Geometric deep learning: going beyond Euclidean data

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SPECTRAL METHODS

- **Spectral CNN (SCNN)**

特征向量 describing the smooth structure of the graph

signal/function

Mapping

$$\mathbf{g}_l = \xi\left(\sum_{l'=1}^{q} \mathbf{\Phi}_k \mathbf{\Gamma}_{l,l'} \boxed{\mathbf{\Phi}_k^\top \mathbf{f}_{l'}}\right)$$

non-linearity

Filter

$\mathbf{\Gamma}_{l,l'}$ is a $k \times k$ diagonal matrix of spectral multipliers

- Using only the first *k* eigenvectors in sets a cutoff frequency which depends on the intrinsic regularity of the graph and also the sample size.

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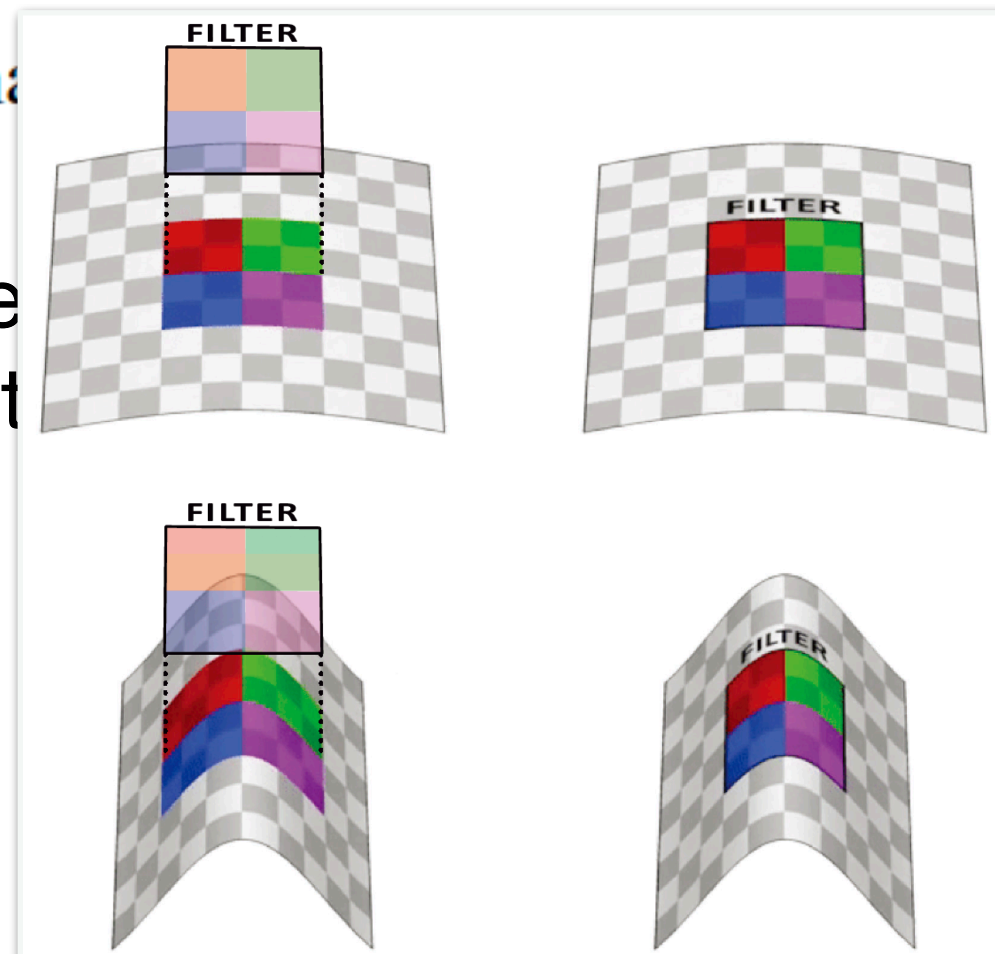
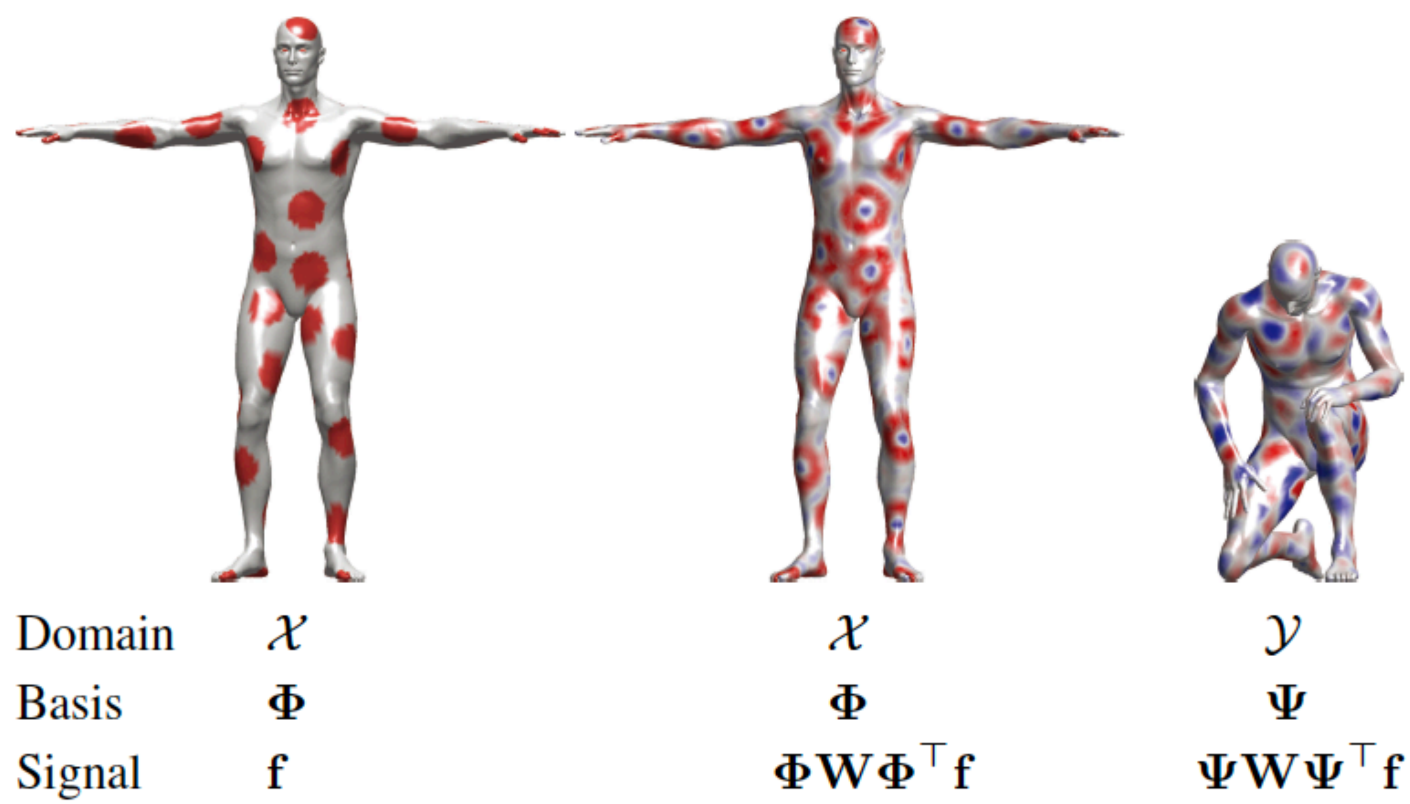


Euclidean CNN Geometric CNN

- Using only the first *k* eige equency which depends on the int ph and also the sample size.

