



UNIVERSITY OF
CALGARY

Geometric Deep Learning

• • •

Sebastian Crites
Statistical Learning Group 2019

Gameplan

- Review of Euclidean Convolutional Neural Networks
- Laplacian operators in the Euclidean and non-Euclidean domains
- Spectral Analysis
- Constructing non-Euclidean Convolutional Neural Networks

Different formulations of non-Euclidean CNNs



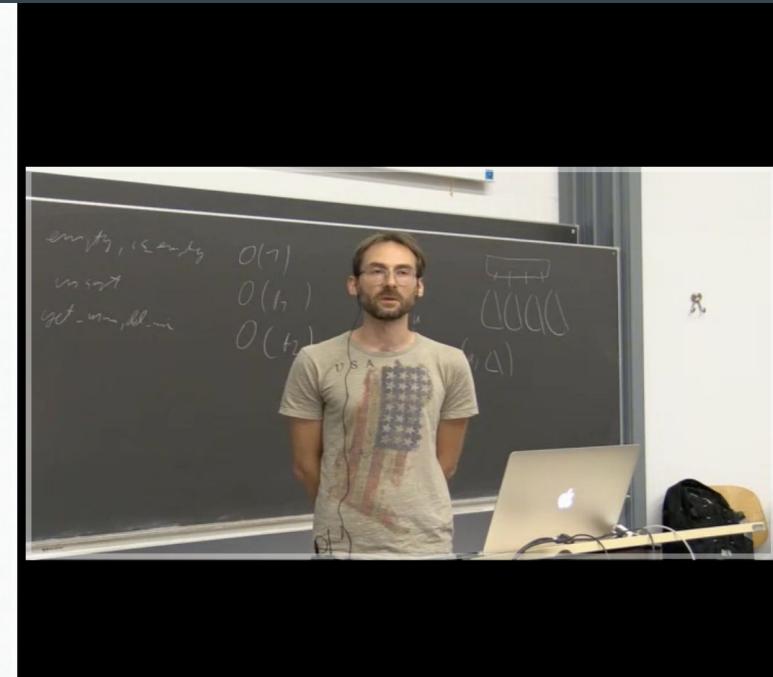
Spectral domain



Spatial domain

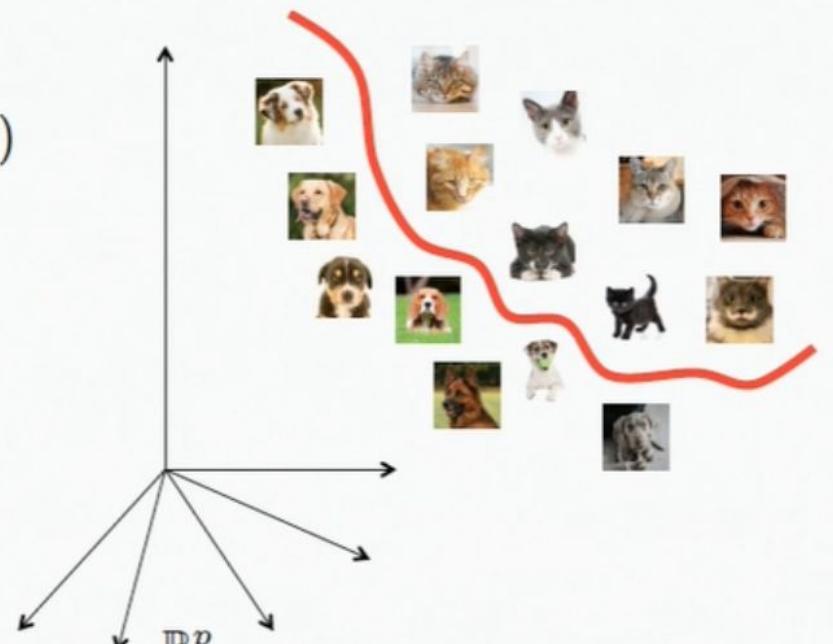


Embedding domain



Euclidean Supervised Learning

- Data vectors $\mathbf{f} \in \mathbb{R}^p$
(e.g. for 512×512 images $p \approx 10^5$)
- Unknown classification functional
 $y : \mathbb{R}^p \rightarrow \{1, \dots, L\}$ in L classes
- Training set
$$S = \{(\mathbf{f}_i \in \mathbb{R}^p, y_i = y(\mathbf{f}_i))\}_{i=1}^T$$
- Parametric model y_Θ of y



Euclidean Supervised Learning

Supervised learning: find optimal model parameters by minimizing the loss ℓ on the training set

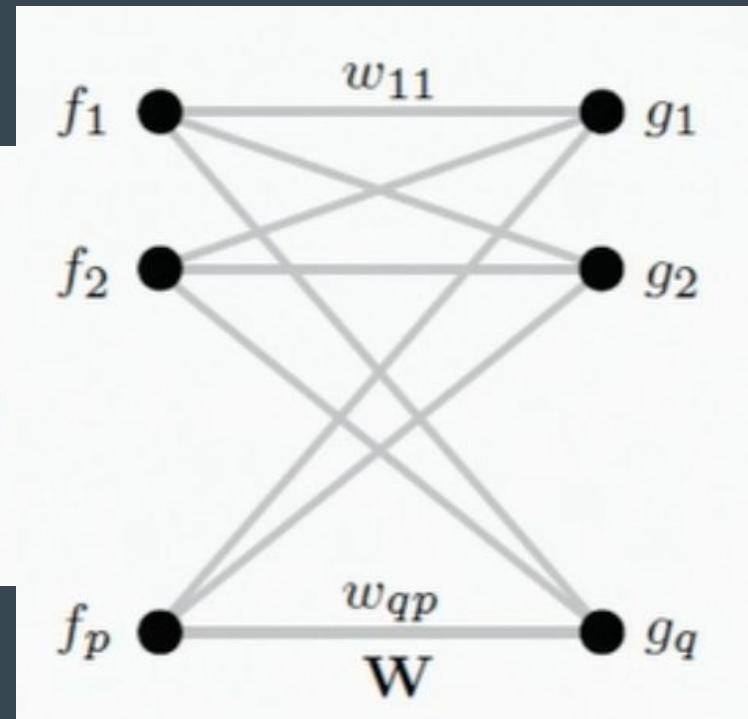
$$\Theta^* = \operatorname{argmin}_{\Theta} \sum_{i=1}^T \ell(y_{\Theta}(\mathbf{f}_i), y_i)$$

Single Dense Layer

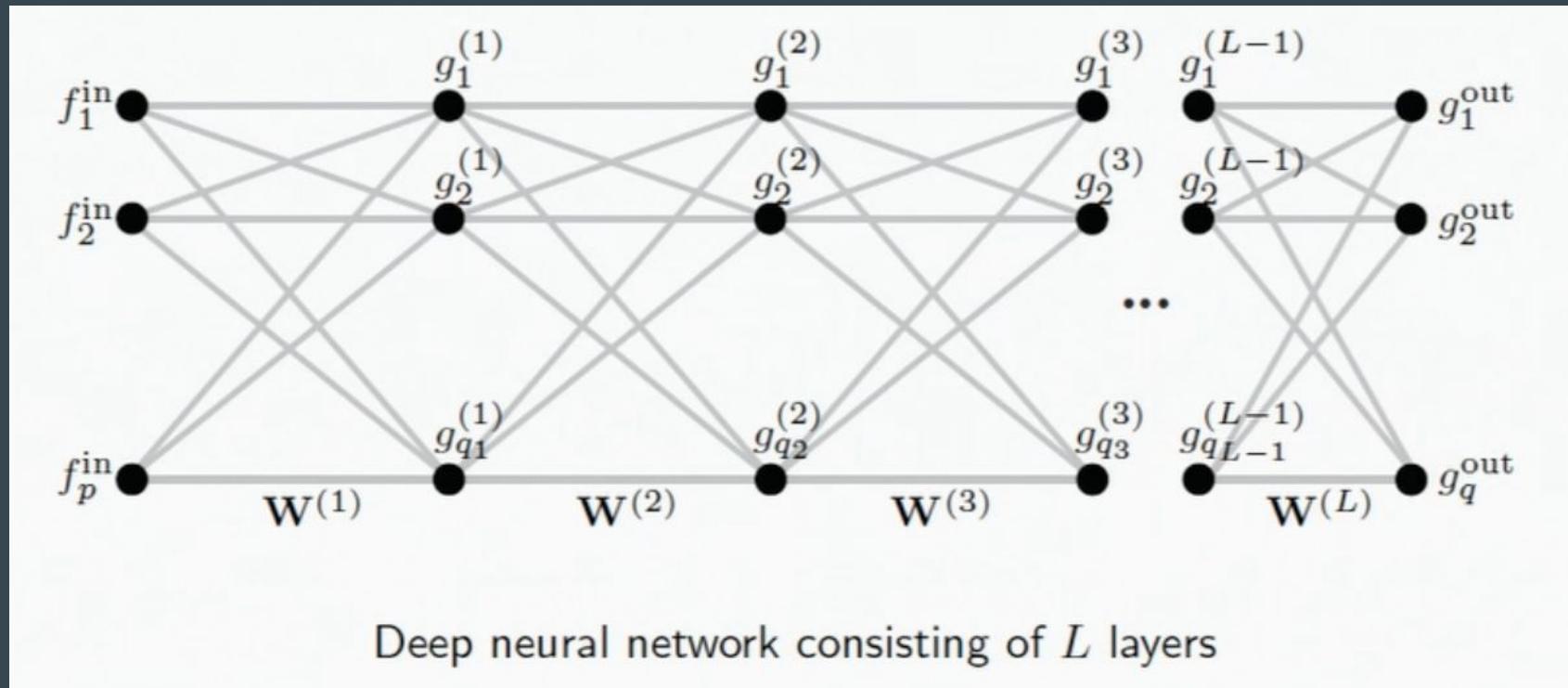
$$g_l = \xi \left(\sum_{l'=1}^p f_{l'} w_{l,l'} \right) \quad l = 1, \dots, q \\ l' = 1, \dots, p$$

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

layer weights \mathbf{W} (including bias)

