UC San Diego

Lecture 19:

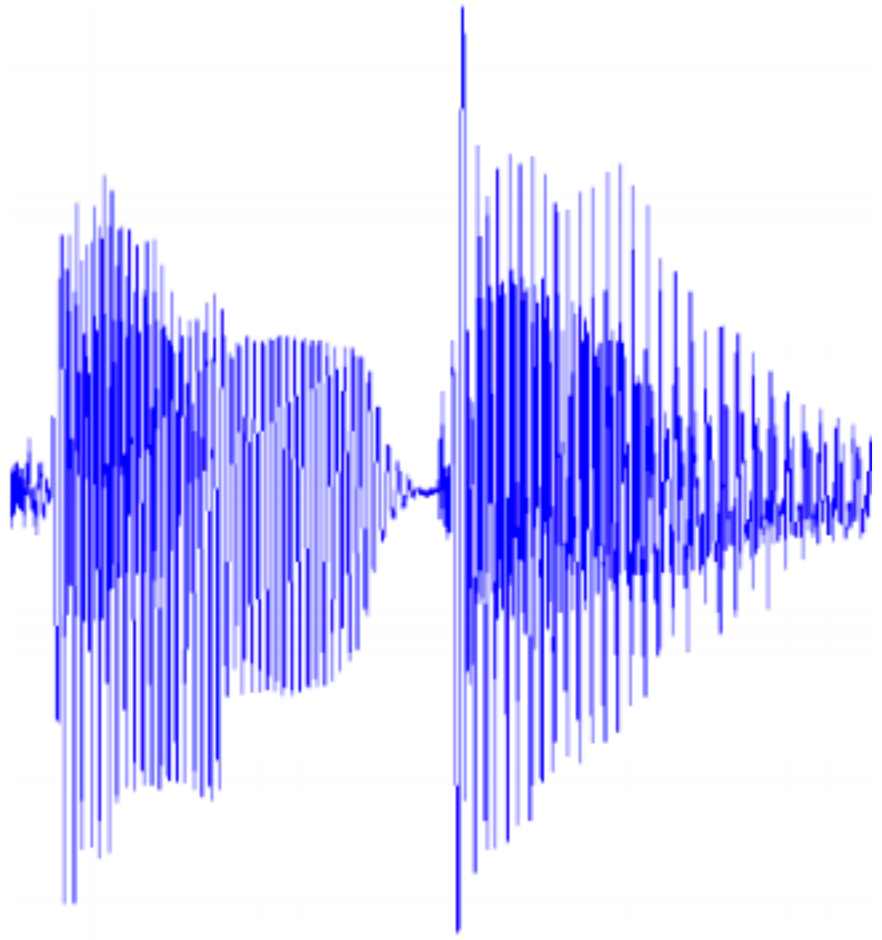
Deep Learning on Graph Data

Instructor: Hao Su

Mar 16, 2018

Slides ack: Li Yi

CNN has been very successful