SPECTRAL METHODS

- **Limitations of spectral CNN (SCNN)**
  - Basis dependent



  - Too much parameters

$$pqk = O(n)$$

SPECTRAL METHODS

- **Spectral CNN with smooth spectral multipliers**
  - To reduce the number of free parameters
  - Convolutional kernels with small spatial support (Euclidean domains)
    - The number of parameters independent of the input size
  - How to restrict the class of spectral multipliers?
- **Virtue of the Parseval Identity**

$$\int_{-\infty}^{+\infty} |x|^{2k} |f(x)|^2 dx = \int_{-\infty}^{+\infty} \left| \frac{\partial^k \hat{f}(\omega)}{\partial \omega^k} \right|^2 d\omega,$$

  - Smooth spectral multipliers = features (shared across locations and well localized)
  - Smoothness can be prescribed by learning only a subsampled set of frequency multipliers and using an interpolation kernel to obtain the rest, such as cubic splines.

SPECTRAL METHODS

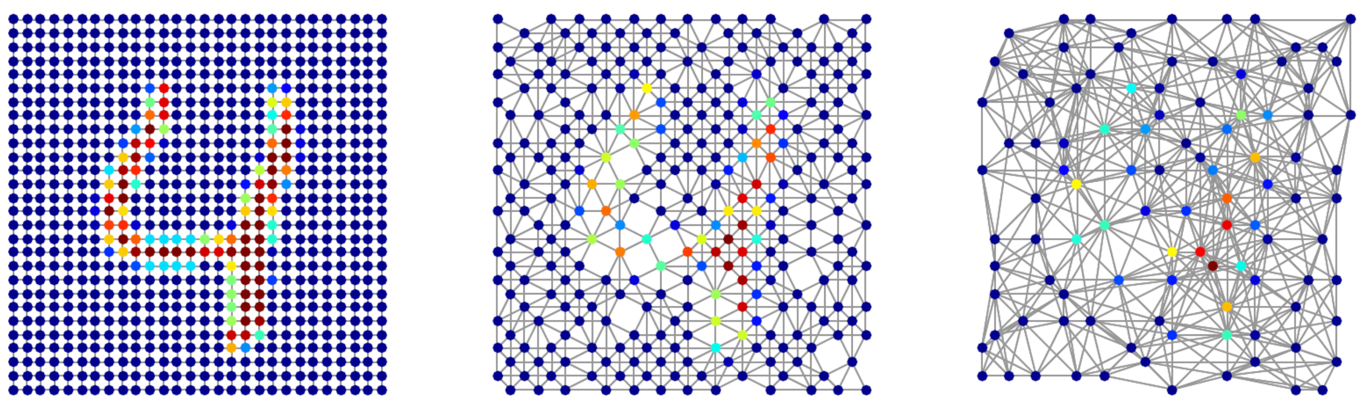
- **Spectral CNN with smooth spectral multipliers**
  - Interpolation kernel for the smoothness
    - to learn only a subsampled set of frequency multipliers and using an interpolation kernel to obtain the rest.

$$\mathrm{diag}(\underbrace{\boldsymbol{\Gamma}_{l,l'}}_{\text{Filter:frequency multipliers}}) = \underbrace{\mathbf{B}}_{\text{interpolation kernel}}\underbrace{\boldsymbol{\alpha}_{l,l'}}_{\text{interpolation coefficients}},$$

- Trainable parameters
  - O(log n), the same as CNNs on Euclidean grids

SPECTRAL METHODS

- **Graph coarsening**
  - The non-Euclidean analogy of pooling



$$\tilde{\mathbf{\Phi}} \approx \mathbf{P}\mathbf{\Phi} \begin{pmatrix} \mathbf{I}_{\alpha n} \\ \mathbf{0} \end{pmatrix}$$

Laplacian eigenvectors (Coarsening)