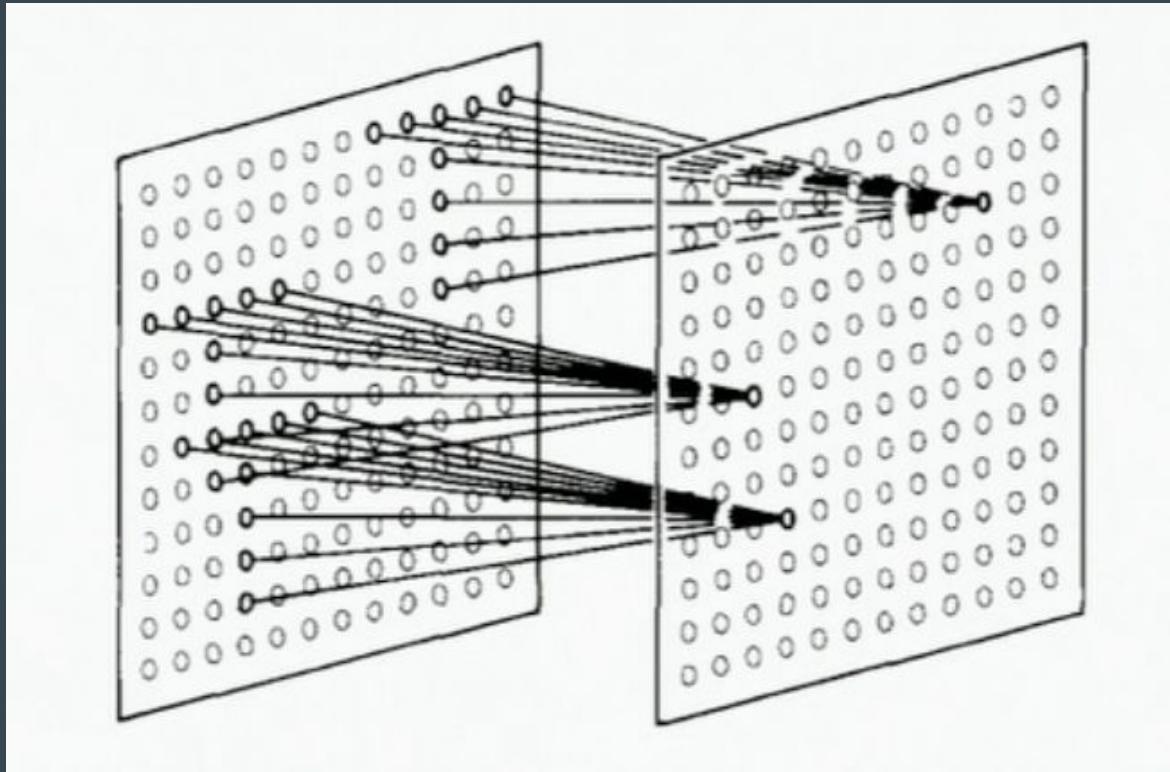


Composing Dense Layers

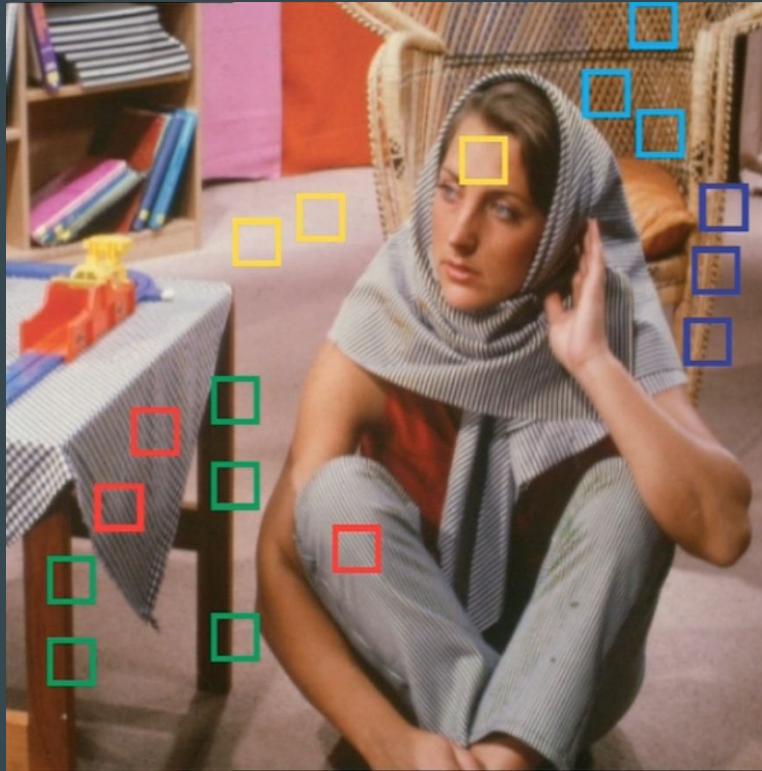


Properties of Image Data

Locality



Self-Similarity

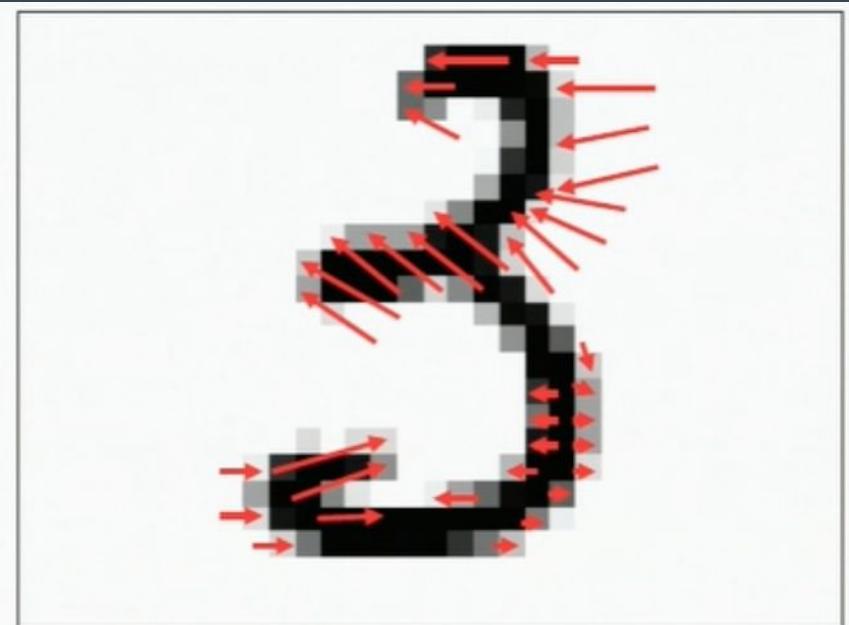
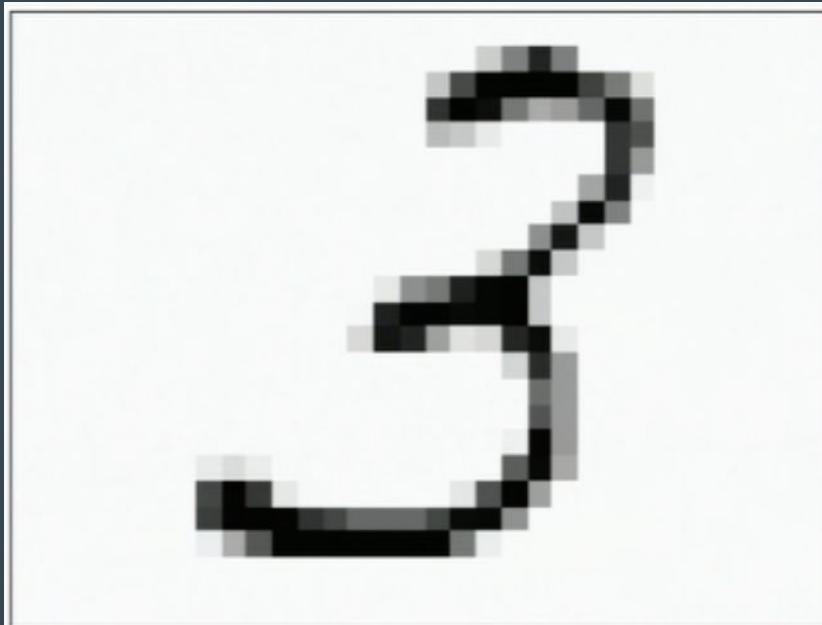


Translation Invariance



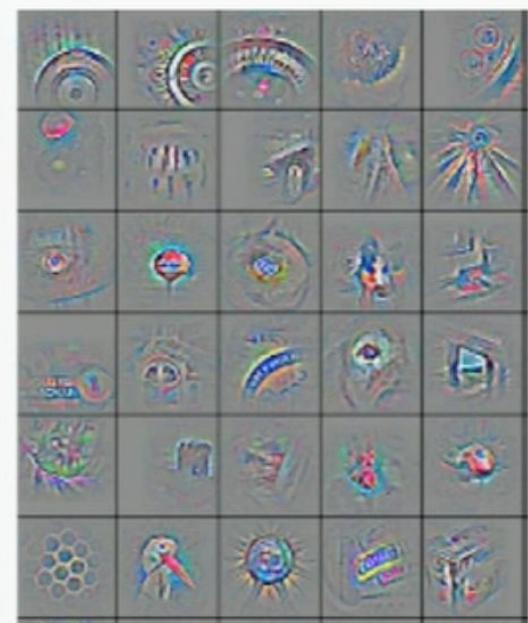
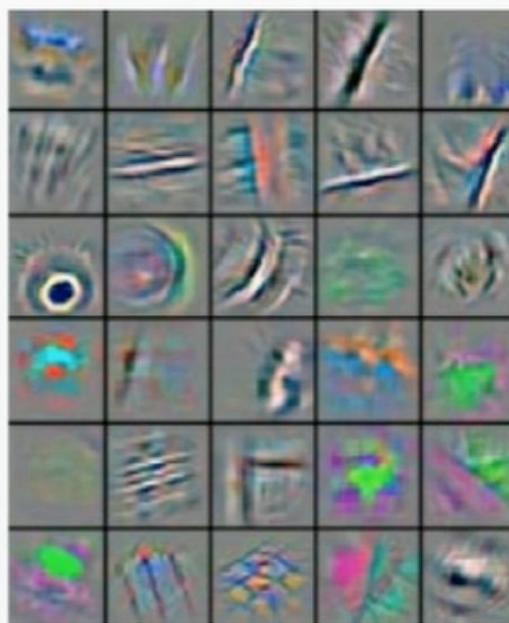
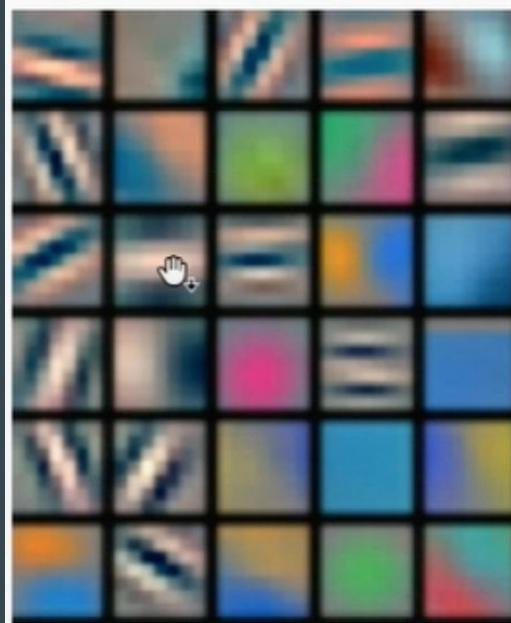
$$y(\mathcal{T}_v f) = y(f) \quad \forall f, v$$

Deformation Tolerance



$$|y(\mathcal{L}_\tau f) - y(f)| \approx \|\nabla \tau\| \quad \forall f, \tau$$

Hierarchical & Composable



Typical features learned by a CNN becoming increasingly complex at deeper layers

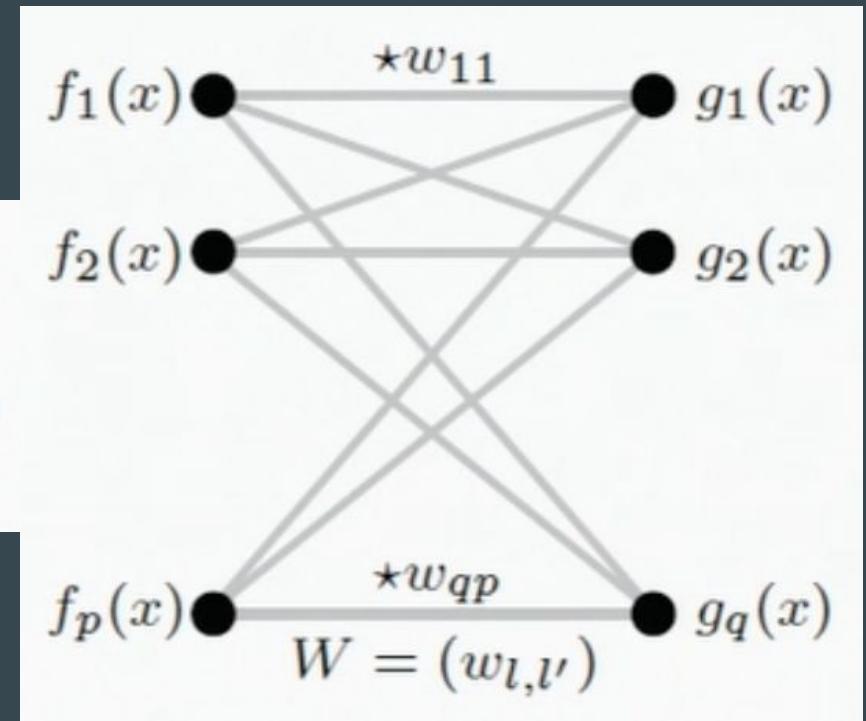
Convolutional Neural Networks

Convolutional Neural Network (CNN) Layer

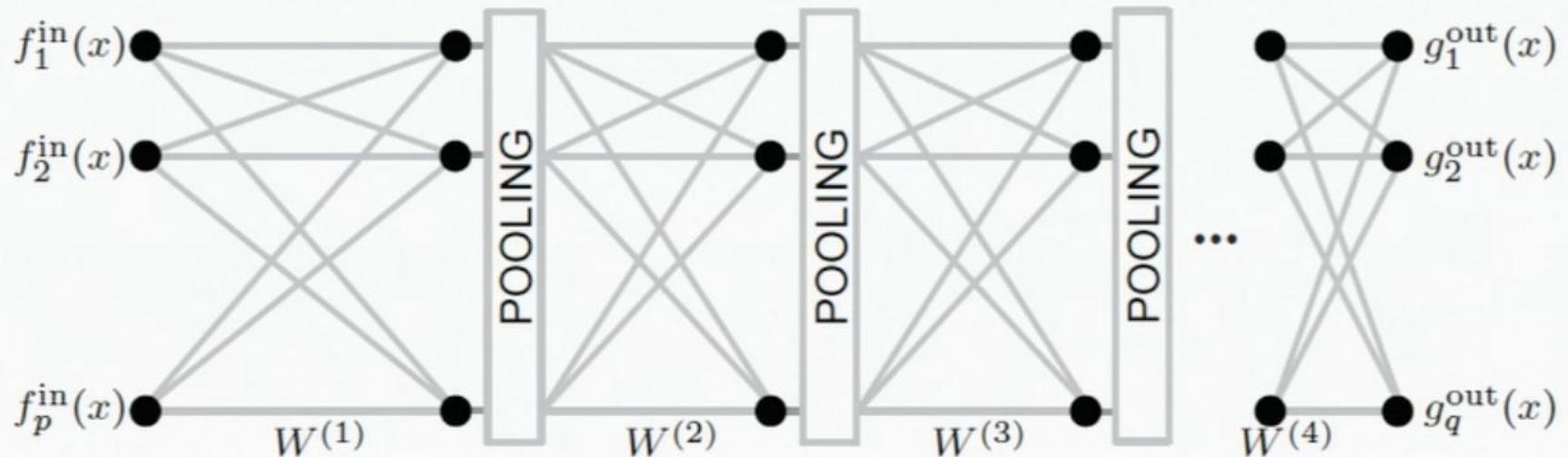
$$g_l(x) = \xi \left(\sum_{l'=1}^p (f_{l'} \star w_{l,l'})(x) \right) \quad l = 1, \dots, q$$

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

filters W



Composing Convolutional Layers



CNN consisting of L convolutional layers interleaved with pooling

Image Convolution Example

3	3	2	1	0	0
3	3	2	1	0	0
3	3	2	1	0	0
3	3	3	2	0	0
3	3	2	1	0	0
3	2	1	1	0	0

Input image

$$\begin{matrix} * & \begin{matrix} 1 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 1 \end{matrix} & = \end{matrix}$$

Filter

6	8	6	3	1	0
9	13	10	5	2	0
9	14	11	6	3	0
9	13	11	6	2	0
8	13	10	5	3	0
6	7	5	3	1	0

Feature map

13	10	2
14	11	3
13	10	3

Max pooling

Key Properties of CNNs

😊 Convolutional filters (**Translation invariance**)

Key Properties of CNNs

- ☺ Convolutional filters (**Translation invariance**)
- ☺ Multiple layers (**Compositionality**)

Key Properties of CNNs

- ☺ Convolutional filters (**Translation invariance**)
- ☺ Multiple layers (**Compositionality**)
- ☺ Filters localized in space (**Locality**)

Key Properties of CNNs

- 😊 Convolutional filters (**Translation invariance**)
- 😊 Multiple layers (**Compositionality**)
- 😊 Filters localized in space (**Locality**)
- 😊 Weight sharing (**Self-similarity**)

Key Properties of CNNs

- 😊 Convolutional filters (**Translation invariance**)
- 😊 Multiple layers (**Compositionality**)
- 😊 Filters localized in space (**Locality**)
- 😊 Weight sharing (**Self-similarity**)
- 😊 $\mathcal{O}(1)$ parameters per filter (independent of input image size n)

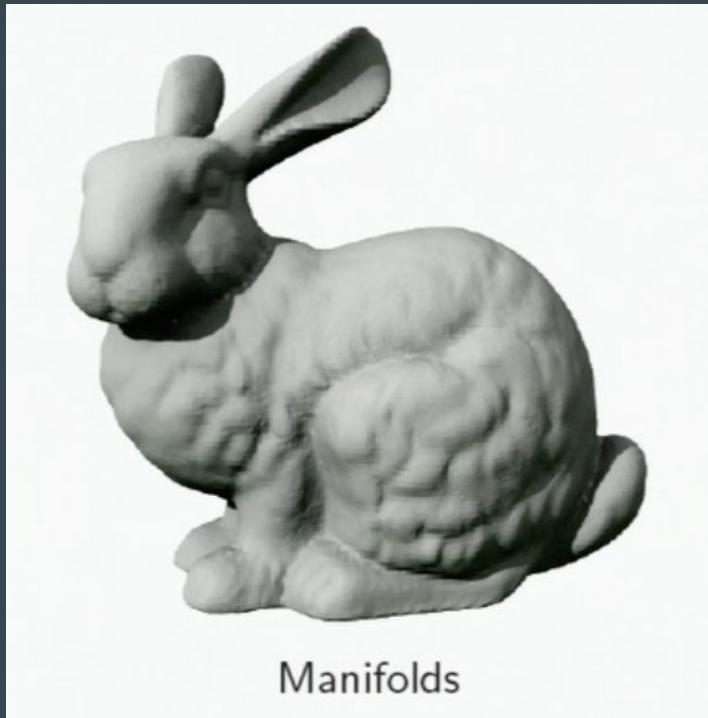
Key Properties of CNNs

- ☺ Convolutional filters (**Translation invariance**)
- ☺ Multiple layers (**Compositionality**)
- ☺ Filters localized in space (**Locality**)
- ☺ Weight sharing (**Self-similarity**)
- ☺ $\mathcal{O}(1)$ parameters per filter (independent of input image size n)
- ☺ $\mathcal{O}(n)$ complexity per layer (filtering done in the spatial domain)

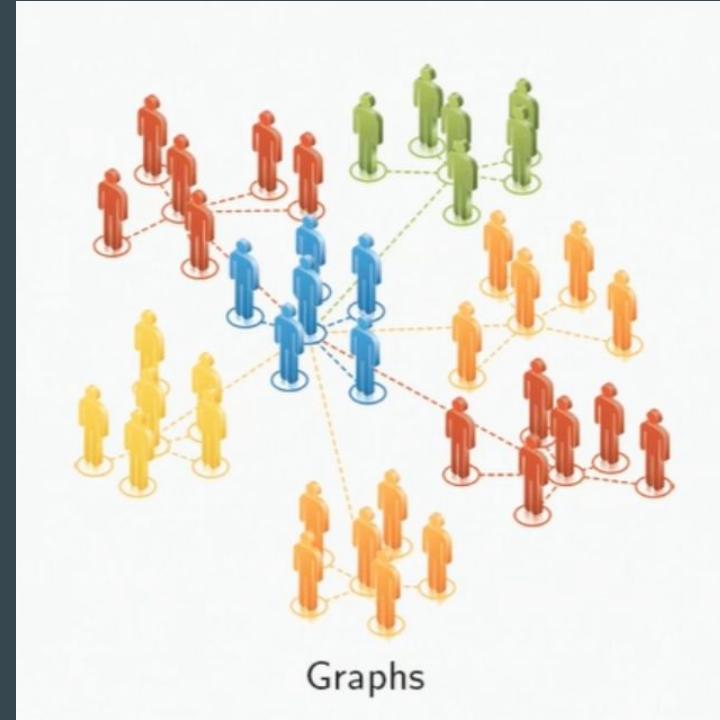
Key Properties of CNNs

- ☺ Convolutional filters (**Translation invariance**)
- ☺ Multiple layers (**Compositionality**)
- ☺ Filters localized in space (**Locality**)
- ☺ Weight sharing (**Self-similarity**)
- ☺ $\mathcal{O}(1)$ parameters per filter (independent of input image size n)
- ☺ $\mathcal{O}(n)$ complexity per layer (filtering done in the spatial domain)
- ☺ $\mathcal{O}(\log n)$ layers in classification tasks

