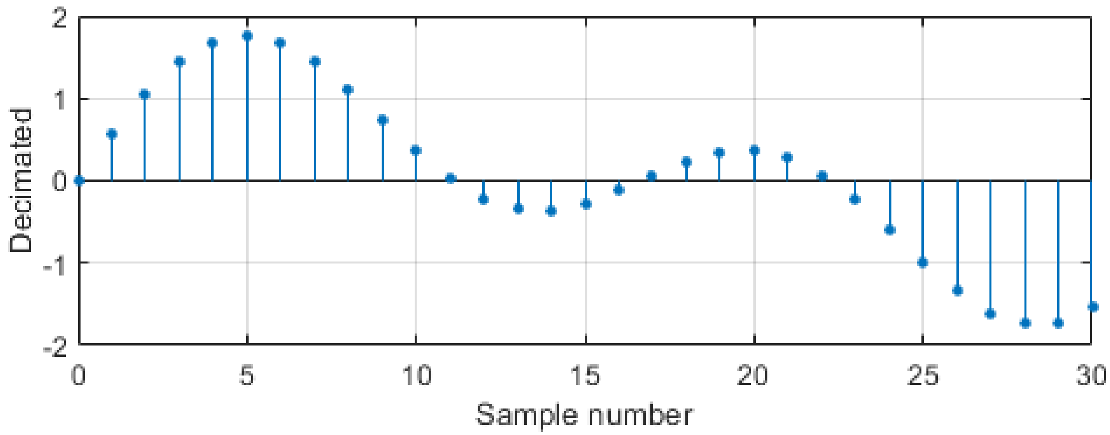
$$\Delta x = -K\,x$$

$$K = \begin{pmatrix} 2 & -1 & & & -1 \\ \boxed{-1} & \boxed{2} & \boxed{-1} & & \\ & \ddots & \ddots & \ddots & \\ & & -1 & 2 & -1 \\ -1 & & & -1 & 2 \end{pmatrix}$$

Spectral methods on graphs

- Illustration from the 1-D case
  - The sampled function is defined over a uniform 1-D grid
  - The eigendecomposition yields

$$\Delta \phi_j = \lambda_j \phi_j \qquad \phi_j : \begin{cases} \sqrt{1/n} & \text{if } j = 1 \\ \sqrt{2/n}\,\sin(2\pi h \lfloor j/2 \rfloor / n) & \text{if } j \text{ is even} \\ \sqrt{2/n}\,\cos(2\pi h \lfloor j/2 \rfloor / n) & \text{if } j \text{ is odd}\,. \end{cases}$$



$$\Delta x = -K\,x$$

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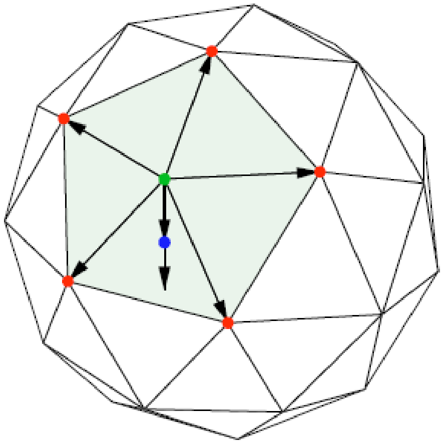
Spectral methods on graphs

- The graph Laplacian
  - Multiple definitions have been proposed
  - The straight-forward generalization is known as the combinatorial Laplacian
    - Also called unnormalized Laplacian



$$\mathbf{\Delta} = \mathbf{D} - \mathbf{A}$$

$$A_{ij} = \begin{cases} 1 & i \text{ and } j \text{ are neighbors} \\ 0 & \text{otherwise} \end{cases}$$

$$D_{ij} = \begin{cases} d_i = |N(i)| & \text{if } i = j, \\ 0 & \text{otherwise.} \end{cases}$$

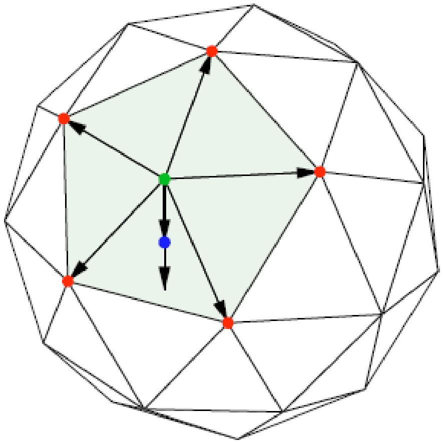
1-D case

$$\boldsymbol{\Delta x} = -K\boldsymbol{x}$$

$$K = \begin{pmatrix} 2 & -1 & & & -1 \\ -1 & 2 & -1 & & \\ & \ddots & \ddots & \ddots & \\ & & -1 & 2 & -1 \\ -1 & & & -1 & 2 \end{pmatrix}$$

Spectral methods on graphs

- The graph Laplacian
  - Multiple definitions have been proposed
  - The straight-forward generalization is known as the combinatorial Laplacian
    - Also called unnormalized Laplacian
    - The adjacency can be further generalized to edge weights **W**



$$\mathbf{\Delta} = \mathbf{D} - W$$

$$W_{ij} = w(e_{ij}) = w_{ij}$$

$$w : E \to \mathbb{R}^{+}, \text{ whenever } (i, j) \in E.$$

$$D_{ii} = \sum_{j \in N(i)} w_{ij}.$$

Spectral methods on graphs

- The graph Laplacian
  - Multiple definitions have been proposed
  - The straight-forward generalization is known as the combinatorial Laplacian

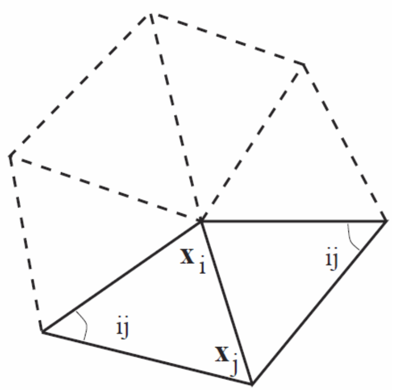
$$\mathbf{\Delta} = \mathbf{D} - \mathbf{A}$$

- Normalized Laplacian

$$\mathbf{\Delta} = \mathbf{I} - \mathbf{D}^{-1/2}\mathbf{A}\mathbf{D}^{-1/2}$$

- Laplace-Beltrami Operator
  - Geometric Laplacian

$$\mathbf{L}(\mathbf{x}_i) = \frac{1 \;\; b_i}{2A_M} \sum_{j \in N_1(\mathbf{x}_i)} \left(\cot\alpha_{ij} + \cot\beta_{ij}\right)\left(\mathbf{x}_i - \mathbf{x}_j\right)$$



Spectral methods on graphs

- The Laplacian on a graph of n vertices
  - Can be decomposed in n eigenvectors

$$\boldsymbol{\Delta}\phi_k = \lambda_k \phi_k, \quad k = 1, 2, \ldots \qquad \boldsymbol{\Delta} = \boldsymbol{\Phi}^T \boldsymbol{\Lambda} \boldsymbol{\Phi}$$

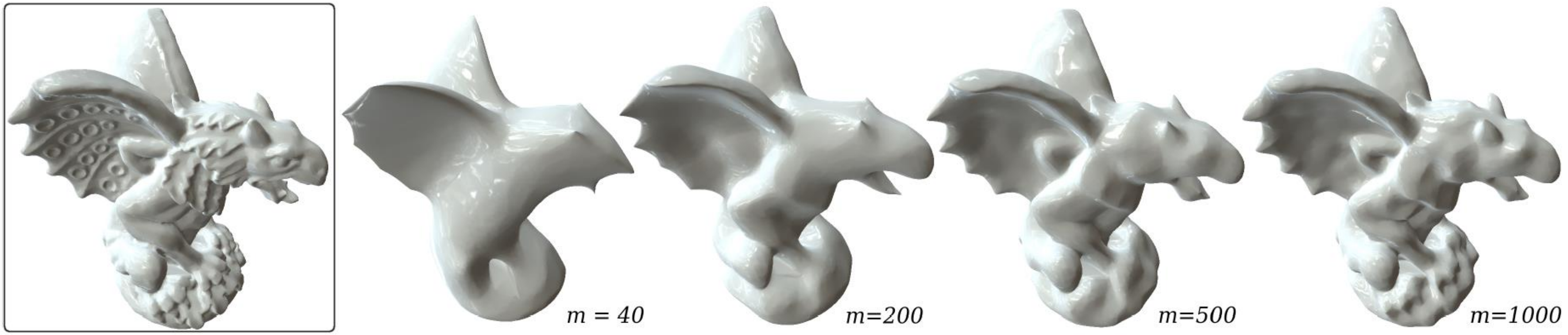
  - Eigenvectors are real and orthonormal

$$\langle \phi_k, \phi_{k'} \rangle_{L^2(\mathcal{V})} = \delta_{kk'}$$

  - The eigenvectors of the Lalpacian are analogous to the Fourier basis functions on the graph
    - Later, we take advantage of this and use the **convolution theorem**

Spectral methods on graphs

- Have been applied to a wide variety of problems
  - Mesh segmentation & correspondence
  - Surface smoothing and reconstruction
  - Watermarking



Reconstructions obtained with an increasing number of eigenfunctions.