Laplacian eigenvectors (Original)

```
[1 1 0]
[1 1 0]
[0 0 4]
```

```
[4 0 0]
[0 1 1]
[0 1 1]
```

```
[ 0.70710678 -0.70710678  0.        ]
[ 0.70710678  0.70710678  0.        ]
[ 0.          0.          1.        ]
```

```
[ 0.          0.          1.        ]
[ 0.70710678  0.70710678  0.        ]
[ 0.70710678 -0.70710678  0.        ]
```

PECTRUM-FREE METHODS

- **Represent the filters via a polynomial expansion**

$$\boldsymbol{\Gamma}_{l,l'} = g_{\boldsymbol{\alpha}_{l,l'}}(\boldsymbol{\Lambda})$$

$$\mathbf{g}_l = \xi\left(\sum_{l'=1}^{q} \boldsymbol{\Phi}_k \boldsymbol{\Gamma}_{l,l'} \boldsymbol{\Phi}_k^\top \mathbf{f}_{l'}\right)$$

$$g_{\boldsymbol{\alpha}}(\boldsymbol{\Lambda}) \;=\; \mathrm{diag}(g_{\boldsymbol{\alpha}}(\lambda_1), \ldots, g_{\boldsymbol{\alpha}}(\lambda_n))$$

$$g_{\boldsymbol{\alpha}}(\lambda) = \sum_{j=0}^{r-1} \alpha_j \lambda^j$$

- It automatically yields localized filters
  - The Laplacian is a local operator, the action of its j-th power is constrained to j-hops.
  - The filter is a linear combination of powers of the Laplacian, overall behaves like a diffusion operator limited to r-hops around each vertex.

PECTRUM FREE METHODS

- **Graph CNN (GCNN) a.k.a. ChebNet**
  - Chebyshev polynomial

$$
\begin{aligned}
T_j(\lambda) &= 2\lambda T_{j-1}(\lambda) - T_{j-2}(\lambda); \\
T_0(\lambda) &= 1; \\
T_1(\lambda) &= \lambda.
\end{aligned}
$$

Recurrence relation

  - A filter can be parameterized uniquely via an expansion

$$
\begin{aligned}
g_{\boldsymbol{\alpha}}(\tilde{\boldsymbol{\Delta}}) &= \sum_{j=0}^{r-1} \alpha_j \boldsymbol{\Phi} T_j(\tilde{\boldsymbol{\Lambda}}) \boldsymbol{\Phi}^\top \\
&= \sum_{j=0}^{r-1} \alpha_j T_j(\tilde{\boldsymbol{\Delta}}),
\end{aligned}
$$

$$
\bar{\mathbf{f}}^{(j)} = T_j(\tilde{\boldsymbol{\Delta}})\mathbf{f}
$$

$$
\bar{\mathbf{f}}^{(j)} = 2\tilde{\boldsymbol{\Delta}}\bar{\mathbf{f}}^{(j-1)} - \bar{\mathbf{f}}^{(j-2)}
$$

Computational complexity is O(rn)
Does not require an explicit computation of the Laplacian eigenvectors

PECTRUM-FREE METHODS

- **Graph Convolutional Network**
  - Assuming r = 2 and $\lambda_n \approx 2$
  - One obtains filters represented by a single parameter

$$g_\alpha(\mathbf{f}) \quad = \quad \alpha(\mathbf{I} + \mathbf{D}^{-1/2}\mathbf{W}\mathbf{D}^{-1/2})\mathbf{f}.$$

  - ChebNet and GCN (spectral domain) boil down to applying simple filters acting on the r-or 1-hop neighborhood of the graph in the spatial domain.