Non-Euclidean Domains



Manifolds



Graphs

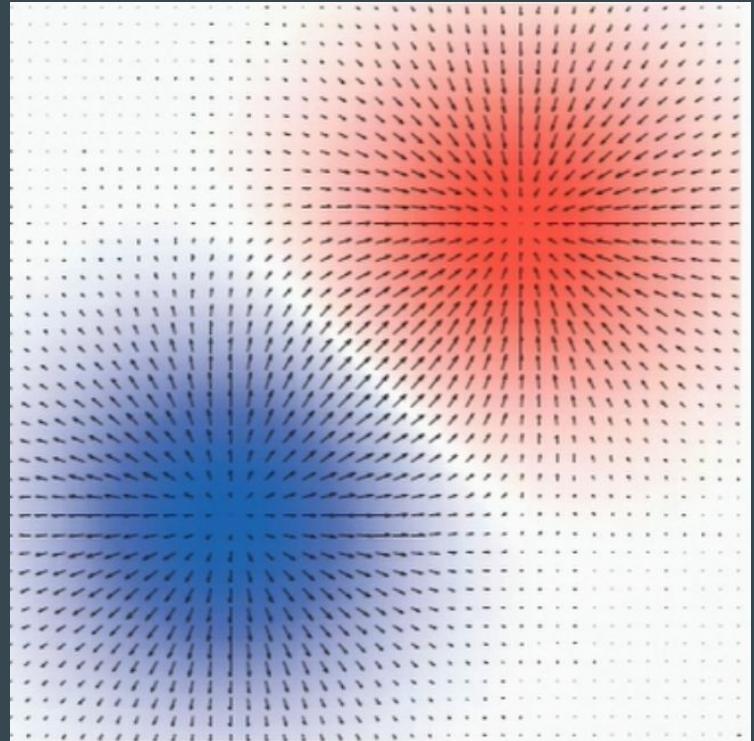
Laplacian Operators

Euclidean Laplacian Operator



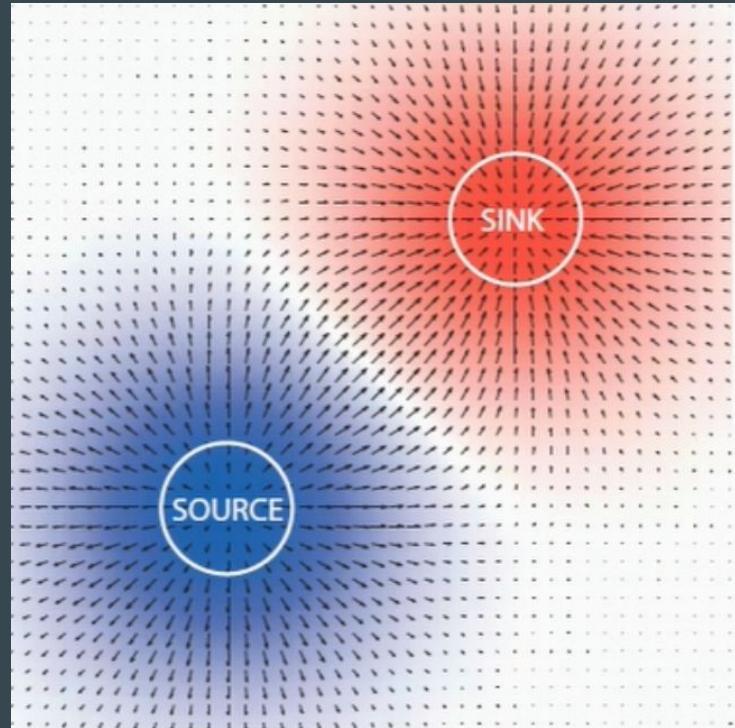
Laplacian Operator

Gradient $\nabla f(x) = \text{'direction of the steepest increase of } f \text{ at } x'$



Laplacian Operator

Divergence $\operatorname{div}(F(x))$ = 'density of an outward flux of F from an infinitesimal volume around x '



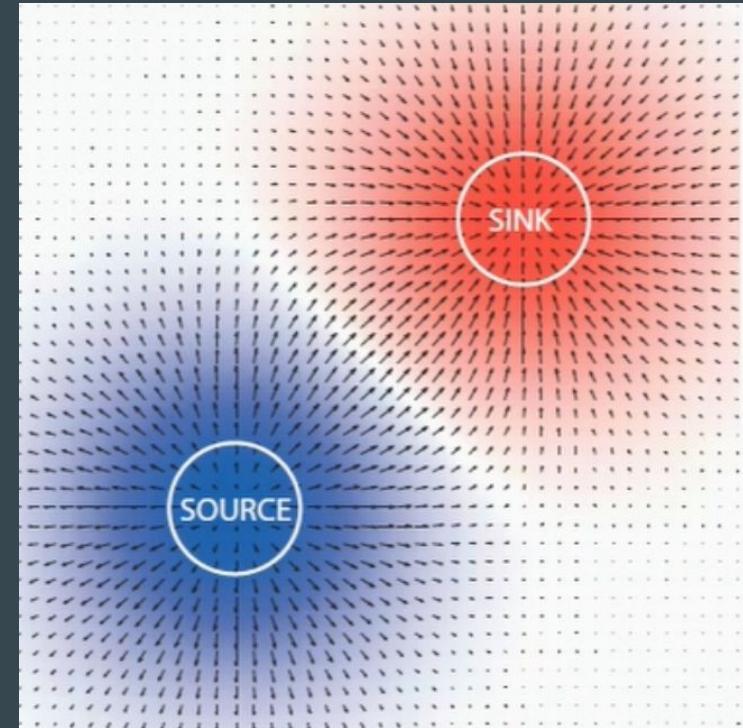
Smooth vector field F

Laplacian Operator

Divergence theorem:

$$\int_V \operatorname{div}(F) dV = \int_{\partial V} \langle F, \hat{n} \rangle dS$$

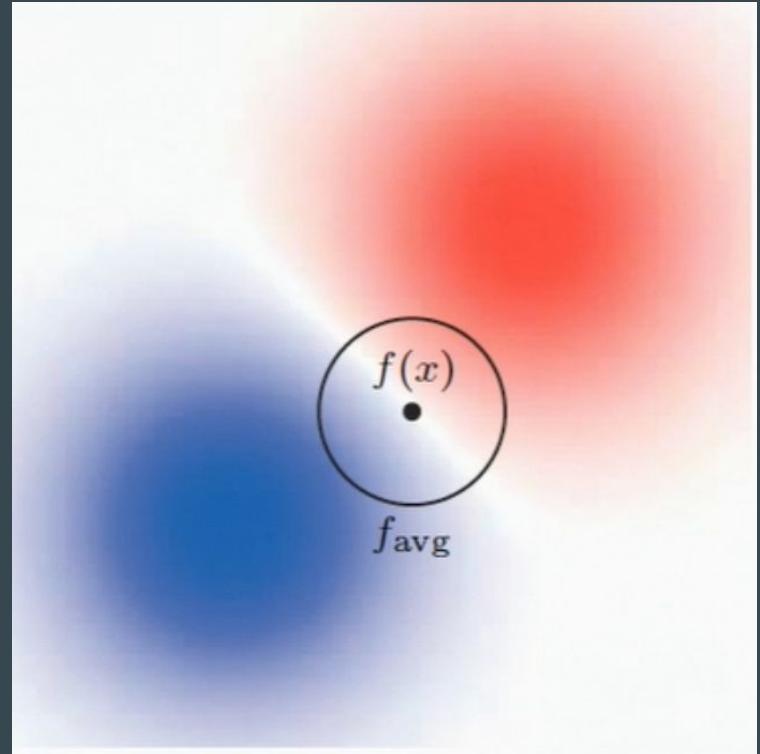
' \sum sources + sinks = net flow'



Smooth vector field F

Laplacian Operator

Laplacian $\Delta f(x) = -\text{div}(\nabla f(x))$

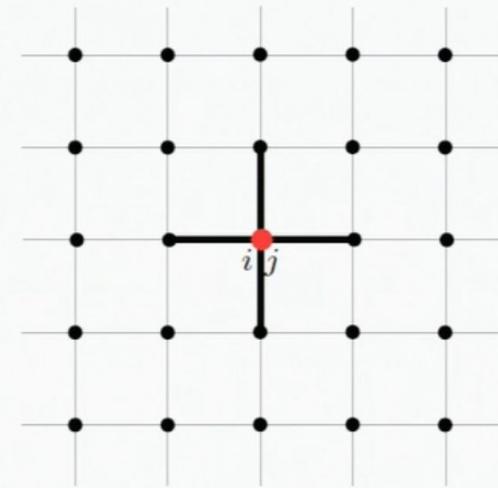


Laplacian in 1D and 2D



One-dimensional

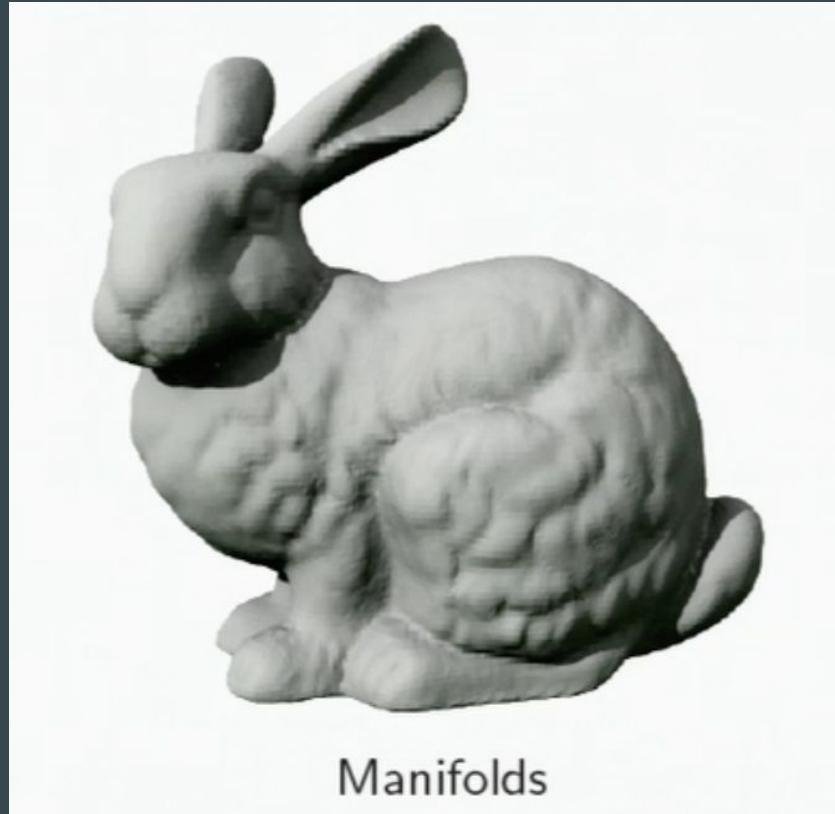
$$(\Delta f)_i \approx 2f_i - f_{i-1} - f_{i+1}$$



Two-dimensional

$$\begin{aligned} (\Delta f)_{ij} \approx & 4f_{ij} - f_{i-1,j} - f_{i+1,j} \\ & - f_{i,j-1} - f_{i,j+1} \end{aligned}$$

Non-Euclidean Domains



Manifolds

Riemannian Manifolds

Manifold \mathcal{X} = topological space

No global Euclidean structure

Tangent plane $T_x \mathcal{X}$ = local Euclidean representation of manifold \mathcal{X} around x

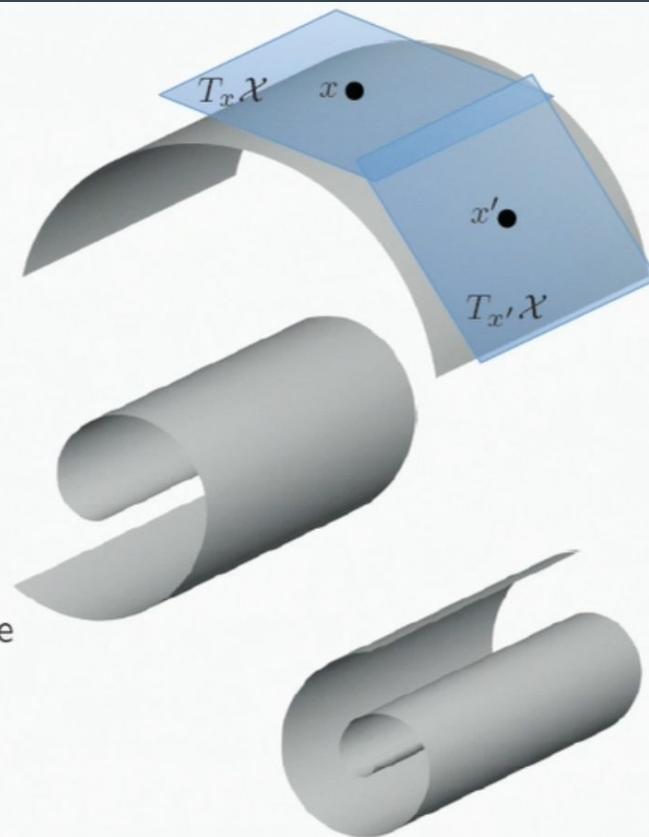
Riemannian metric

$$\langle \cdot, \cdot \rangle_{T_x \mathcal{X}} : T_x \mathcal{X} \times T_x \mathcal{X} \rightarrow \mathbb{R}$$

depending smoothly on x

Isometry = metric-preserving shape deformation

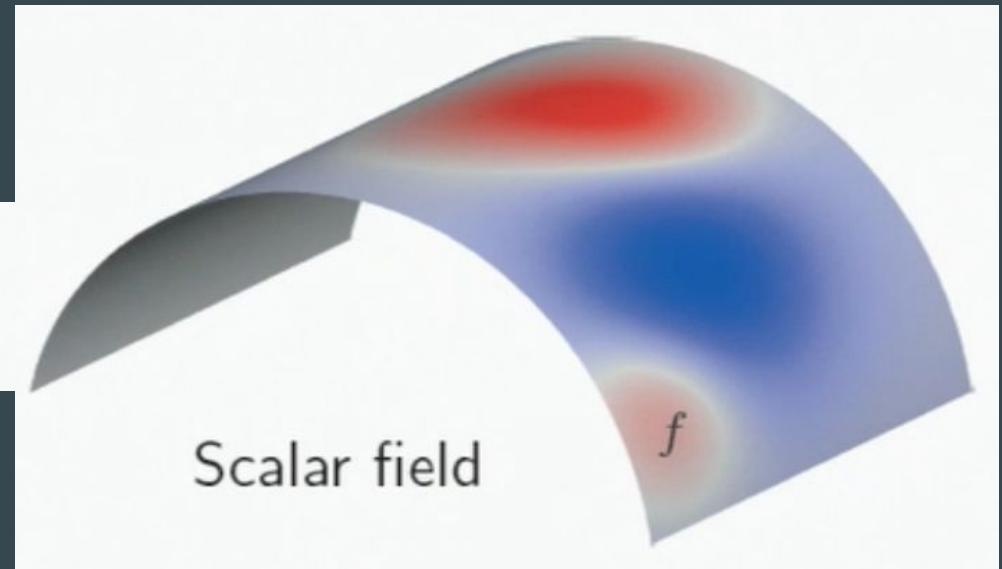
Intrinsic = expressed solely in terms of the Riemannian metric