Spectral convolution

- Given two continuous functions f, g
  - Their convolution defined as

$$(f \star g)(x) = \int_{-\pi}^{\pi} f(x')g(x - x')dx'$$

  - Maps into a product in the Fourier domain

$$\mathcal{F}\{f \star g\} = \mathcal{F}\{f\} \cdot \mathcal{F}\{g\}$$

- In the case of discrete signals (vectors)

$$\mathbf{f} = (f_1, \ldots, f_n)^\top \text{ and } \mathbf{g} = (g_1, \ldots, g_n)^\top$$

$$\mathbf{f} \star \mathbf{g} \quad = \quad \mathbf{\Phi}\left(\mathbf{\Phi}^\top \mathbf{g} \circ \mathbf{\Phi}^\top \mathbf{f}\right)$$

Fourier basis

Spectral convolution

- In graphs, we work ***by analogy*** to the discrete case

$$\mathbf{f} = (f_1, \ldots, f_n)^\top \text{ and } \mathbf{g} = (g_1, \ldots, g_n)^\top$$

$$\mathbf{f} \star \mathbf{g} \quad = \quad \mathbf{\Phi}(\mathbf{\Phi}^\top \mathbf{g} \circ \mathbf{\Phi}^\top \mathbf{f})$$

- Where the Fourier basis comes from the Laplacian

$$\mathbf{\Delta} = \mathbf{\Phi}^T \mathbf{\Lambda} \mathbf{\Phi}$$

- Therefore

$$\mathbf{f} \star \mathbf{g} \quad = \quad \overset{\mathscr{F}^{-1}}{\boxed{\mathbf{\Phi}}}(\underbrace{\overset{\mathscr{F}}{\boxed{\mathbf{\Phi}^\top}}\mathbf{g}}_{\hat{g}_\theta(\Lambda) = \mathrm{diag}(\theta)} \circ \overset{\mathscr{F}}{\boxed{\mathbf{\Phi}^\top}}\mathbf{f})$$

$$= \quad \mathbf{\Phi}\hat{g}(\mathbf{\Lambda})\mathbf{\Phi}^\top \mathbf{f}$$

$\theta \in \mathbb{R}^n$ is a vector of Fourier coefficients

Spectral convolution

- In graphs, we work ***by analogy*** to the discrete case

$$\mathbf{f} = (f_1, \ldots, f_n)^\top \text{ and } \mathbf{g} = (g_1, \ldots, g_n)^\top$$

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- Theretore

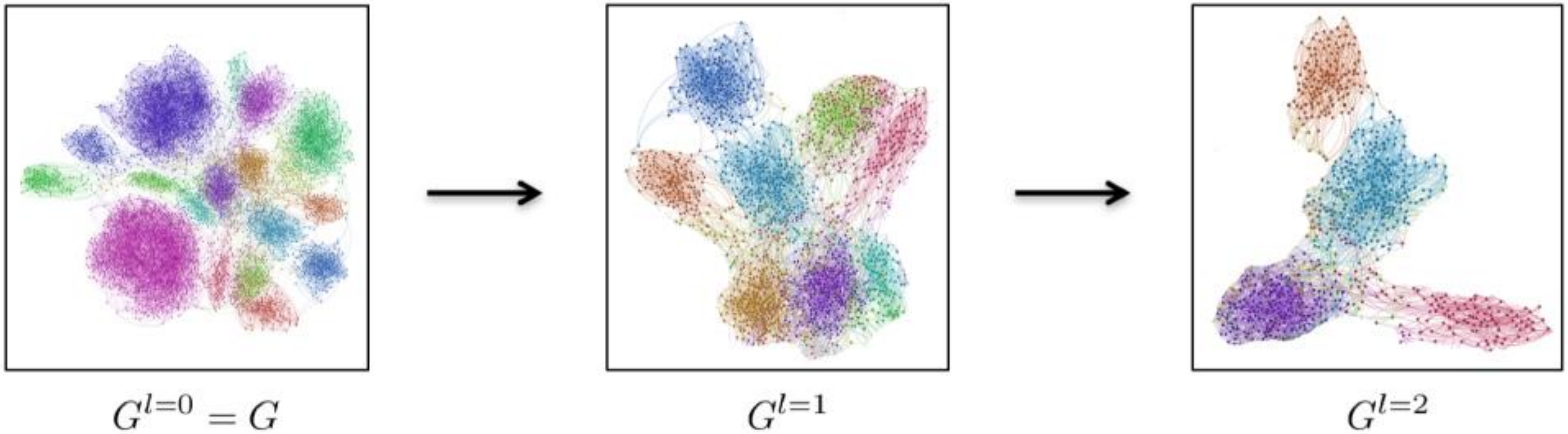
$$\mathbf{f} \star \mathbf{g} \quad = \quad \mathbf{\Phi}\,(\underbrace{\mathbf{\Phi}^\top \mathbf{g}}_{\hat{g}_\theta(\Lambda) = \mathrm{diag}(\theta)} \circ \mathbf{\Phi}^\top \mathbf{f})$$

$$= \quad \mathbf{\Phi} \hat{g}(\mathbf{\Lambda}) \mathbf{\Phi}^\top \mathbf{f} = \hat{g}(\mathbf{\Phi} \mathbf{\Lambda} \mathbf{\Phi}^\top) \mathbf{f} = \hat{g}(\mathbf{\Delta}) \mathbf{f}$$

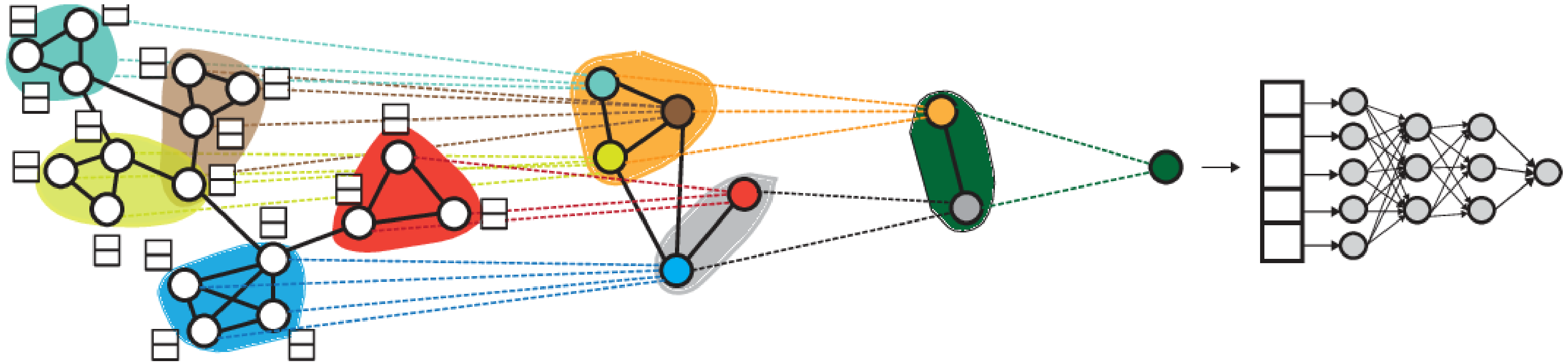
$\theta \in \mathbb{R}^n$ is a vector of Fourier coefficients

Graph pooling

- Equivalent to graph downsampling
  - Graph coarsening
  - Graph partitioning
  - Lots of research
  - But NP-hard problem



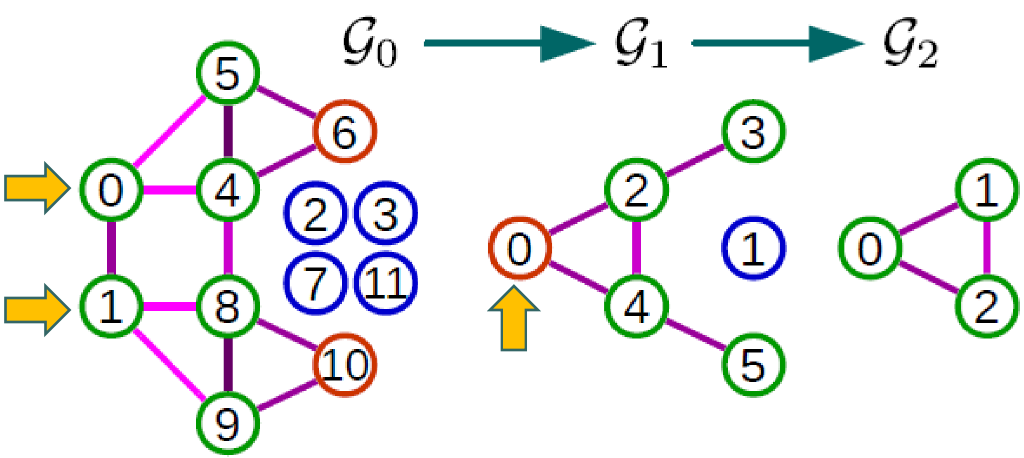
Graph pooling

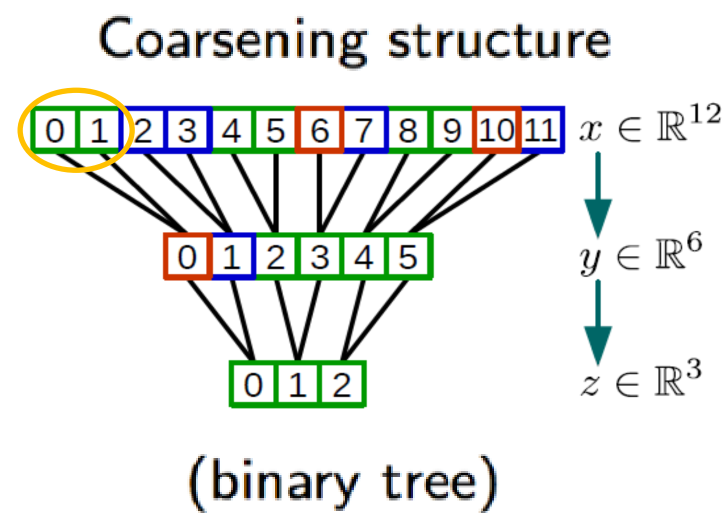


- Approximate solutions
  - Not guaranteed to be optimal
  - But often suffice for our needs
- Structured pooling
  - Arrangement of the node indexing
  - Adjacent nodes are hierarchically merged