PECTRUM-FREE METHODS

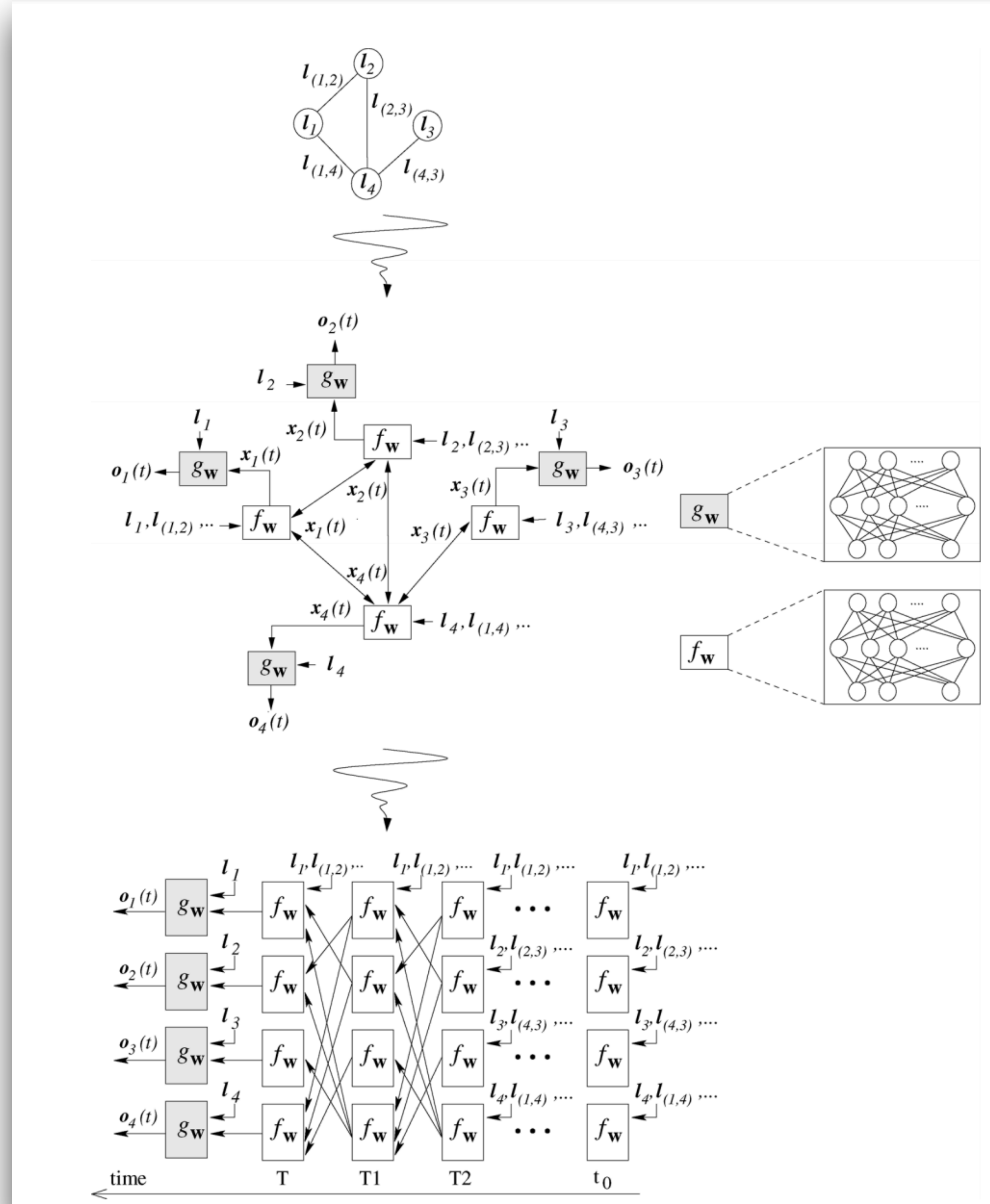
- **Graph Neural Network (GNN)**
  - Graph Neural Networks generalize the notion of applying the filtering operations directly on the graph via the graph weights.