Manifold Definitions

Scalar field $f : \mathcal{X} \rightarrow \mathbb{R}$

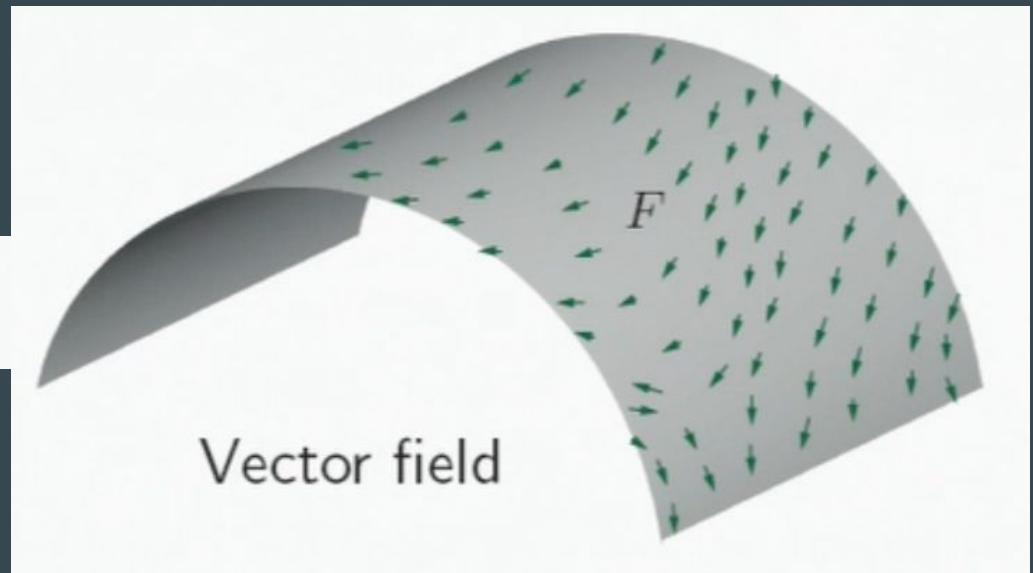
$$\langle f, g \rangle_{L^2(\mathcal{X})} = \int_{\mathcal{X}} f(x)g(x)dx$$



Manifold Definitions

Vector field $F : \mathcal{X} \rightarrow T\mathcal{X}$

$$\langle F, G \rangle_{L^2(T\mathcal{X})} = \int_{\mathcal{X}} \langle F(x), G(x) \rangle_{T_x\mathcal{X}} dx$$

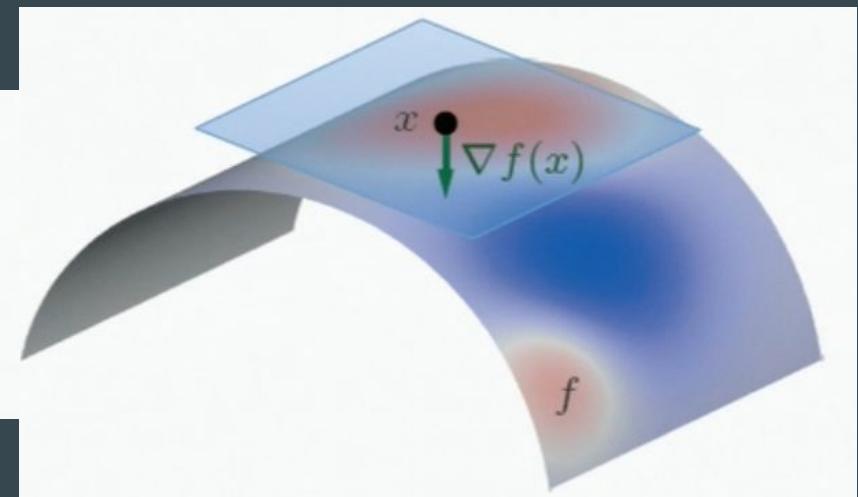


Laplacian on Manifolds

Intrinsic gradient operator

$$\nabla f : L^2(\mathcal{X}) \rightarrow L^2(T\mathcal{X})$$

“direction of steepest change of f ”

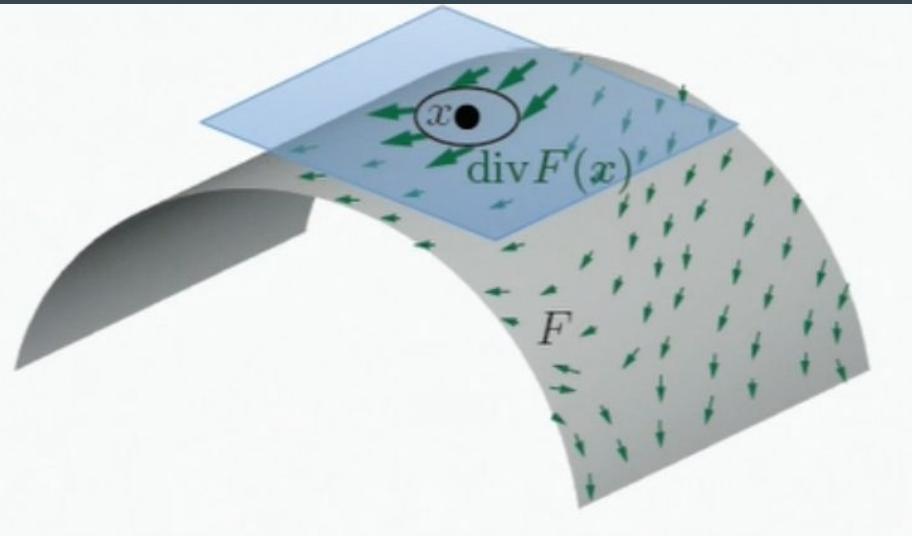


Laplacian on Manifolds

Intrinsic divergence operator

$$\operatorname{div} : L^2(T\mathcal{X}) \rightarrow L^2(\mathcal{X})$$

“net flow of field F at x ”

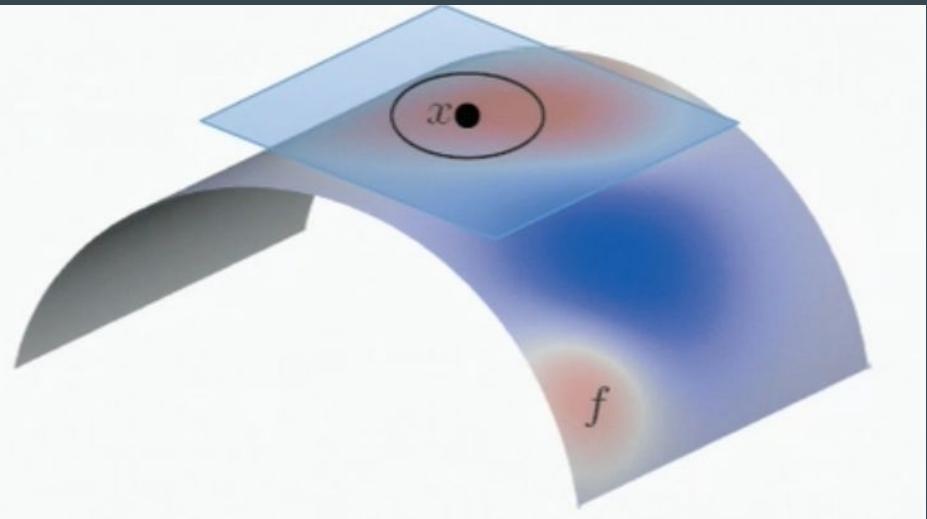


Laplacian on Manifolds

Laplacian $\Delta : L^2(\mathcal{X}) \rightarrow L^2(\mathcal{X})$

$$\Delta f = -\text{div}(\nabla f)$$

“difference between $f(x)$ and average value of f around x ”



Laplacian on Manifolds

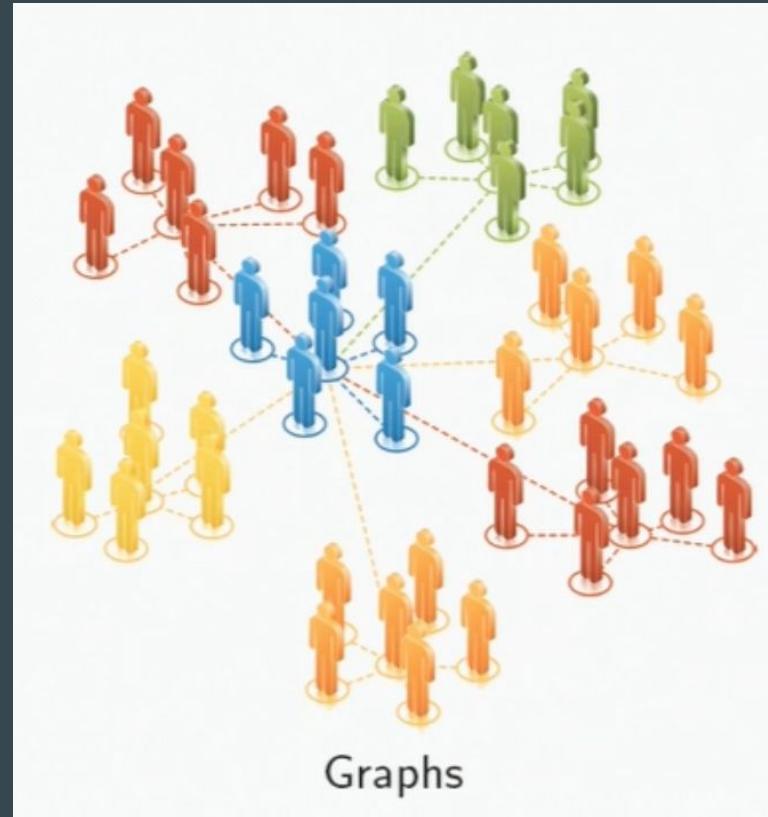
Intrinsic

Isometry-invariant

Self-adjoint $\langle \Delta f, g \rangle_{L^2(\mathcal{X})} = \langle f, \Delta g \rangle_{L^2(\mathcal{X})} \Rightarrow$ orthogonal eigenfunctions

Positive semidefinite \Rightarrow non-negative eigenvalues

Non-Euclidean Domains

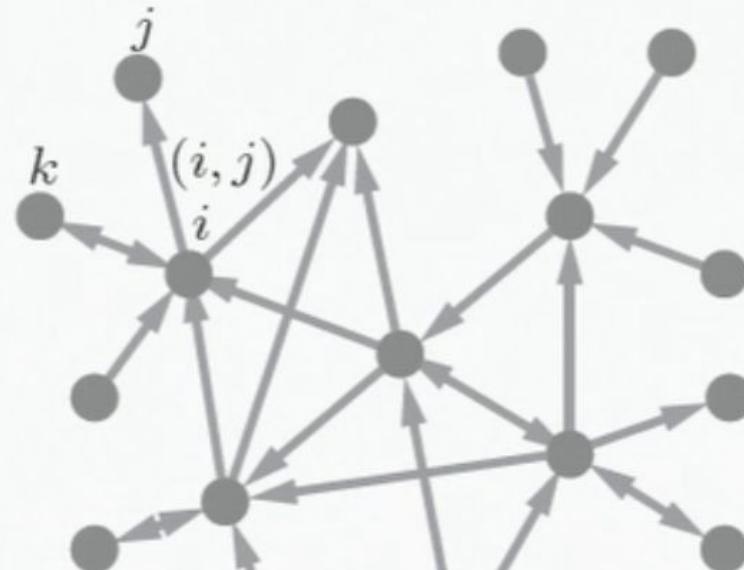


Graph Definitions

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

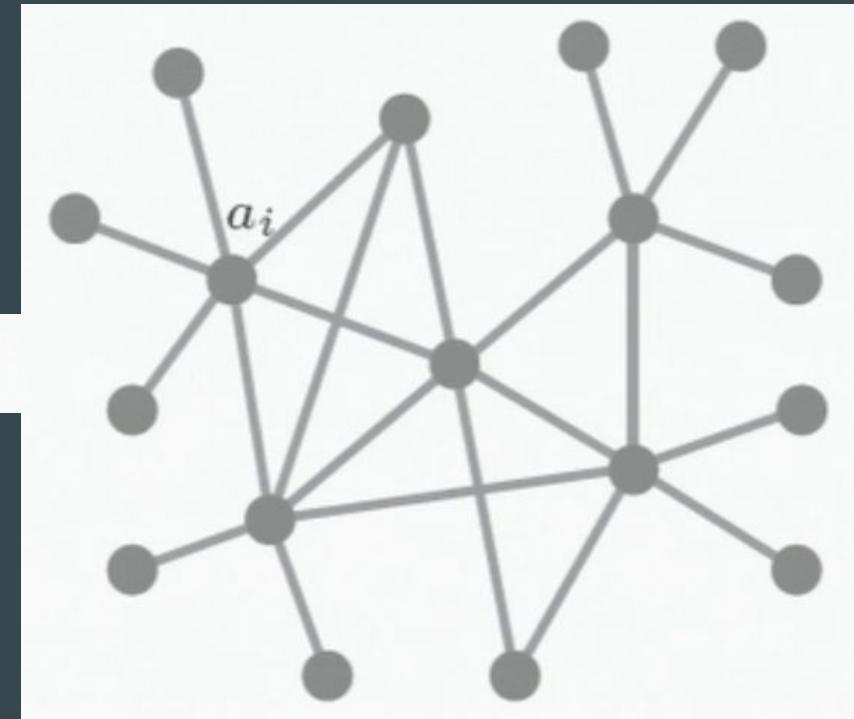
Vertices $\mathcal{V} = \{1, \dots, n\}$