Graph pooling

- Structured pooling
  - Arrangement of the node indexing
  - Adjacent nodes are hierarchically merged
    - Requires adding “ghost” nodes
  - As efficient as a 1D-Euclidean grid pooling





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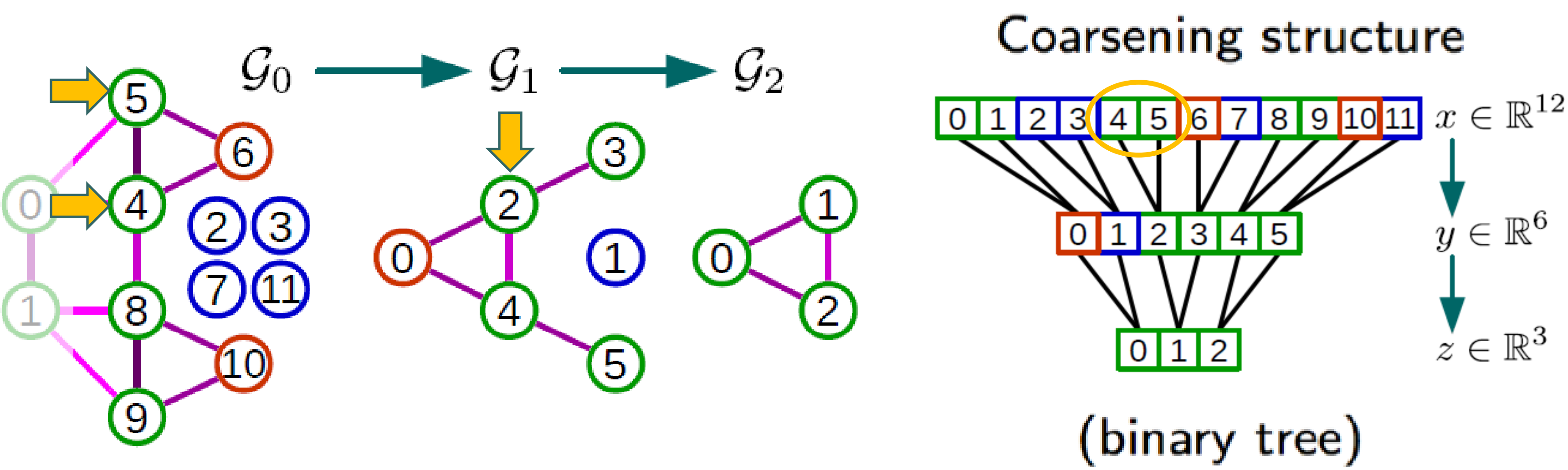

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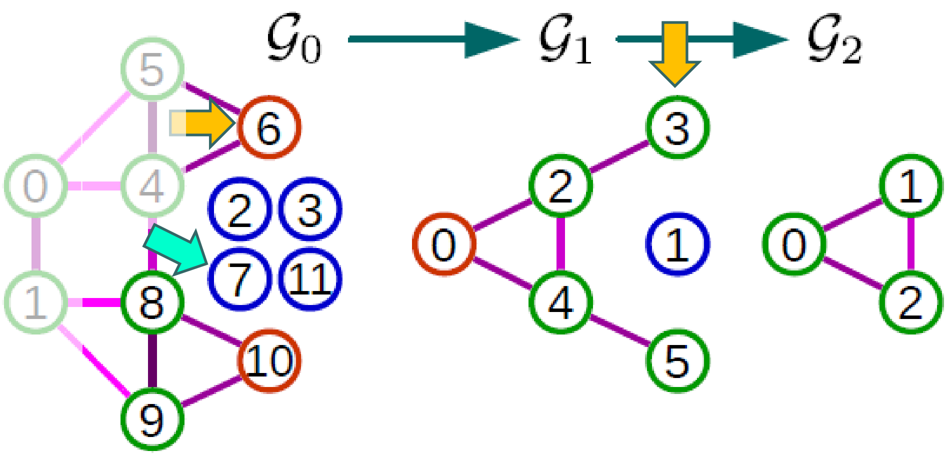

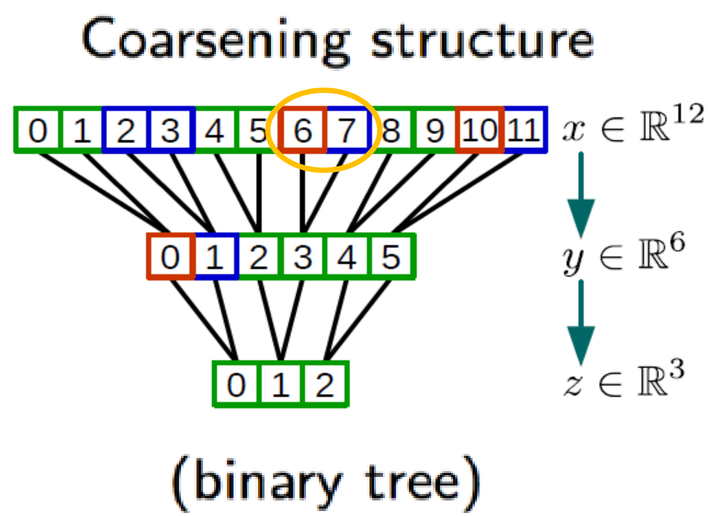

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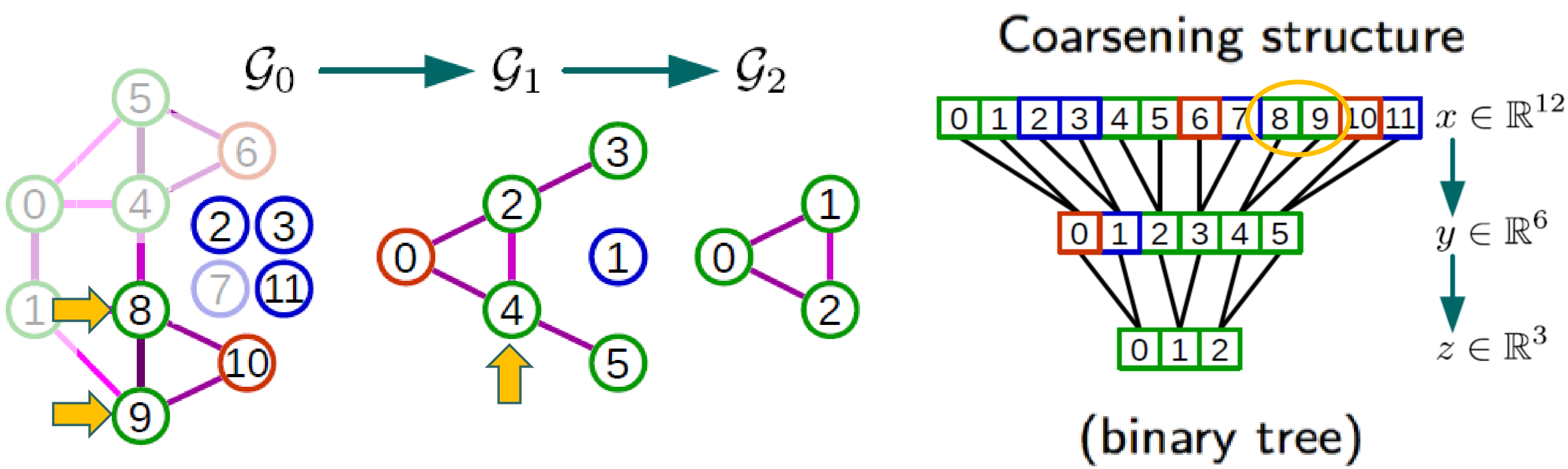

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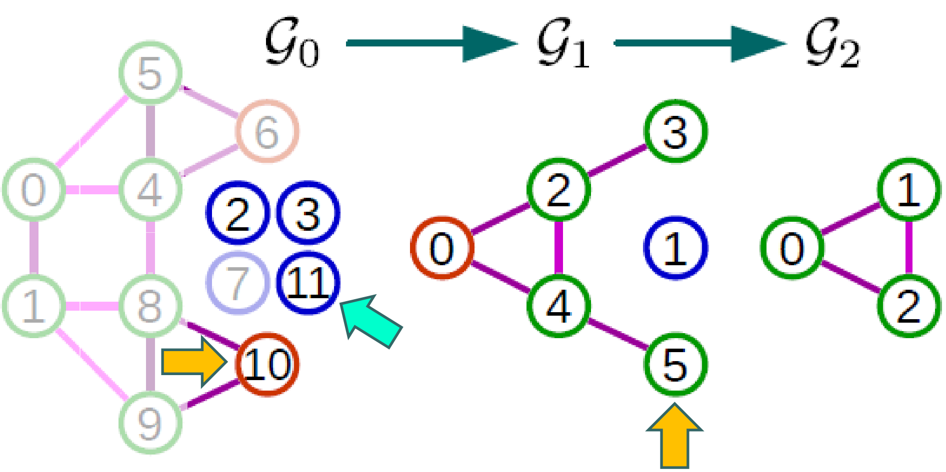