audio

video

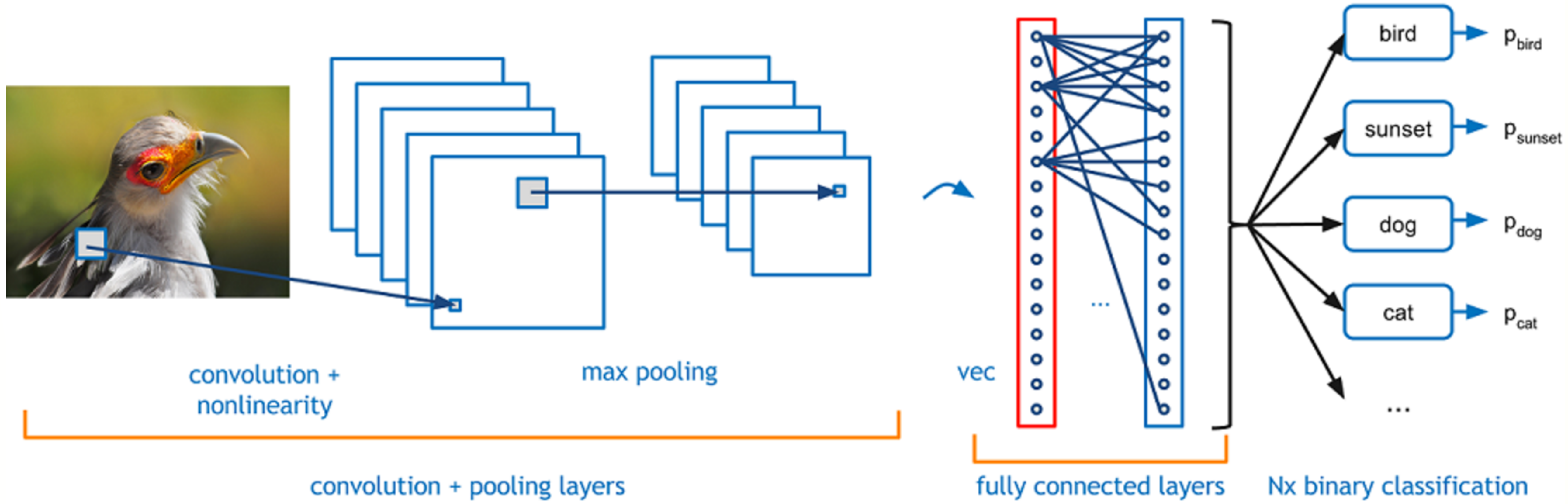


image credit: Adit Deshpande

image

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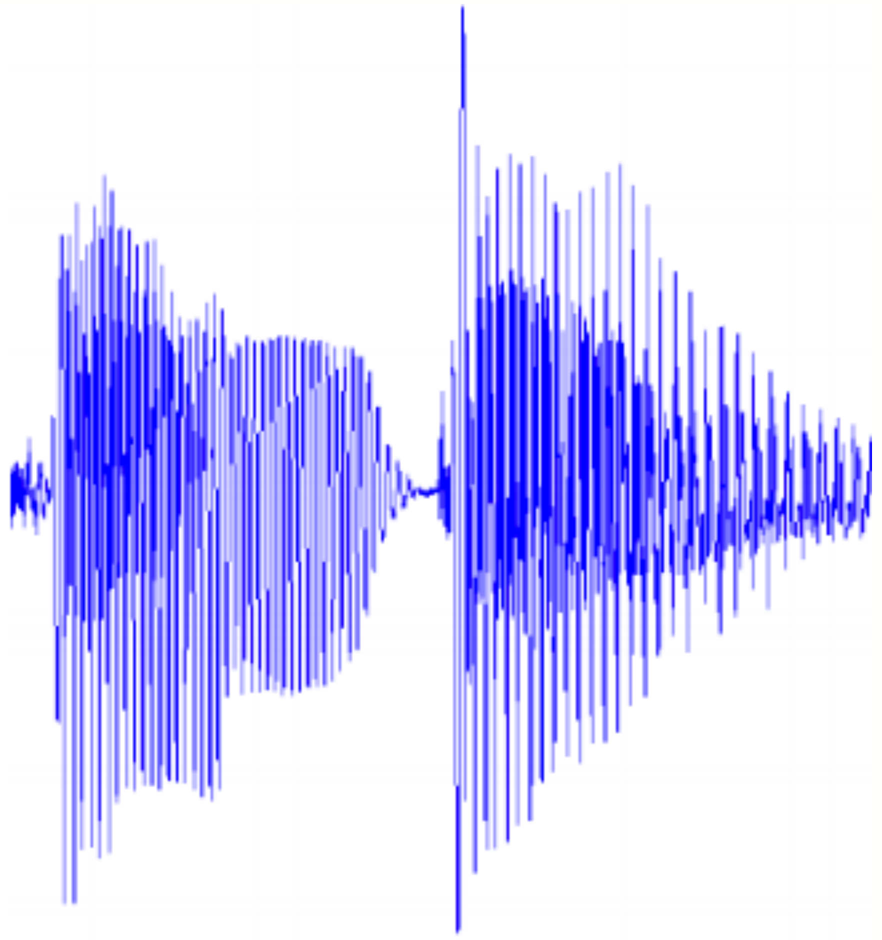