Edges $\mathcal{E} \subseteq \mathcal{V} \times \mathcal{V}$



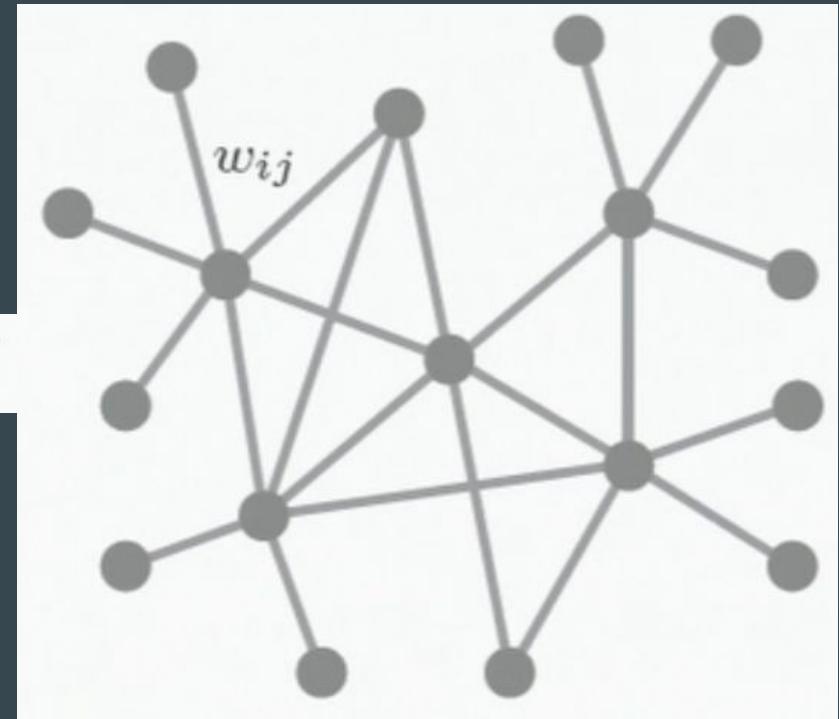
Graph Definitions

Vertex weights $a_i > 0$ for $i \in \mathcal{V}$



Graph Definitions

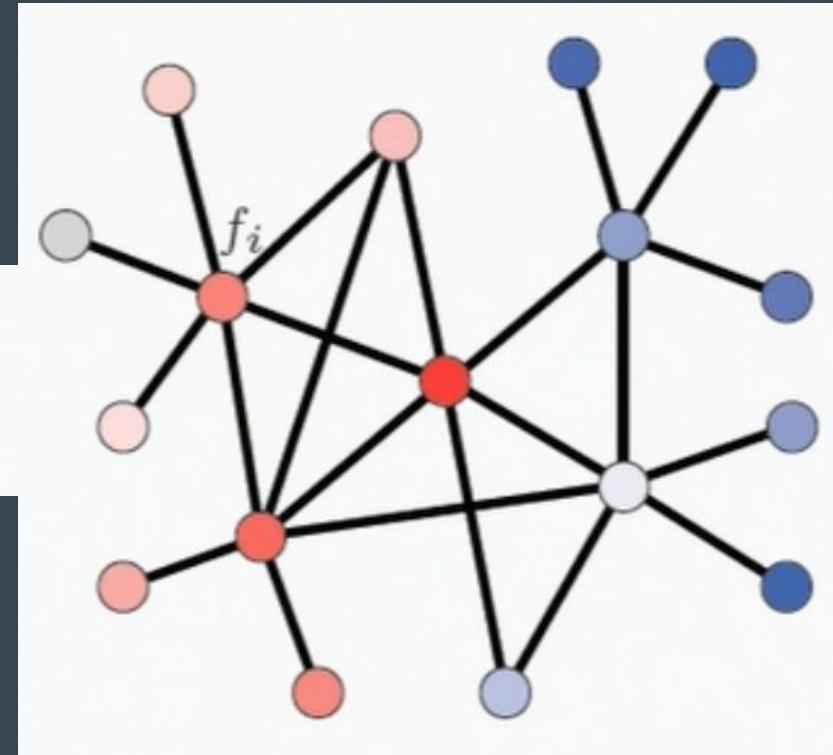
Edge weights $w_{ij} \geq 0$ for $(i, j) \in \mathcal{E}$



Graph Definitions

Vertex field $f : \mathcal{V} \rightarrow \mathbb{R}$

$$\langle f, g \rangle_{L^2(\mathcal{V})} = \sum_{i \in \mathcal{V}} a_i f_i g_i$$

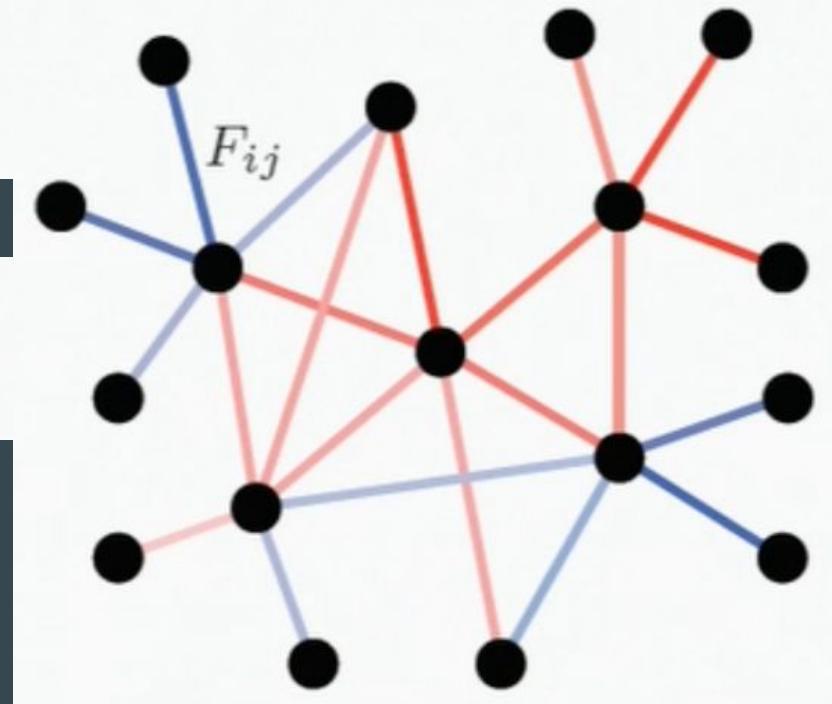


Graph Definitions

Edge field $F : \mathcal{E} \rightarrow \mathbb{R}$

assumed alternating $F_{ij} = -F_{ji}$

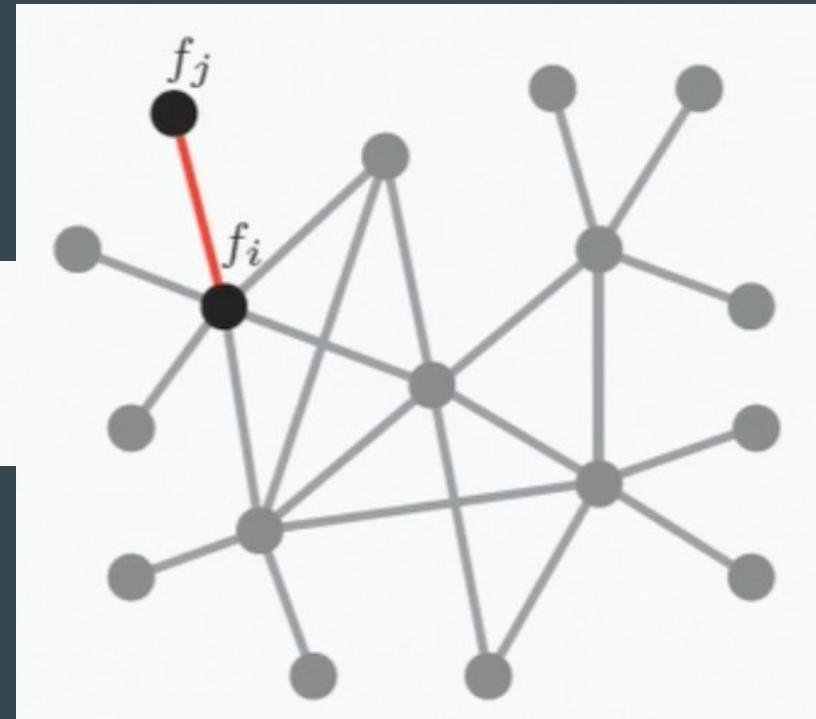
$$\langle F, G \rangle_{L^2(\mathcal{E})} = \sum_{i \in \mathcal{E}} w_{ij} F_{ij} G_{ij}$$



Laplacian on Graphs

Gradient operator $\nabla : L^2(\mathcal{V}) \rightarrow L^2(\mathcal{E})$

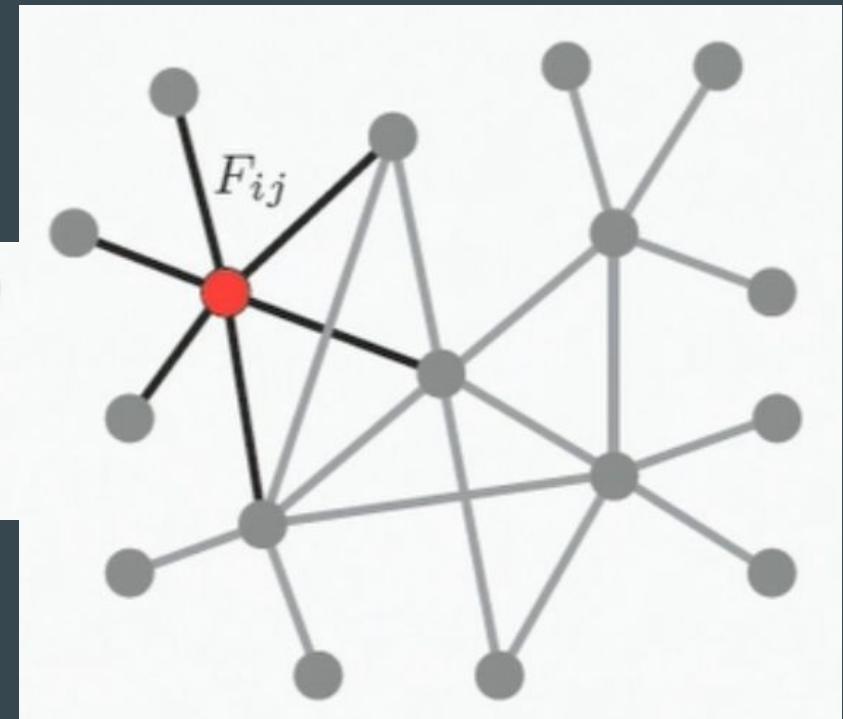
$$(\nabla f)_{ij} = f_i - f_j$$



Laplacian on Graphs

Divergence operator $\operatorname{div} : L^2(\mathcal{E}) \rightarrow L^2(\mathcal{V})$

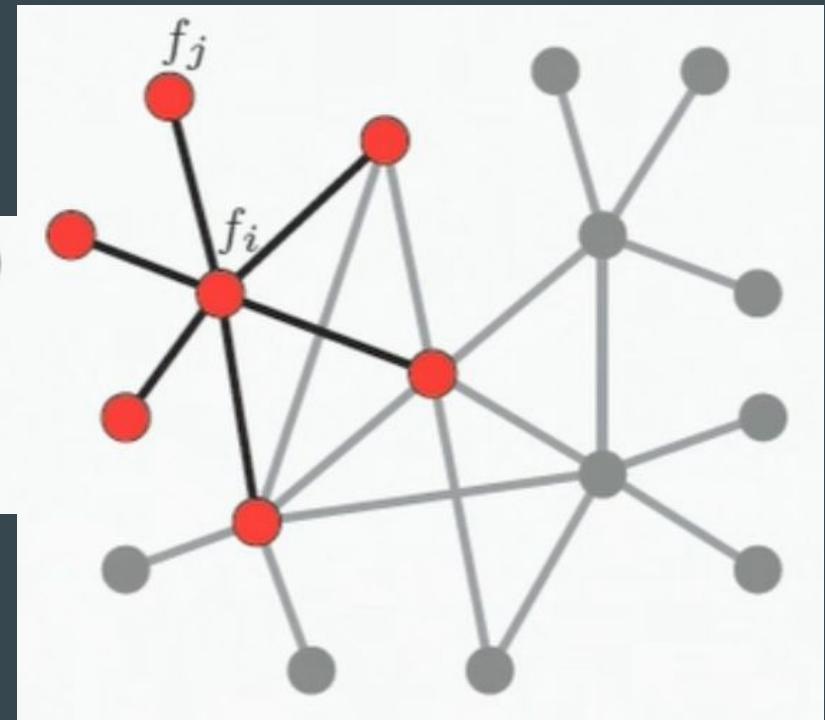
$$(\operatorname{div} F)_i = \frac{1}{a_i} \sum_{j:(i,j) \in \mathcal{E}} w_{ij} F_{ij}$$



Laplacian on Graphs

Laplacian operator $\Delta : L^2(\mathcal{V}) \rightarrow L^2(\mathcal{V})$

$$(\Delta f)_i = \frac{1}{a_i} \sum_{j:(i,j) \in \mathcal{E}} w_{ij} (f_i - f_j)$$



Laplacian on Graphs

Represented as a positive semi-definite $n \times n$ matrix

$$\Delta = A^{-1}(D - W)$$

where $W = (w_{ij})$, $A = \text{diag}(a_1, \dots, a_n)$, and $D = \text{diag}(\sum_{j \neq i} w_{ij})$

Laplacian on Graphs

Represented as a positive semi-definite $n \times n$ matrix

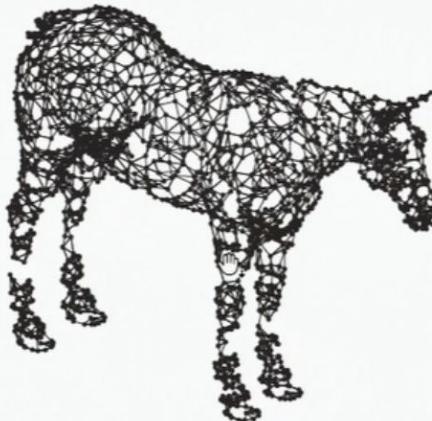
$$\Delta = A^{-1}(D - W)$$

where $W = (w_{ij})$, $A = \text{diag}(a_1, \dots, a_n)$, and $D = \text{diag}(\sum_{j \neq i} w_{ij})$

Unnormalized Laplacian: $\Delta = D - W$ $(A = I)$

Random walk Laplacian: $\Delta = D^{-1}(D - W)$ $(A = D)$

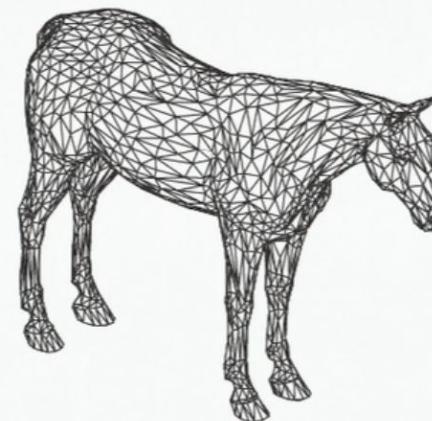
Graphs as Discrete Manifolds



Nearest neighbor graph

Vertices $\mathcal{V} = \{1, \dots, n\}$

Edges $\mathcal{E} \subseteq \mathcal{V} \times \mathcal{V}$



Triangular mesh

Vertices $\mathcal{V} = \{1, \dots, n\}$

Edges $\mathcal{E} \subseteq \mathcal{V} \times \mathcal{V}$

Faces $\mathcal{F} = \{(i, j, k) \in \mathcal{V} \times \mathcal{V} \times \mathcal{V} : (i, j), (j, k), (k, i) \in \mathcal{E}\}$