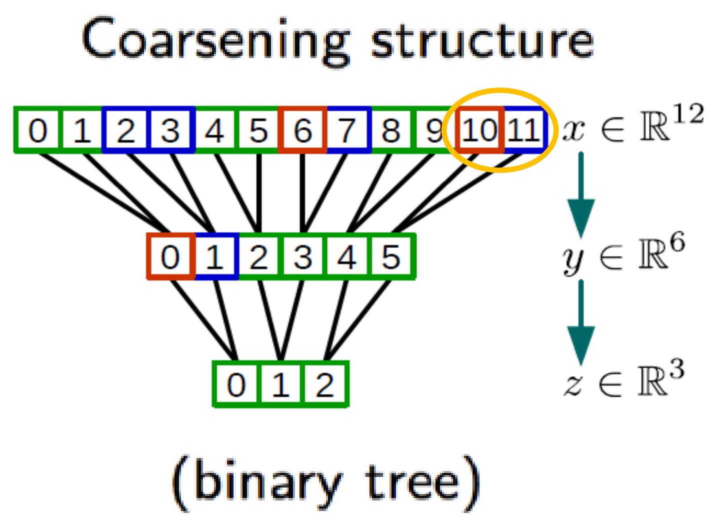

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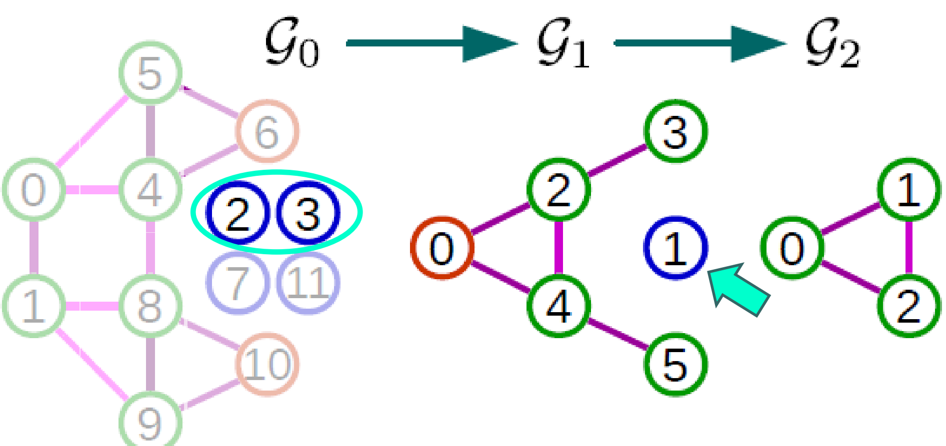
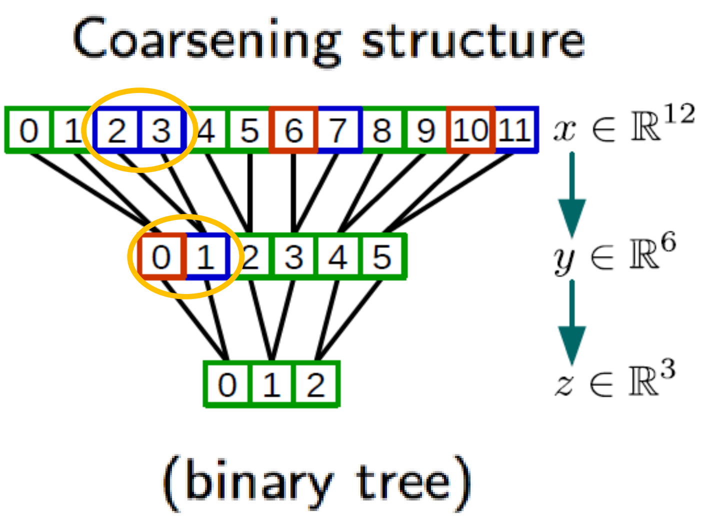
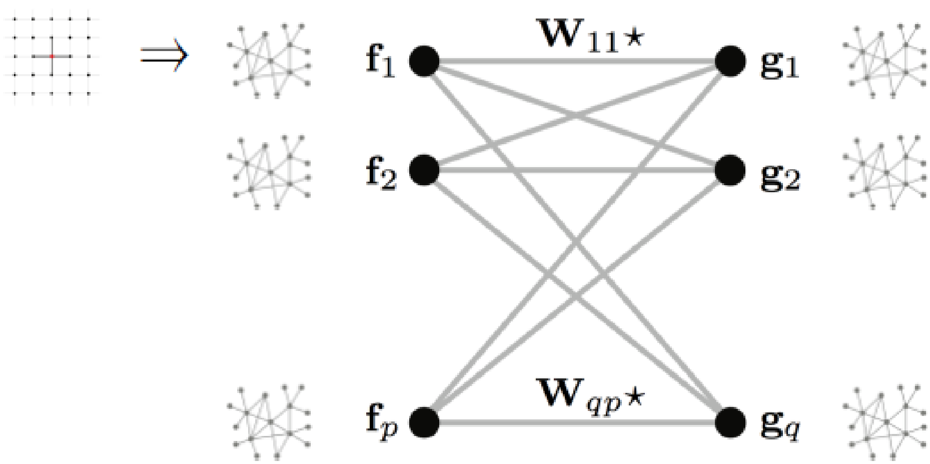




Vanilla graph CNNs

- Graph convolutional layer

$$\begin{aligned} \mathbf{f}_l &= l\text{-th data feature on graphs, } \dim(\mathbf{f}_l) = n \times 1 \\ \mathbf{g}_l &= l\text{-th feature map, } \dim(\mathbf{g}_l) = n \times 1 \end{aligned}$$



Conv. layer $\qquad \mathbf{g}_l = \xi\left(\sum_{l'=1}^{p} \mathbf{W}_{l,l'} \star \mathbf{f}_{l'}\right)$

Activation, e.g. $\quad \xi(x) = \max\{x, 0\}$ $\quad$ rectified linear unit (ReLU)

Vanilla spectral graph CNNs

- The convolutional layer in the spatial domain

$$\mathbf{g}_l = \xi\left(\sum_{l'=1}^{p} \mathbf{W}_{l,l'} \star \mathbf{f}_{l'}\right)$$

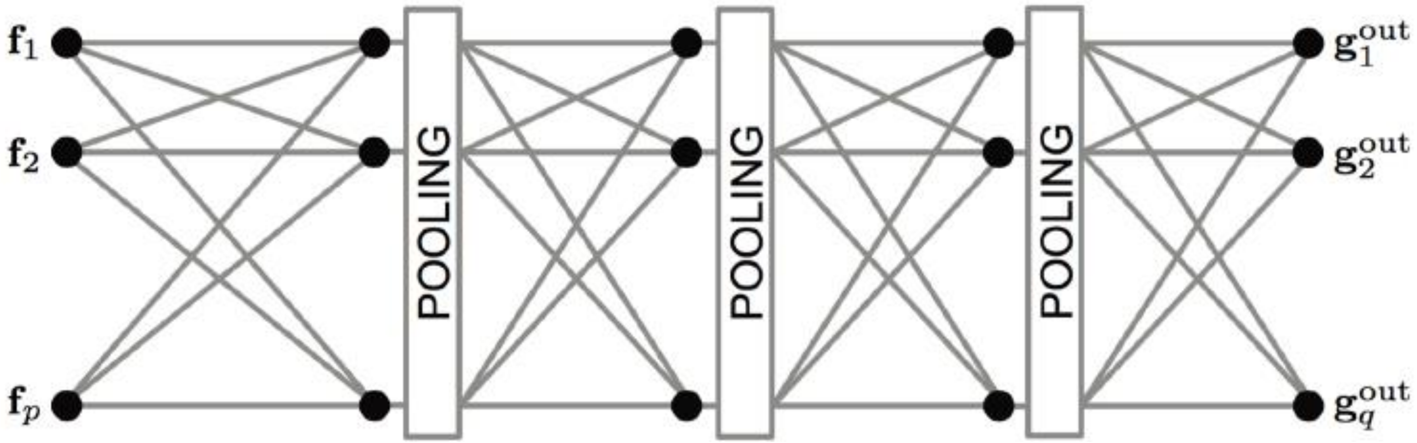
- Can be replaced by a filter expressed in the spectral domain

$$\mathbf{g}_l = \xi\left(\sum_{l'=1}^{p} \boxed{\mathbf{W}_{l,l'} \star \mathbf{f}_{l'}}\right) \qquad \mathbf{g} \star \mathbf{f} = \mathbf{\Phi}\, \hat{g}(\mathbf{\Lambda})\mathbf{\Phi}^\top \mathbf{f}$$

$$\mathbf{\Phi}\hat{\mathbf{W}}_{l,l'}\mathbf{\Phi}^\top \mathbf{f}_{l'}$$

- $(n \times n)$ diagonal matrix
- Filter coefficients in the spectral domain

Graph Compositional layers



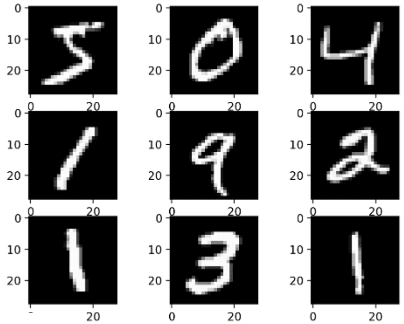
$$\begin{aligned} \mathbf{f}_l &= l\ l\text{-th data feature on graphs, } \dim(\mathbf{f}_l) = n \times 1 \\ \mathbf{g}_l^{(k)} &= l\ l\text{-th feature map, } \dim(\mathbf{g}_l) = n \times 1 \end{aligned}$$

Convolutional layer $\quad \mathbf{g}_l^{(k)} = \xi \left(\sum_{l'=1}^{q^{(k-1)}} \mathbf{\Phi} \widehat{\mathbf{W}}_{l,l'}^{(k)} \mathbf{\Phi}^\top \underbrace{\mathbf{g}_{l'}^{(k-1)}}_{\mathbf{f}_l} \right)$

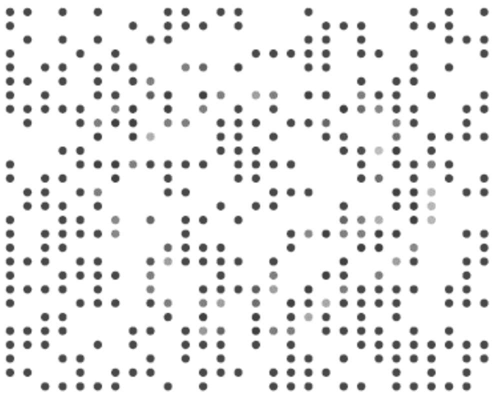
Activation, e.g. $\quad \xi(x) = \max\{x, 0\}$ rectified linear unit (ReLU)