$$\mathbf{g}_i = \eta_{\boldsymbol{\theta}}\left((\mathbf{W}\mathbf{f})_i, (\mathbf{D}\mathbf{f})_i\right)$$

  - Laplacian operator $\eta(\mathbf{a}, \mathbf{b}) = \mathbf{b} - \mathbf{a}$
  - Nonlinear choices for η yield trainable, task-specific diffusion operators

PECTRUM-FREE METHODS

- **Graph Neural Network**
  -



CHARTING-BASED METHODS

- Inherent drawback of inability to adapt the model across different domains
  - Resort to the convolution in the spatial domain
  - One of the major problems in applying the same paradigm to non-Euclidean domains is the lack of shift-invariance, implying that the '**patch operator**' extracting a local 'patch' would be position-dependent.

$$D_j(x)f = \int_{\mathcal{X}} f(x')v_j(x,x')dx', \quad j = 1, \ldots, J,$$

$$(f \star g)(x) = \sum_j g_j D_j(x) f,$$

CHARTING-BASED METHODS

- Geodesic CNN

$$v_{ij}(x, x') = e^{-(\rho(x') - \rho_i)^2 / 2\sigma_\rho^2} \, e^{-(\theta(x') - \theta_j)^2 / 2\sigma_\theta^2}$$

- Anisotropic CNN

$$\Delta_{\alpha\theta} f(x) = -\mathrm{div}(\mathbf{A}_{\alpha\theta}(x) \nabla f(x))$$

- Mixture model network (MoNet)

$$v_j(\mathbf{u}) = \exp\left(-\tfrac{1}{2}(\mathbf{u} - \boldsymbol{\mu}_j)^\top \boldsymbol{\Sigma}_j^{-1} (\mathbf{u} - \boldsymbol{\mu}_j)\right)$$

COMBINED SPATIAL /SPECTRAL METHODS

- Windowed Fourier transform

$$
\begin{aligned}
(Sf)(x,\omega) &= \int_{-\infty}^{\infty} f(x')\, \underbrace{g(x'-x)e^{-i\omega x'}}_{\overline{g_{x,\omega}}(x')}\, dx' \\
&= \langle f, g_{x,\omega} \rangle_{L^2(\mathbb{R})}.
\end{aligned}
$$

spatial location of the window x

modulation frequency w

window function

- Wavelets (Haar wavelets)
- Localized Spectral CNN (LSCNN)

CHARTING-BASED METHODS

Dichotomy of Geometric deep learning methods

Method	Domain	Data
Spectral CNN [52]	spectral	graph
GCNN/ChebNet [45]	spec. free	graph
GCN [77]	spec. free	graph
GNN [78]	spec. free	graph
Geodesic CNN [47]	charting	mesh
Anisotropic CNN [48]	charting	mesh/point cloud
MoNet [54]	charting	graph/mesh/point cloud
LSCNN [89]	combined	mesh/point cloud

APPLICATIONS

- Network analysis
  - Classification application (citation network)
  - Ranking (PageRank algorithm) and community detection.
  - Recommender systems (matrix completion)
    - Geometric matrix completion
    - Multi-Graph CNN
  - Computer vision and graphics
  - Particle physics and Chemistry (Classification)
    - Chemical properties of a molecule are determined by the relative positions of its atoms
  - Molecule design
    - A key problem in material- and drug design is predicting the physical, chemical, or biological properties of a novel molecule
  - Medical imaging (non-Euclidean domains)

OPEN PROBLEMS AND FUTURE DIRECTIONS

- **Generalization**
  - Spectral formulation of convolution allows designing CNNs on a graph, but the model learned this way on one graph cannot be straightforwardly applied to another one, since the spectral representation of convolution is domain-dependent.
    - Spatial transformer networks
  - The spatial methods, on the other hand, allow generalization across different domains
- **Time-varying domains**
- **Directed graphs**
- **Synthesis problems**
- **Computation**