Spectral Analysis

Eigendecomposition of the Laplacian

Laplacian of a compact manifold \mathcal{X} has countably many eigenfunctions

$$\Delta\phi_k(x) = \lambda_k\phi_k(x), \quad k = 1, 2, \dots$$

Eigenfunctions are real and orthonormal

Eigenvalues are non-negative $0 = \lambda_1 \leq \lambda_2 \leq \dots$

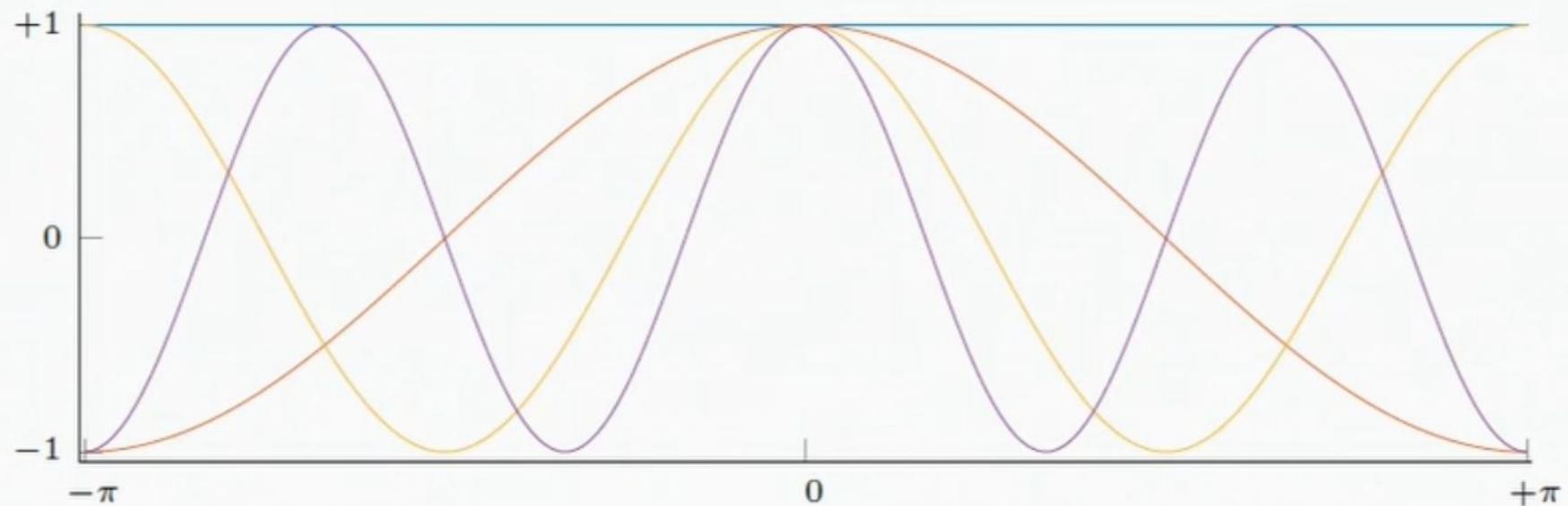
Eigendecomposition of the Laplacian

Eigendecomposition of a graph Laplacian

$$\Delta \Phi = \Phi \Lambda$$

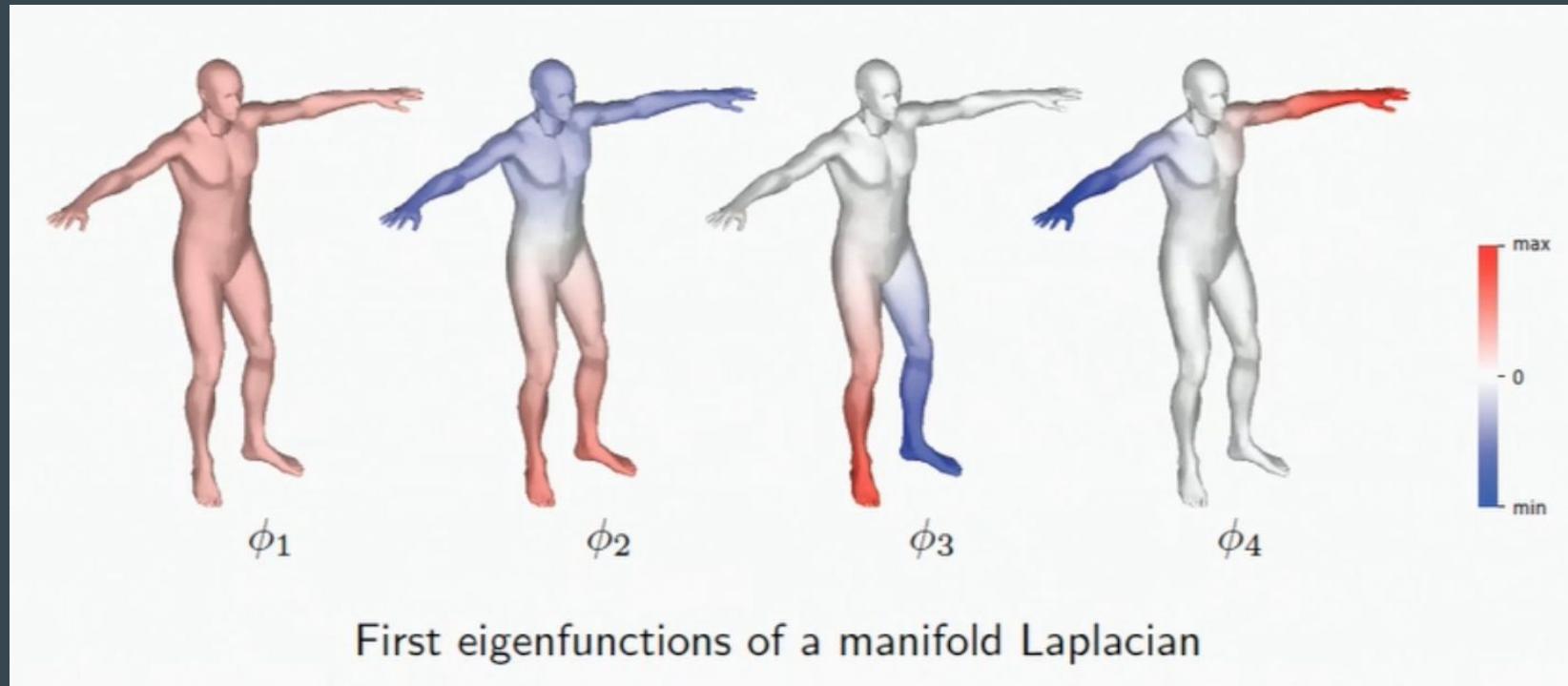
where $\Phi = (\phi_1, \dots, \phi_n)$ and $\Lambda = \text{diag}(\lambda_1, \dots, \lambda_n)$

Eigendecomposition of the Laplacian

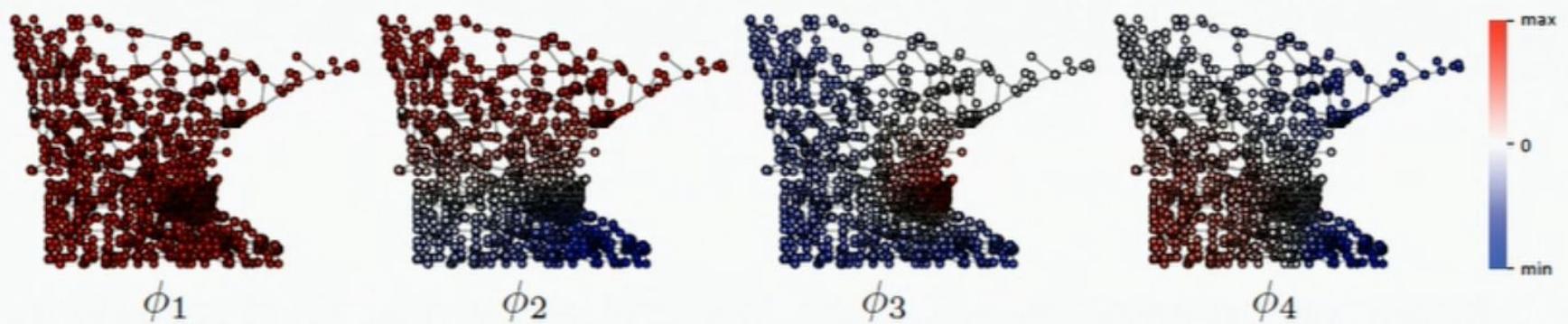


First eigenfunctions of 1D Euclidean Laplacian = standard Fourier basis

Eigendecomposition of the Laplacian

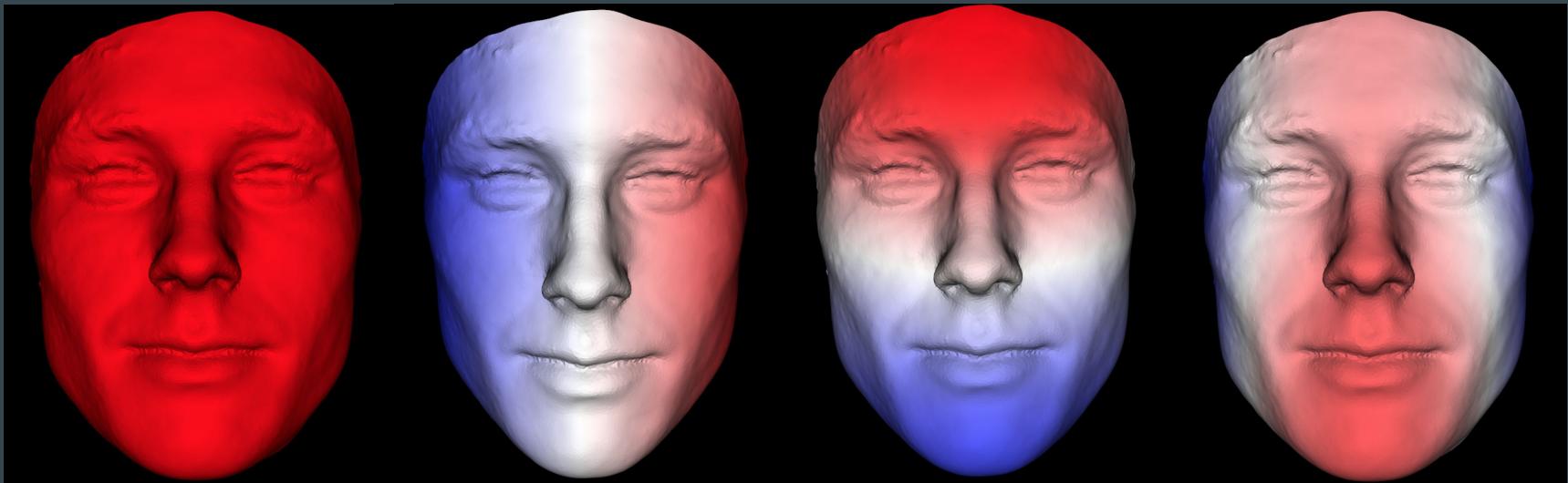


Eigendecomposition of the Laplacian

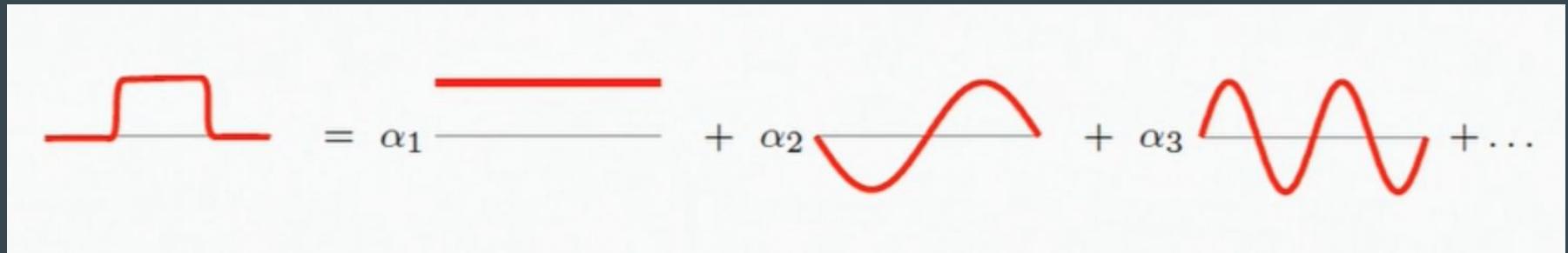


First eigenfunctions of a graph Laplacian

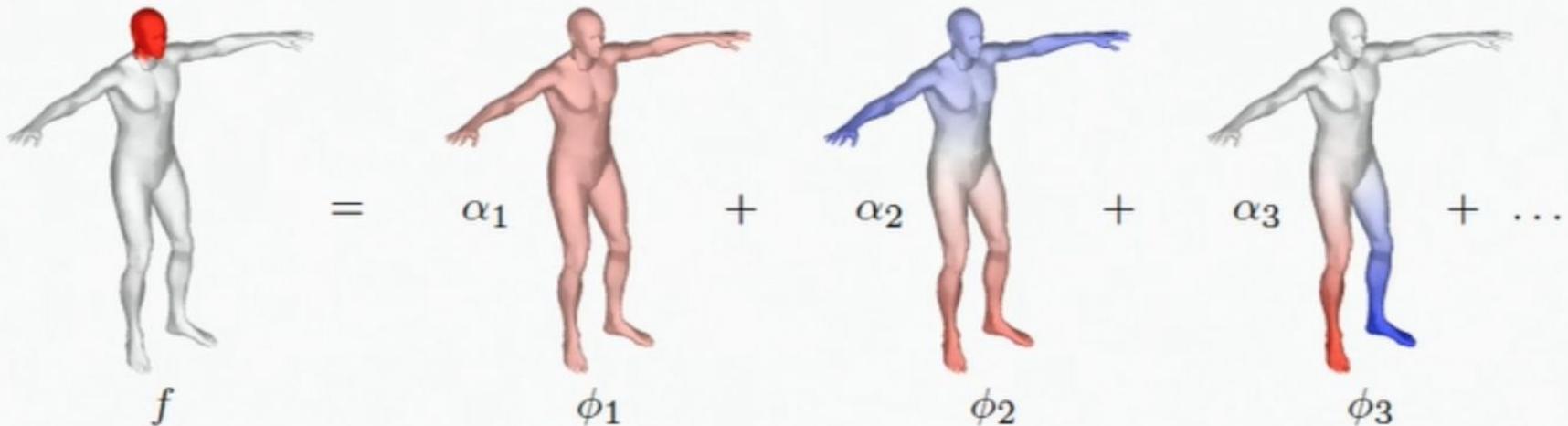
Eigendecomposition of the Laplacian



Fourier Analysis



Fourier Analysis



Fourier basis = Laplacian eigenfunctions: $\Delta\phi_k(x) = \lambda_k\phi_k(x)$

Convolution in the Euclidean Domain

Given two functions $f, g : [-\pi, \pi] \rightarrow \mathbb{R}$ their convolution is a function

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

- Shift-invariance: $f(x - x_0) \star g(x) = (f \star g)(x - x_0)$
- Convolution operator commutes with Laplacian: $(\Delta f) \star g = \Delta(f \star g)$
- Convolution theorem: Fourier transform diagonalizes the convolution operator \Rightarrow convolution can be computed in the Fourier domain as

$$\widehat{(f \star g)} = \hat{f} \cdot \hat{g}$$

- Efficient computation using FFT with $\mathcal{O}(n \log n)$ complexity

Convolution in the Euclidean Domain

Convolution of two vectors $\mathbf{f} = (f_1, \dots, f_n)^\top$ and $\mathbf{g} = (g_1, \dots, g_n)^\top$

$$\mathbf{f} * \mathbf{g} = \begin{bmatrix} g_1 & g_2 & \dots & \dots & g_n \\ g_n & g_1 & g_2 & \dots & g_{n-1} \\ \vdots & \vdots & \ddots & \ddots & \vdots \\ g_3 & g_4 & \dots & g_1 & g_2 \\ g_2 & g_2 & \dots & \dots & g_1 \end{bmatrix} \begin{bmatrix} f_1 \\ \vdots \\ f_n \end{bmatrix}$$

Convolution in the Spectral Domain

$$\Phi \begin{bmatrix} \hat{g}_1 \\ \ddots \\ \hat{g}_n \end{bmatrix} \Phi^\top \mathbf{f}$$