Pooling $\quad \mathbf{g}_l^{(k)}(x) = \|\mathbf{g}_l^{(k-1)}(x') : x' \in \mathcal{N}(x)\|_p \quad p = 1, 2, \text{ or } \infty$

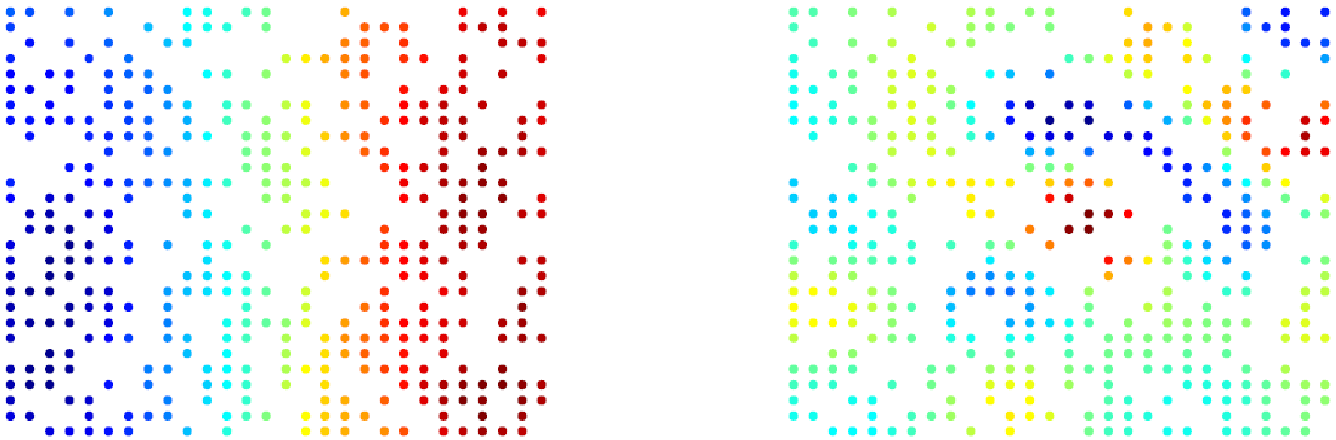
Graph CNNs on a synthesized graph



- MNIST digits database
  - Images were sub-sampled
    - 400 points
    - Non-regular graph



  - Example of the first two eigenvectors of the Laplacian

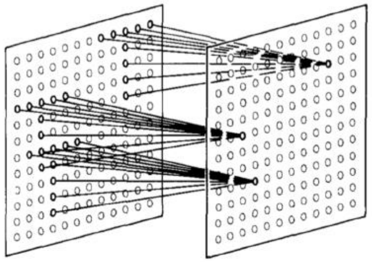


Spectral domain issues

- Direct operation in spectral domain

$$\mathbf{g}_l^{(k)} = \xi \left(\sum_{l'=1}^{q^{(k-1)}} \mathbf{\Phi} \hat{\mathbf{W}}_{l,l'}^{(k)} \mathbf{\Phi}^\top \mathbf{g}_{l'}^{(k-1)} \right)$$

  - Allows to compute convolutions on a graph
  - But is computationally expensive
    - O(n) parameters to be learned in each layer
    - $O(n^2)$ complexity to transform between domains
      - Fourier and invers Fourier
    - $O(n^3)$ complexity for the eigen-decomposition of the Laplacian
  - No guarantee of spatial localization of filters



Toward spatial localization

- Localization in space
  - Implies smoothness in the spectrum
- SplineNet
  - Re-define the spectral filter parameters
    - As linear combinations of smooth kernel functions
    - Based on splines
- ChebNet
  - Re-define the spectral filter parameters
    - With polynomials of the Laplacian eigenvalues

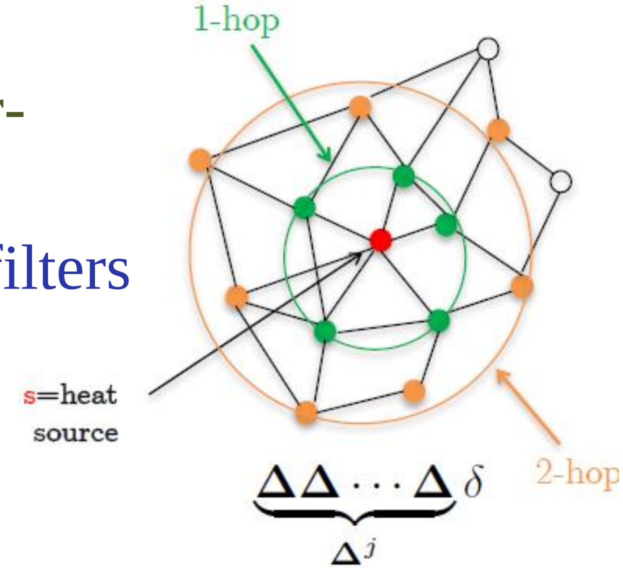
$$w_{\boldsymbol{\alpha}}(\lambda) = \sum_{j=0}^{r} \alpha_j \lambda^j$$

ChebNet

- Re-define the spectral filter parameters
  - With polynomials of the Laplacian eigenvalues

$$w_{\boldsymbol{\alpha}}(\lambda) = \sum_{j=0}^{r} \alpha_j \lambda^j$$

- Spectral filters of this type will be r-localized (in space)
  - Equivalent spatial coefficients beyond r-neighbors will be zero
- Exact control of the spatial support of the filters
- Parameter complexity reduced to O(r)



ChebNet

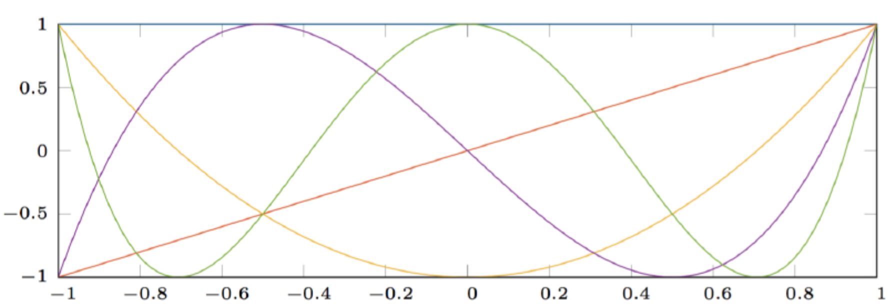
- Chebynet
  - Spectral GCNN $$\mathbf{g}_l^{(k)} = \xi\left(\sum_{l'=1}^{q^{(k-1)}} \mathbf{\Phi}\mathbf{W}_{l,l'}^{(k)}\mathbf{\Phi}^\top \mathbf{g}_{l'}^{(k-1)}\right)$$
  - Spectral polynomials $$\mathbf{g}_l^{(k)} = \xi\left(\sum_{l'=1}^{q^{(k-1)}} w_{\boldsymbol{\alpha}}^{(k)}(\mathbf{\Delta})\,\mathbf{g}_{l'}^{(k-1)}\right)$$
- Therefore
  - ~~O(n) parameters~~ $\Rightarrow$ O(r) parameters
  - ~~$O(n^2)$ complexity to transform between domains~~
    - Reduced to approximately O(n) for sparse graphs
  - ~~$O(n^3)$ complexity for eigen-decomposition of Laplacian~~
    - No need to explicitly compute the spectrum of the graph

6K29VN

ChebNet

- Recursive formulation of filters
  - Using Chebyshev polynomial expansion
  - More stable under perturbations
    - Better behavior for optimization
  - Approximate solution
    - The Laplacian must be scaled appropriately

$$w_{\boldsymbol{\alpha}}(\boldsymbol{\Delta})\mathbf{f} = \sum_{j=0}^{r} \alpha_j \boldsymbol{\Delta}^j \mathbf{f} \quad \Rightarrow \quad w_{\boldsymbol{\alpha}}(\tilde{\boldsymbol{\Delta}})\mathbf{f} = \sum_{j=0}^{r} \alpha_j T_j(\tilde{\boldsymbol{\Delta}})\mathbf{f}$$



T_0, T_1, T_2, T_3

$$T_j(\tilde{\lambda}) = 2\tilde{\lambda}T_{j-1}(\tilde{\lambda}) - T_{j-2}(\tilde{\lambda})$$

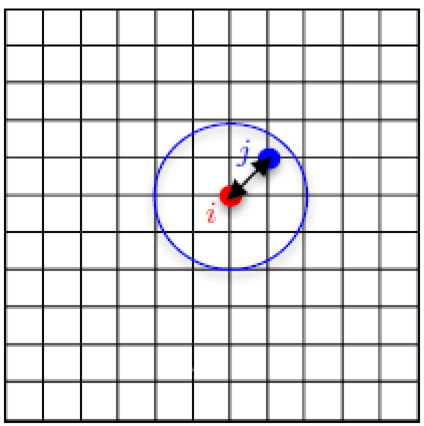
$$T_0(\tilde{\lambda}) = 1, \quad T_1(\tilde{\lambda}) = \tilde{\lambda}$$

Experiments in a Euclidean grid

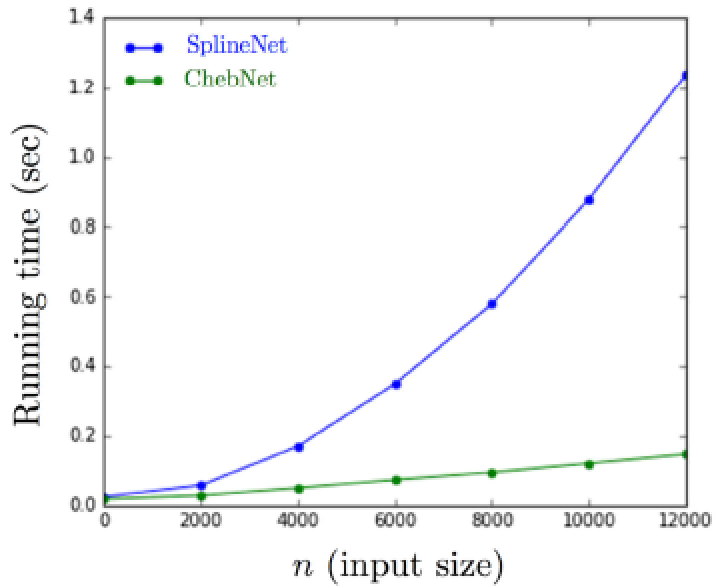
- Digit recognition
  - MNIST database

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

Graph: a 8-NN graph of the Euclidean grid



- Running time



Beyond ChebNet I: CayleyNet

- Some graphs are difficult for ChebNet
  - For example, community graphs
  - In such cases ChebNet requires relatively high-order polynomials

Synthetic graph with 15 communities

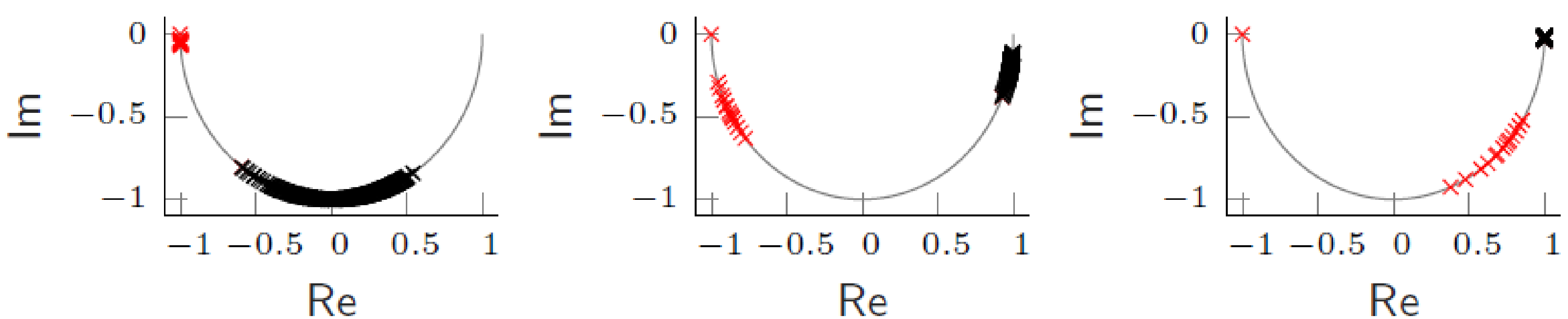
Beyond ChebNet I: CayleyNet

- CayleyNet
  - Use the Cayley transform

$$C(\lambda) = \frac{\lambda - i}{\lambda + i}$$

  - To map the (scaled) eigenvalues of the Laplacian
    - Non-linearly to the unit circle
    - Spectral zoom

$$C(h\lambda) = (h\lambda - i)(h\lambda + i)^{-1}$$



Cayley transform $C(h\lambda)$ for (left-to-right) $h = 0.1$, 1, and 10 of the 15-communities graph Laplacian spectrum

Beyond ChebNet I: CayleyNet

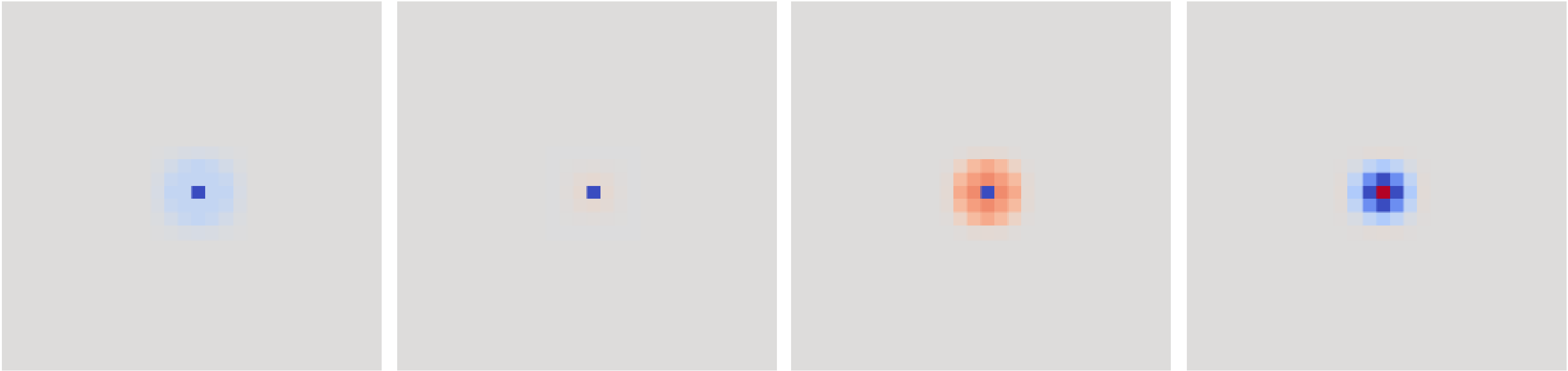
- Cayley polynomials of order r
  - Are a family of real-valued rational functions
  - With complex coefficients

$$\tau_{\mathbf{c}}(h\mathbf{\Delta}) = \mathbf{\Phi}\left(c_0 + \sum_{j=1}^{r} c_j C(h\mathbf{\Lambda})^j + \sum_{j=1}^{r} \bar{c_j} C(h\mathbf{\Lambda})^{-j}\right)\mathbf{\Phi}^T =$$

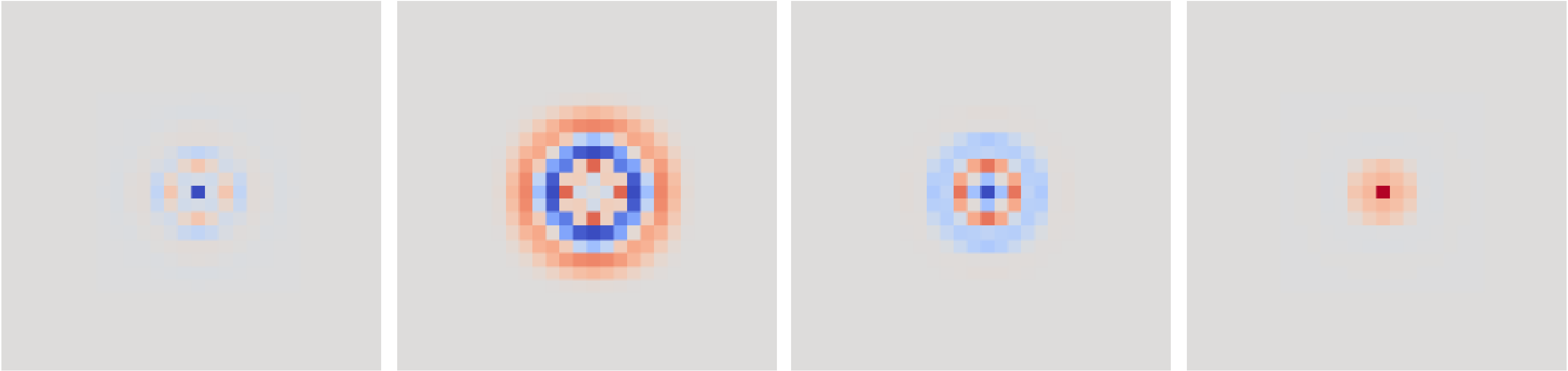
$$= c_0 + \sum_{j=1}^{r} c_j C(h\mathbf{\Delta})^j + \sum_{j=1}^{r} \bar{c_j} C(h\mathbf{\Delta})^{-j}$$