Convolution in the Spectral Domain

$$\Phi \begin{bmatrix} \hat{g}_1 \\ \ddots \\ \hat{g}_n \end{bmatrix} \Phi^\top f = \Phi \begin{bmatrix} \hat{g}_1 \\ \ddots \\ \hat{g}_n \end{bmatrix} \begin{bmatrix} \hat{f}_1 \\ \vdots \\ \hat{f}_n \end{bmatrix}$$

Convolution in the Spectral Domain

$$\Phi \begin{bmatrix} \hat{g}_1 \\ \ddots \\ \hat{g}_n \end{bmatrix} \Phi^\top f = \Phi \begin{bmatrix} \hat{g}_1 \\ \ddots \\ \hat{g}_n \end{bmatrix} \begin{bmatrix} \hat{f}_1 \\ \vdots \\ \hat{f}_n \end{bmatrix}$$

$$= \Phi \begin{bmatrix} \hat{f}_1 \cdot \hat{g}_1 \\ \vdots \\ \hat{f}_n \cdot \hat{g}_n \end{bmatrix}$$

Generalized Spectral Convolution

Generalized convolution of $f, g \in L^2(\mathcal{X})$ can be defined by analogy

$$f \star g = \underbrace{\sum_{k \geq 1} \underbrace{\langle f, \phi_k \rangle_{L^2(\mathcal{X})} \langle g, \phi_k \rangle_{L^2(\mathcal{X})}}_{\text{product in the Fourier domain}} \phi_k}_{\text{inverse Fourier transform}}$$

Generalized Spectral Convolution

In matrix-vector notation

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

Generalized Spectral Convolution

In matrix-vector notation

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

$$\mathbf{f} \star \mathbf{g} = \Phi \operatorname{diag}(\hat{g}_1, \dots, \hat{g}_n) \Phi^\top \mathbf{f}$$

Generalized Spectral Convolution

In matrix-vector notation

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

$$\mathbf{f} \star \mathbf{g} = \underbrace{\Phi \operatorname{diag}(\hat{g}_1, \dots, \hat{g}_n) \Phi^\top}_{\mathbf{G}} \mathbf{f}$$

Generalized Spectral Convolution

$$\mathbf{f} \star \mathbf{g} = \underbrace{\Phi \operatorname{diag}(\hat{g}_1, \dots, \hat{g}_n) \Phi^\top}_{\mathbf{G}} \mathbf{f}$$

Not shift-invariant! (\mathbf{G} has no circulant structure)

Commutes with Laplacian: $\mathbf{G}\Delta\mathbf{f} = \Delta\mathbf{G}\mathbf{f}$

Filter coefficients depend on basis ϕ_1, \dots, ϕ_n

Generalized Spectral CNNs

Spectral Convolutional Layer

Convolutional layer expressed in the spectral domain

$$\mathbf{g}_l = \xi \left(\sum_{l'=1}^p \Phi \mathbf{W}_{l,l'} \Phi^\top \mathbf{f}_{l'} \right) \quad \begin{matrix} l = 1, \dots, q \\ l' = 1, \dots, p \end{matrix}$$

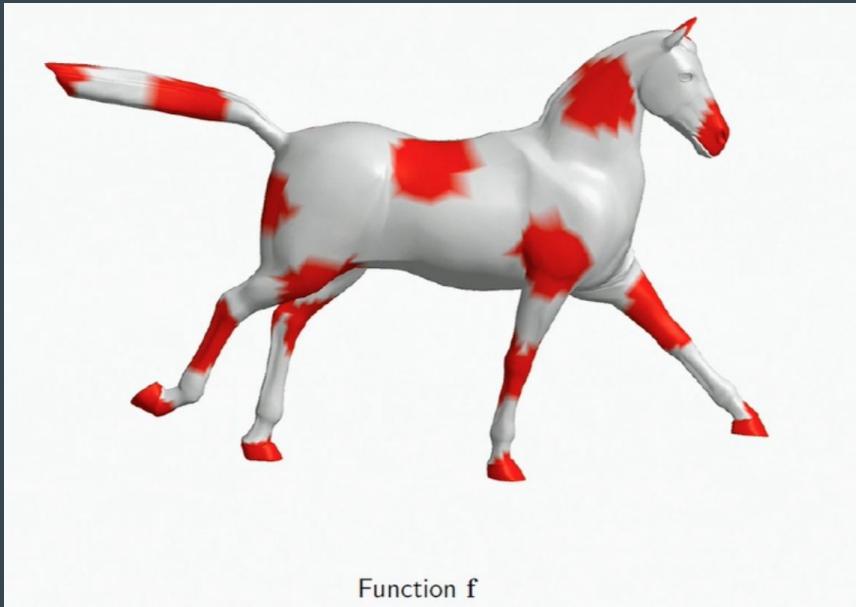
where $\mathbf{W}_{l,l} = n \times n$ diagonal matrix of filter coefficients

Spectral Convolutional Layer

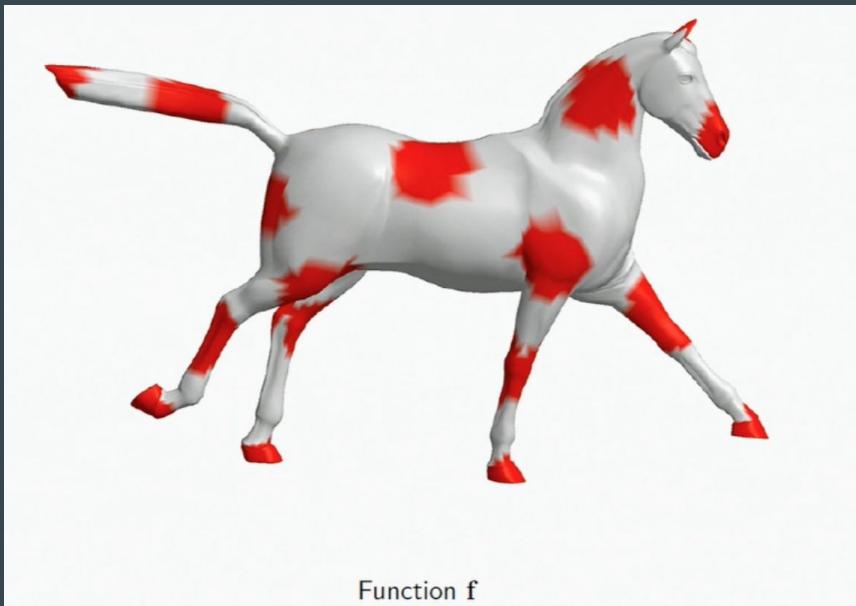
$$\mathbf{g}_l = \xi \left(\sum_{l'=1}^p \Phi \mathbf{W}_{l,l'} \Phi^\top \mathbf{f}_{l'} \right) \quad \begin{matrix} l = 1, \dots, q \\ l' = 1, \dots, p \end{matrix}$$

- ⌚ Filters are basis-dependent \Rightarrow does not generalize across graphs!
- ⌚ $\mathcal{O}(n)$ parameters per layer
- ⌚ $\mathcal{O}(n^2)$ computation of forward and inverse Fourier transforms Φ^\top, Φ (no FFT on graphs)
- ⌚ No guarantee of spatial localization of filters