ChebNet vs CayleyNet on a Euclidean grid

- Chebyshev filters of order 3



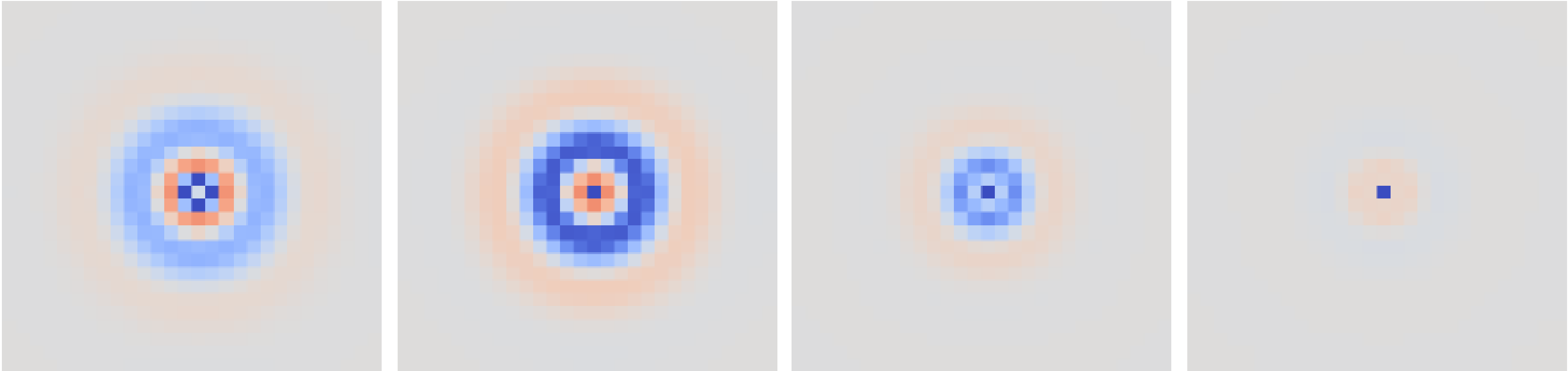
- Chebyshev filters of order 7



ChebNet vs CayleyNet on a Euclidean grid

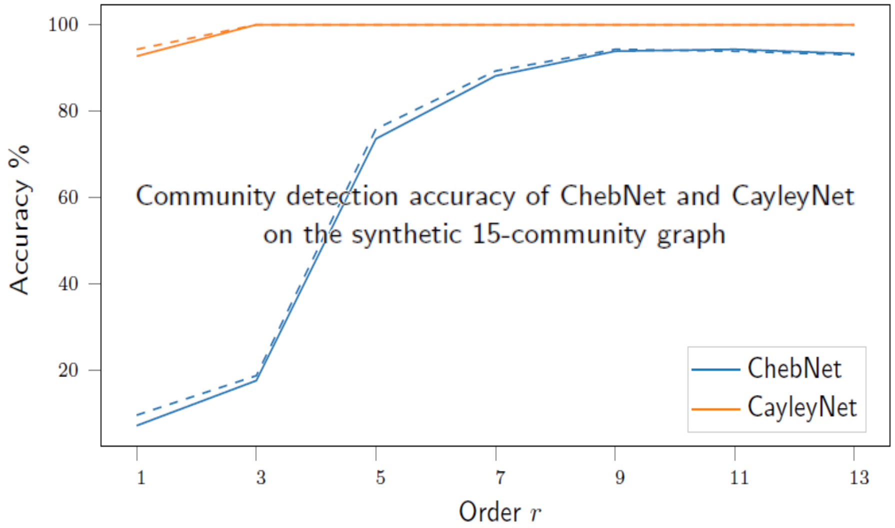
- Chebyshev filters of order 3

- Cayley filters of order 3



ChebNet vs CayleyNet

- Cayley polynomials
  - Are richer than Chebychev polynomials
  - Can be understood as a generalization
  - Improved performance
- Computational cost
  - ChebNet is faster
  - Laplacian inversion
    - Exact $O(n^3)$
    - Approximate solutions $O(n)$

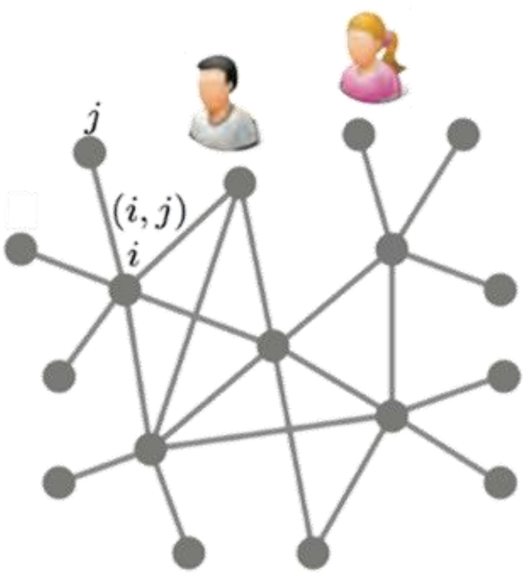


Limitations of Spectral Graph CNNs

- Poor generalization to different graphs
  - Based on the spectrum of the Laplacian
  - Have been developed for fixed graphs only
    - Fourier basis not stable under graph perturbation
    - Difficult to generalize to variable graphs

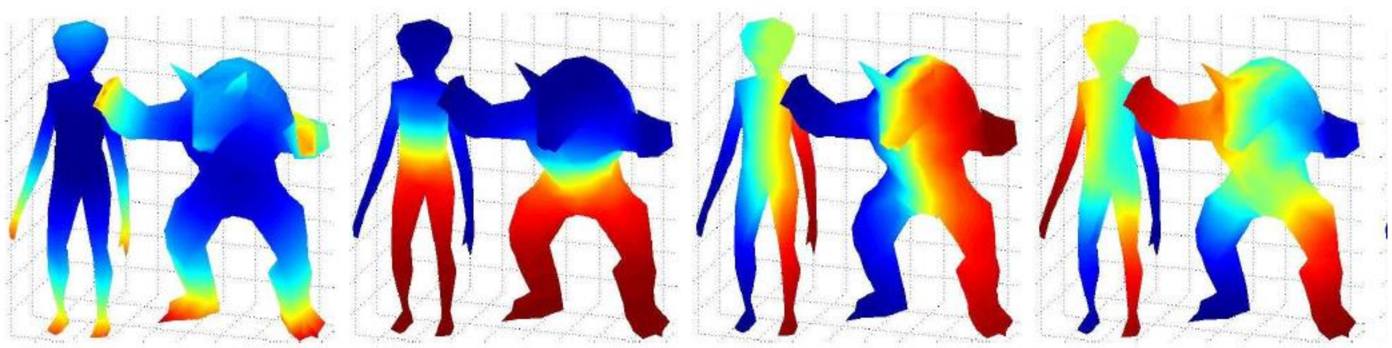
- Graph $\mathcal{G} = (\mathcal{V}, \mathcal{E})$
- Vertices $\mathcal{V} = \{1, \ldots, n\}$
- Edges $\mathcal{E} \subseteq \mathcal{V} \times \mathcal{V}$
- Vertex weights $b_i > 0$ for $i \in \mathcal{V}$
- Edge weights $a_{ij} \geq 0$ for $(i, j) \in \mathcal{E}$
- Vertex fields $L^2(\mathcal{V}) = \{f : \mathcal{V} \to \mathbb{R}^h\}$

  Represented as $\mathbf{f} = (f_1, \ldots, f_n)$



Laplace-Beltrami Spectrum

- Takes into account the geometry of the graph
  - Not only the connectivity
  - Different geometries will have different spectrum
    - But the spectrum should be equivalent
  - Example of the first Laplace Beltrami eigenvectors
    - For two different shapes
      - Most of the times we are not so lucky…..



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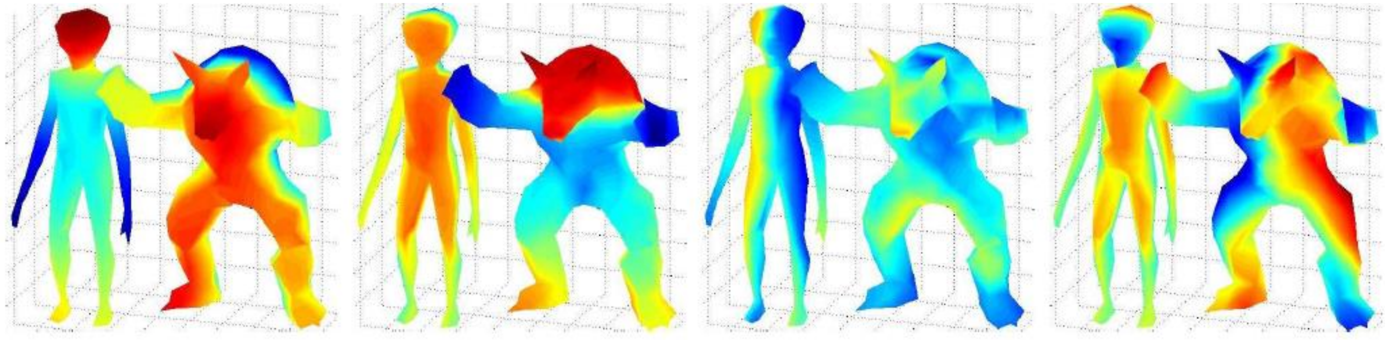
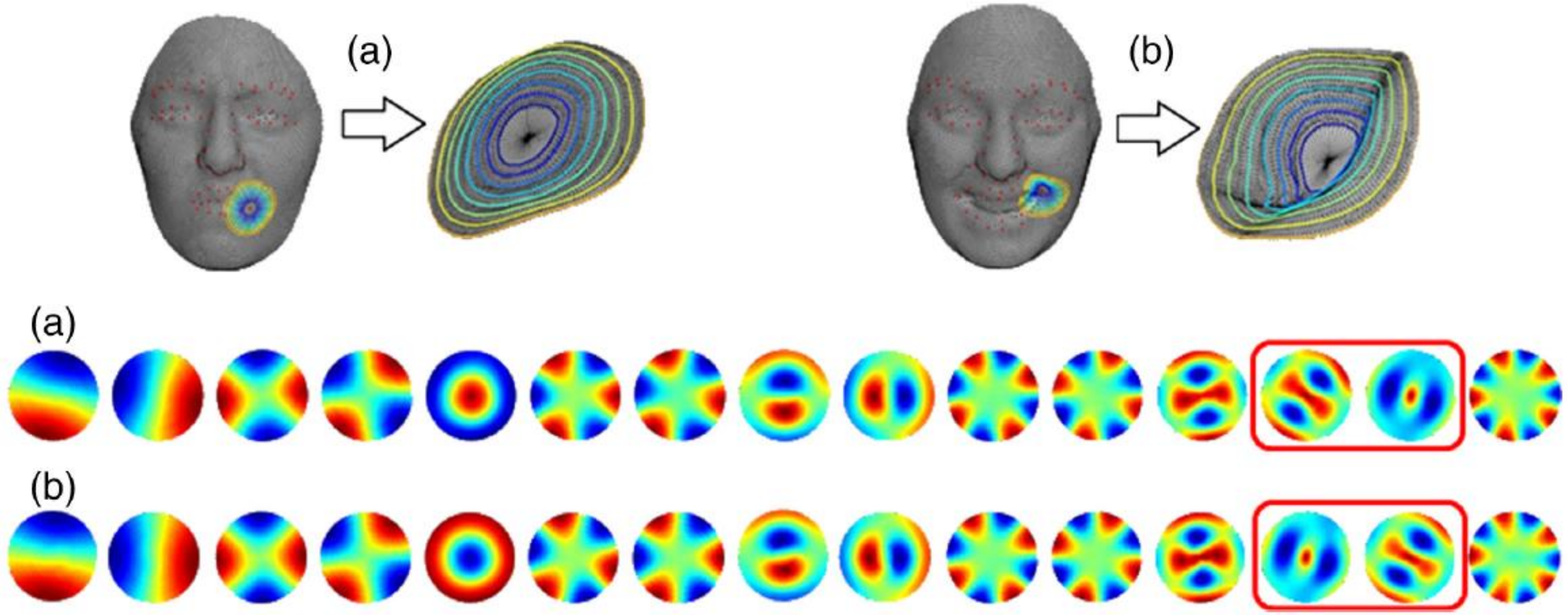
    - For two different shapes
      - Eigenvectors 5 to 8



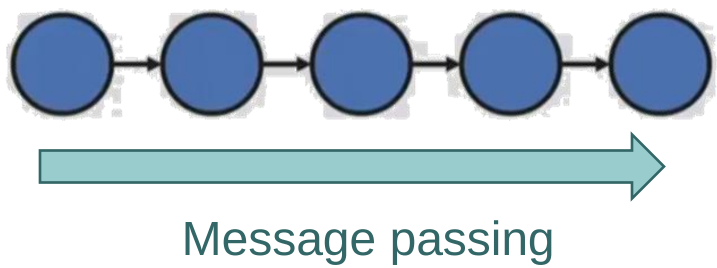
Laplace-Beltrami Spectrum

- Example of the first Laplace Beltrami eigenvectors
  - For two different local patches on the facial surface

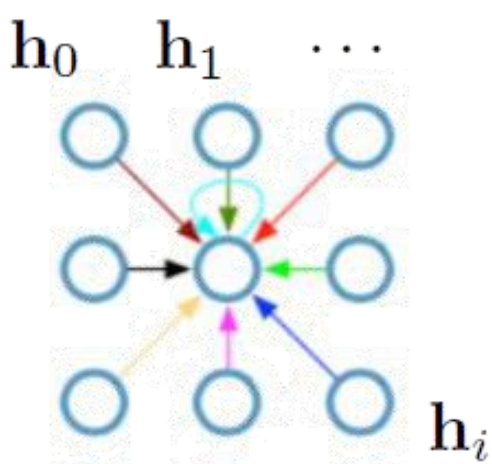


RNN vs CNN motivation for Graph Neural Networks

- A Recurrent Neural Network (RNN)
  - Can be thought of as a special type of graph



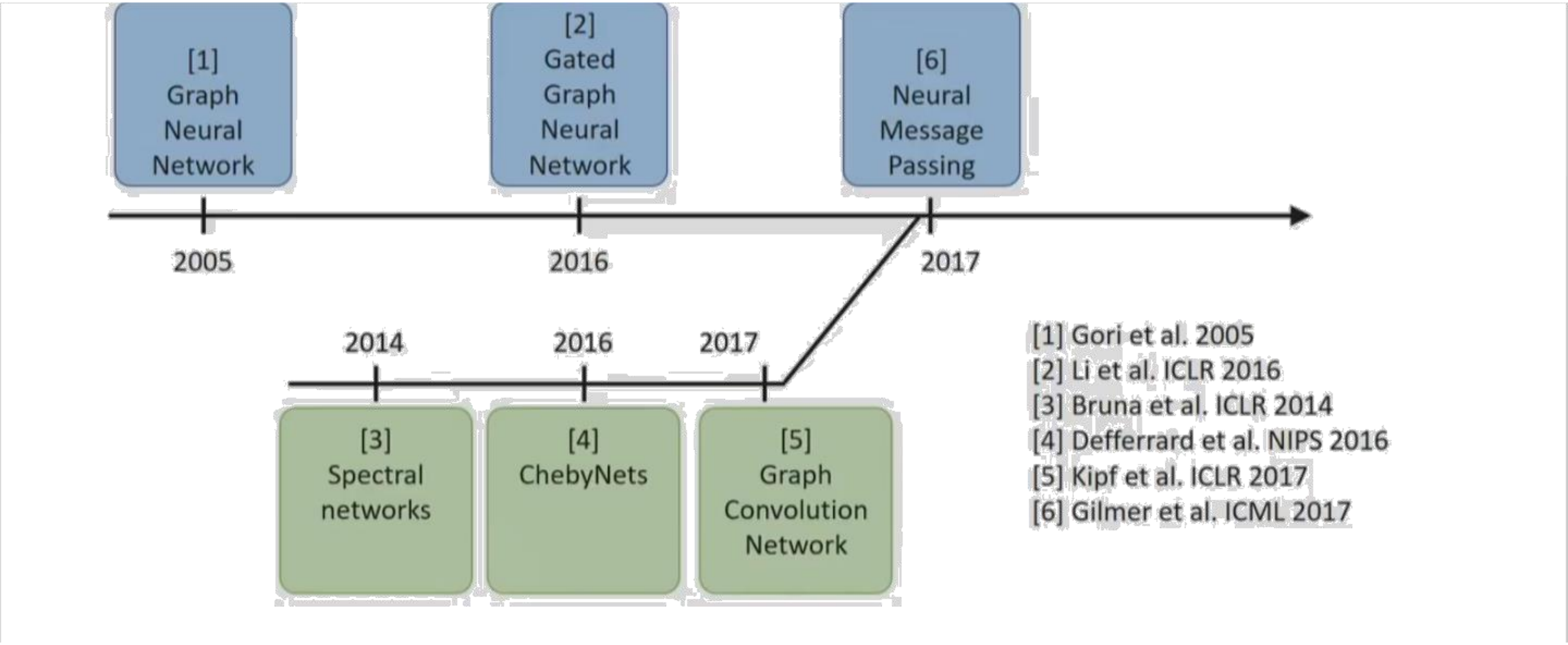
  - Graph Convolutional Nets can be seen equivalently



$$H^{(l+1)} = \sigma\left(\tilde{D}^{-\frac{1}{2}}\tilde{A}\tilde{D}^{-\frac{1}{2}}H^{(l)}W^{(l)}\right)$$

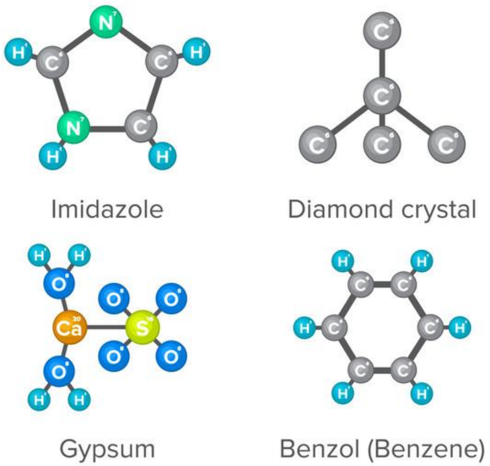
RNN vs CNN motivation for Graph Neural Networks

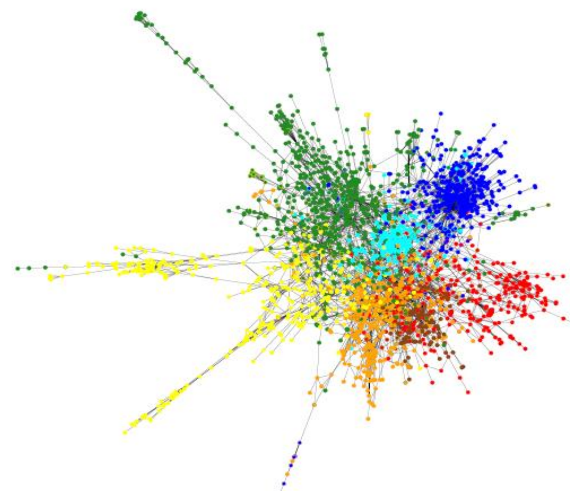
- Both approaches developed from independent paths
  - They were shown to converge to similar formulations



Graph Neural Networks

- Applications to multiple domains
  - Computer graphics
  - Body pose and gestures
  - Citation networks / Social networks
  - Matrix completion
  - Molecule structure





Additional Sources

- Slides inspired from several talks available on-line
  - Xavier Bresson
    - https://www.youtube.com/watch?time_continue=2&v=v3jZRkvIOIM&feature=emb_logo
  - Federico Monti
    - https://www.youtube.com/watch?v=nCv05re-8lQ&t=1316s
  - Alex Gaunt
    - https://www.youtube.com/watch?time_continue=2&v=cWIeTMklzNg&feature=emb_logo

Additional Sources

- J. Bruna, W. Zaremba, A. Szlam, and Y. LeCun, “Spectral networks and locally connected networks on graphs,” in Proc. of ICLR, 2014.
- M. Defferrard, X. Bresson, and P. Vandergheynst, “Convolutional neural networks on graphs with fast localized spectral filtering,” in Proc. of NIPS, 2016
- T. N. Kipf and M. Welling, “Semi-supervised classification with graph convolutional networks,” in Proc. of ICLR, 2017.
- F. Monti, M. Bronstein, and X. Bresson, “Geometric matrix completion with recurrent multi-graph neural networks,” in Proc. of NIPS, 2017,

Reviews

- Wu, Z., Pan, S., Chen, F., Long, G., Zhang, C., & Yu, P. S. (2019). A comprehensive survey on graph neural networks. *arXiv preprint*
- Bronstein, M. M., Bruna, J., LeCun, Y., Szlam, A., & Vandergheynst, P. (2017). Geometric deep learning: going beyond euclidean data. *IEEE Signal Processing Magazine*