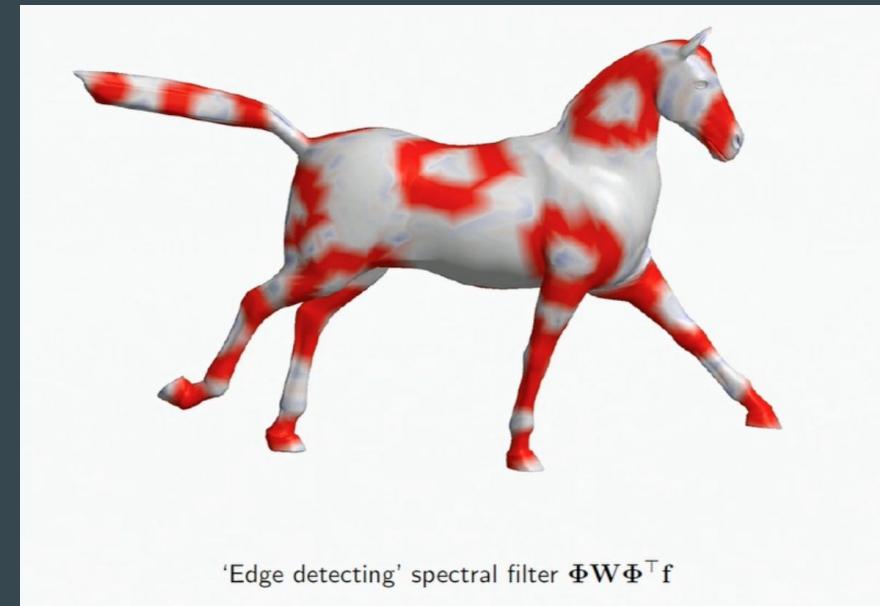
Lack of Generalizability



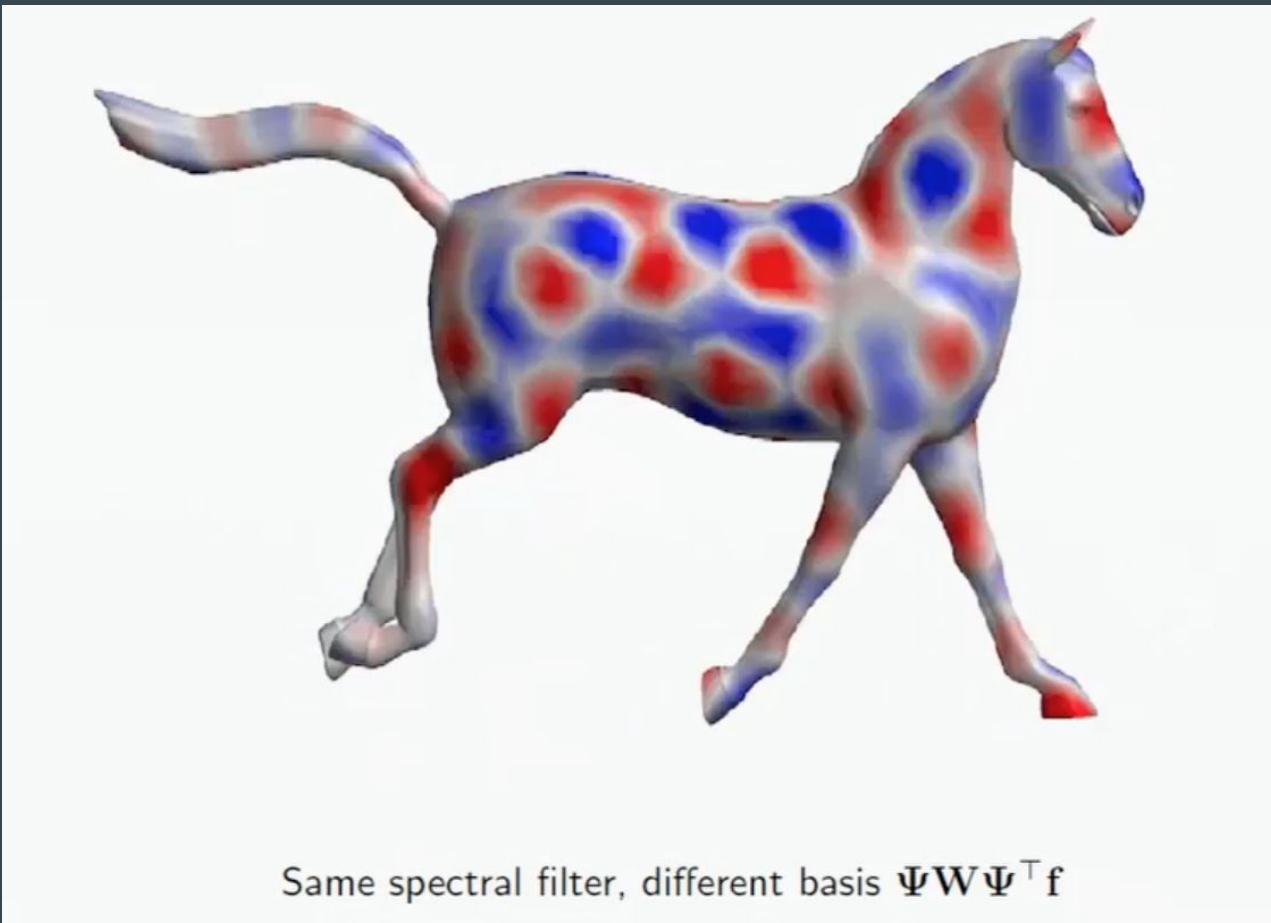
Lack of Generalizability



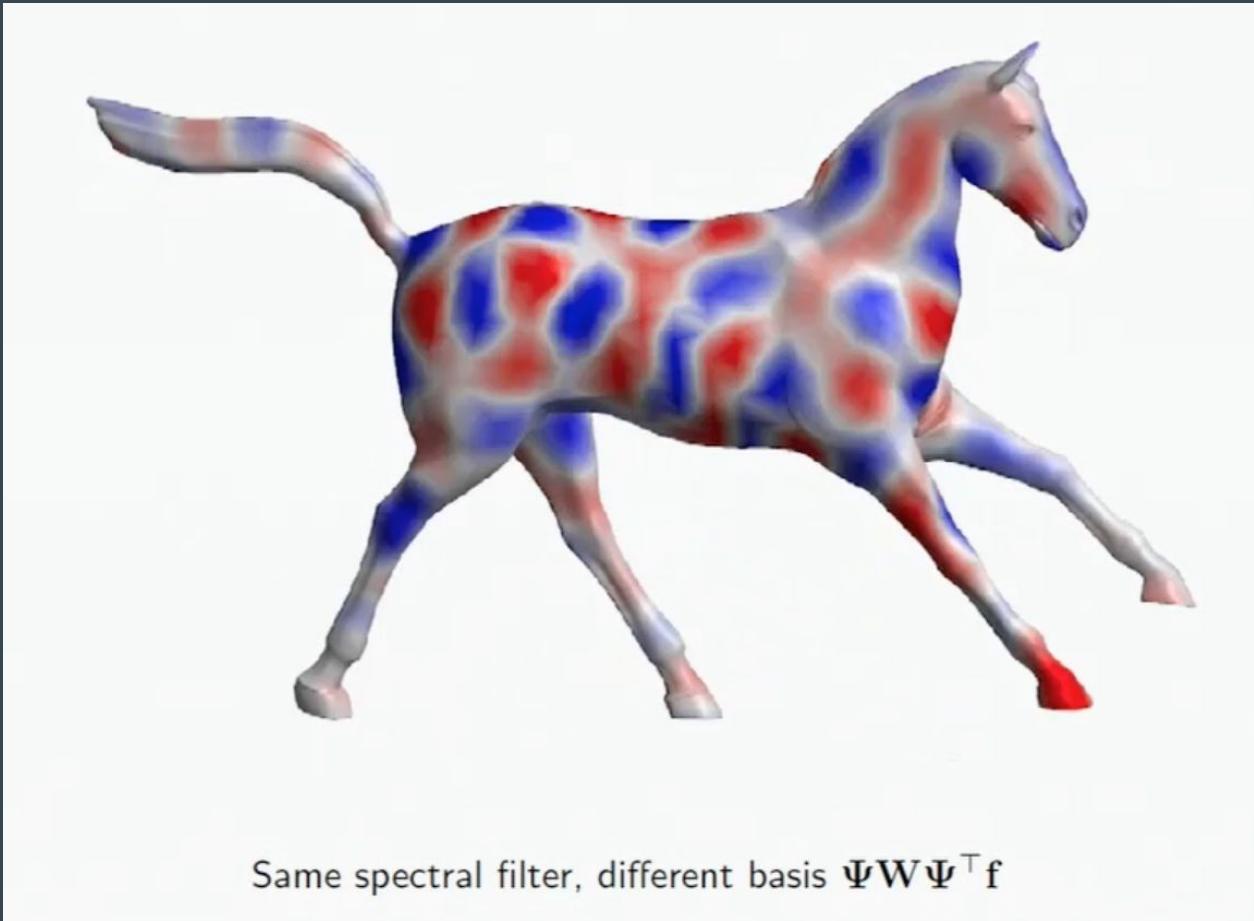
Function f



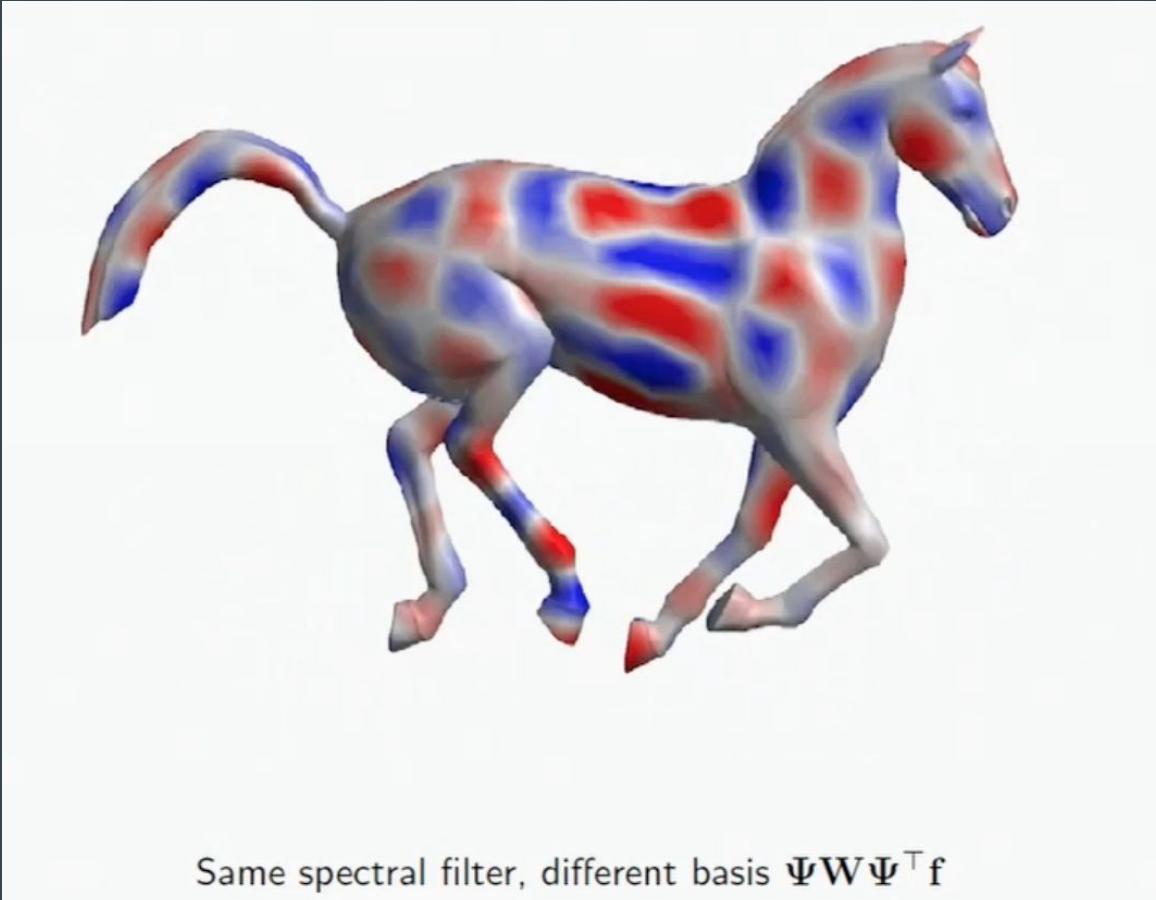
'Edge detecting' spectral filter $\Phi W \Phi^T f$



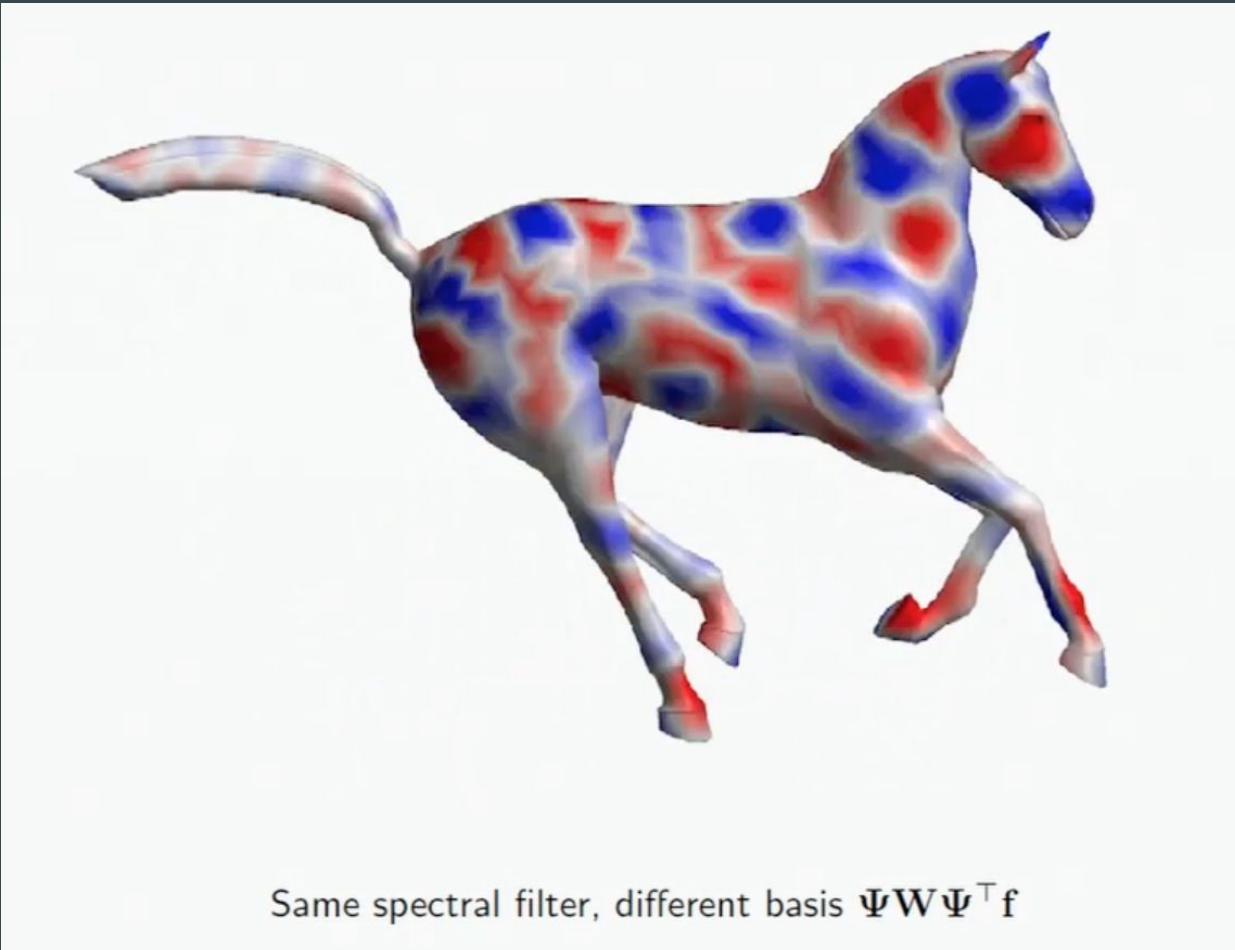
Same spectral filter, different basis $\Psi \mathbf{W} \Psi^\top \mathbf{f}$



Same spectral filter, different basis $\Psi \mathbf{W} \Psi^\top \mathbf{f}$



Same spectral filter, different basis $\Psi \mathbf{W} \Psi^\top \mathbf{f}$



Same spectral filter, different basis $\Psi \mathbf{W} \Psi^\top \mathbf{f}$

Spatial Localization

Localization in space = smoothness in frequency domain

Spatial Localization

Localization in space = smoothness in frequency domain

Parametrize the filter using a smooth spectral transfer function $\tau(\lambda)$

Spatial Localization

Localization in space = smoothness in frequency domain

Parametrize the filter using a smooth spectral transfer function $\tau(\lambda)$

$$\tau(\Delta)\mathbf{f} = \Phi\tau(\Lambda)\Phi^\top\mathbf{f}$$

Spatial Localization

Application of the parametric filter with learnable parameters α

$$\tau_{\alpha}(\Delta)f = \Phi \begin{pmatrix} \tau_{\alpha}(\lambda_1) & & \\ & \ddots & \\ & & \tau_{\alpha}(\lambda_n) \end{pmatrix} \Phi^T f$$

Spatial Localization

Represent spectral transfer function as a **polynomial** or order r

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

where $\alpha = (\alpha_0, \dots, \alpha_r)^{\top}$ is the vector of filter parameters

Application of the filter $\tau_{\alpha}(\Delta)f = \sum_{j=0}^r \alpha_j \Delta^j f$

Spatial Localization

$$\tau_{\alpha}(\Delta)\mathbf{f} = \sum_{j=0}^r \alpha_j \Delta^j \mathbf{f}$$

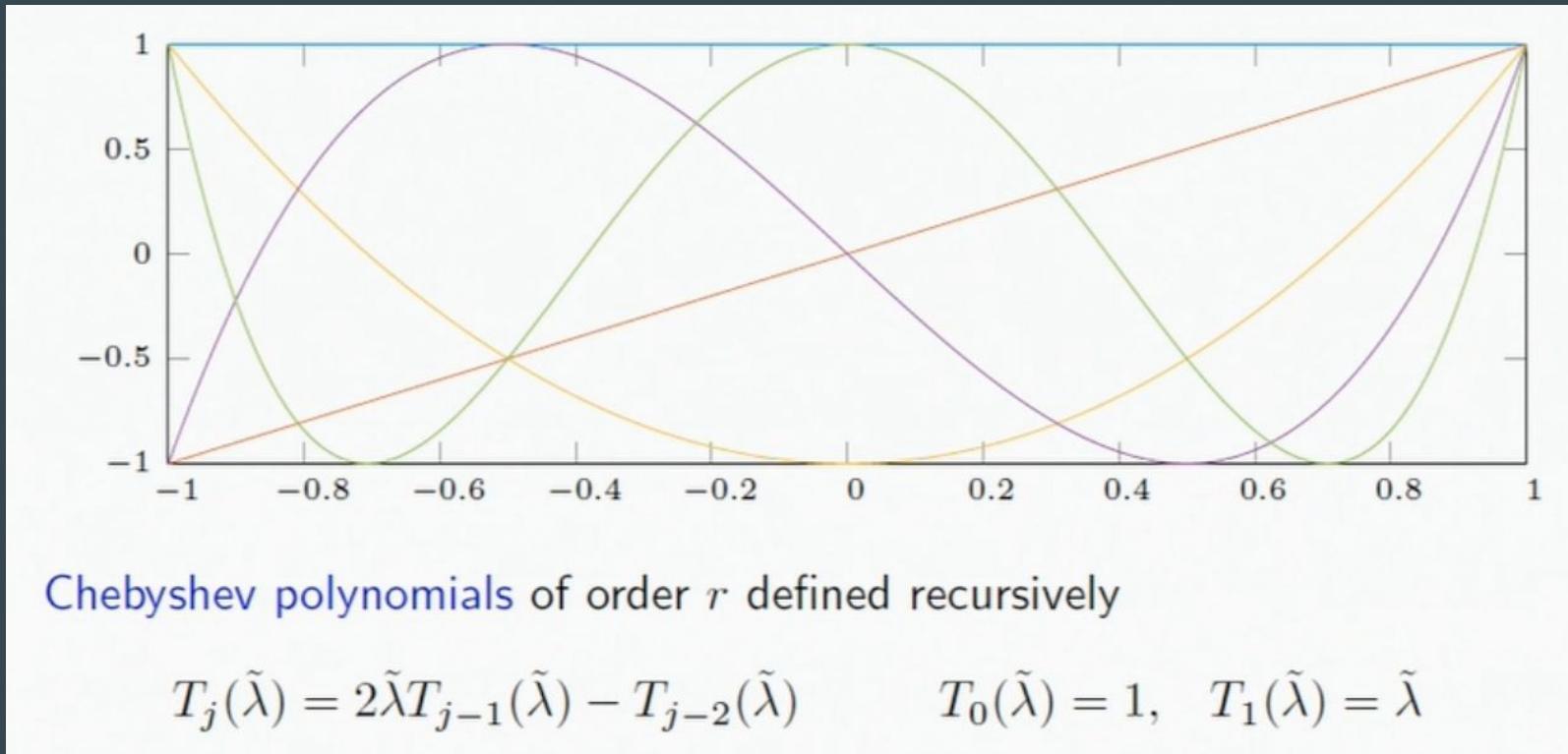
- ☺ $\mathcal{O}(1)$ parameters per layer
- ☺ Filters have guaranteed r -hops support
- ☺ No explicit computation of $\Phi^\top, \Phi \Rightarrow \mathcal{O}(nr)$ computational complexity (assuming sparsely-connected graph)

Almost There...

$$\tau_{\alpha}(\Delta)\mathbf{f} = \sum_{j=0}^r \alpha_j \Delta^j \mathbf{f}$$

- ☺ $\mathcal{O}(1)$ parameters per layer
- ☺ Filters have guaranteed r -hops support
- ☺ No explicit computation of $\Phi^\top, \Phi \Rightarrow \mathcal{O}(nr)$ computational complexity (assuming sparsely-connected graph)
- ☹ Unstable under coefficients perturbation (hard to optimize)

Chebyshev polynomials



Chebyshev approximation

Represent spectral transfer function as a Chebyshev polynomial of order r

$$\tau_{\alpha}(\tilde{\lambda}) = \sum_{j=0}^r \alpha_j T_j(\tilde{\lambda})$$

where $\alpha = (\alpha_0, \dots, \alpha_r)^\top$ is the vector of filter parameters and $-1 \leq \tilde{\lambda} \leq 1$

Application of the filter to scaled Laplacian $\tilde{\Delta} = 2\lambda_n^{-1}\Delta - \mathbf{I}$ recursively

$$\mathbf{g}^{(j)} = 2\tilde{\Delta}\mathbf{g}^{(j-1)} - \mathbf{g}^{(j-2)} \quad \mathbf{g}^{(0)} = \mathbf{f}, \quad \mathbf{g}^{(1)} = \tilde{\Delta}\mathbf{f}$$

Final Construction!

$$\tau_{\alpha}(\tilde{\lambda}) = \sum_{j=0}^r \alpha_j T_j(\tilde{\lambda})$$

$$\mathbf{g}^{(j)} = 2\tilde{\Delta}\mathbf{g}^{(j-1)} - \mathbf{g}^{(j-2)} \quad \mathbf{g}^{(0)} = \mathbf{f}, \quad \mathbf{g}^{(1)} = \tilde{\Delta}\mathbf{f}$$

- ☺ $\mathcal{O}(1)$ parameters per layer
- ☺ Filters have guaranteed r -hops support
- ☺ No explicit computation of $\Phi^\top, \Phi \Rightarrow \mathcal{O}(nr)$ computational complexity (assuming sparsely-connected graph)
- ☺ Stable under coefficients perturbation

Where to go from here?

- Generalizing across graphs
- Pooling on graphs
- Spatial Convolution on graphs
- Wavelet Convolution
- Applications and current results

Thank you!