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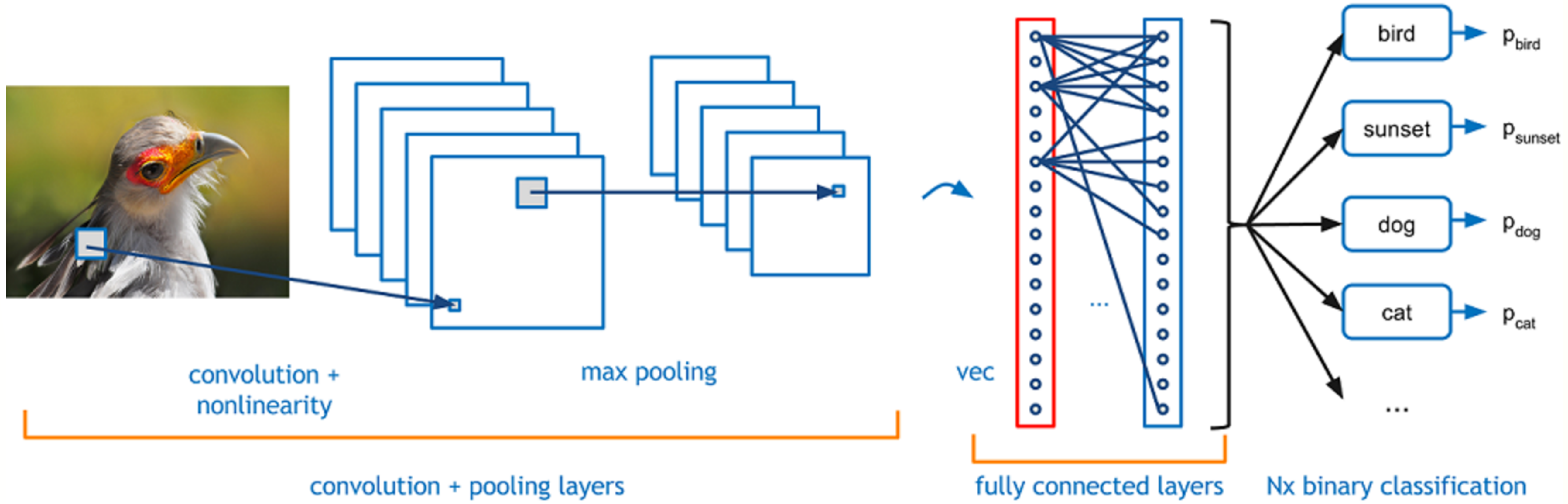

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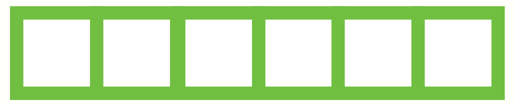
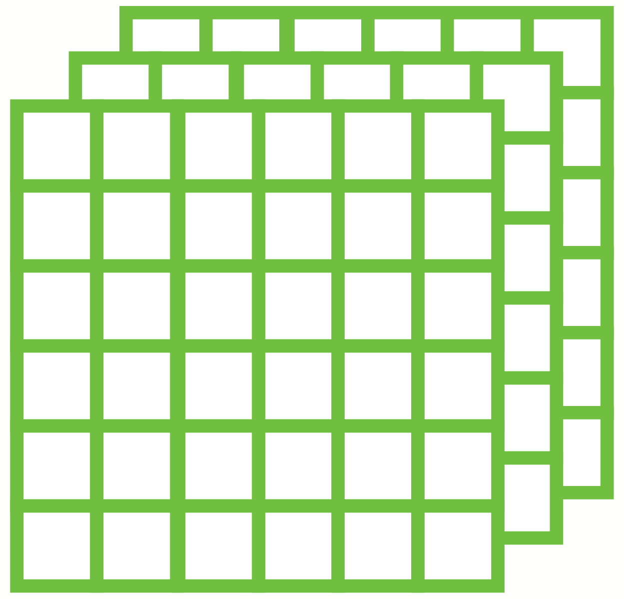
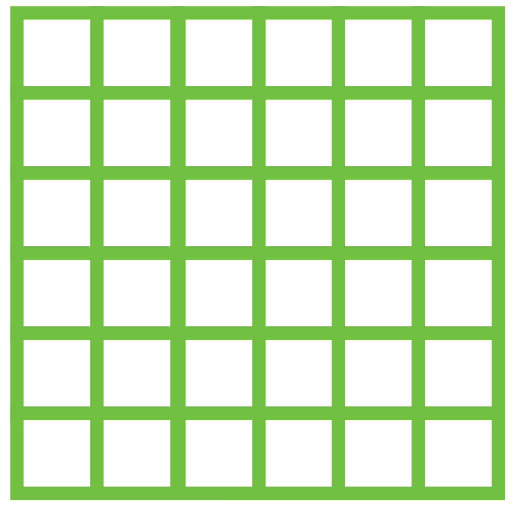
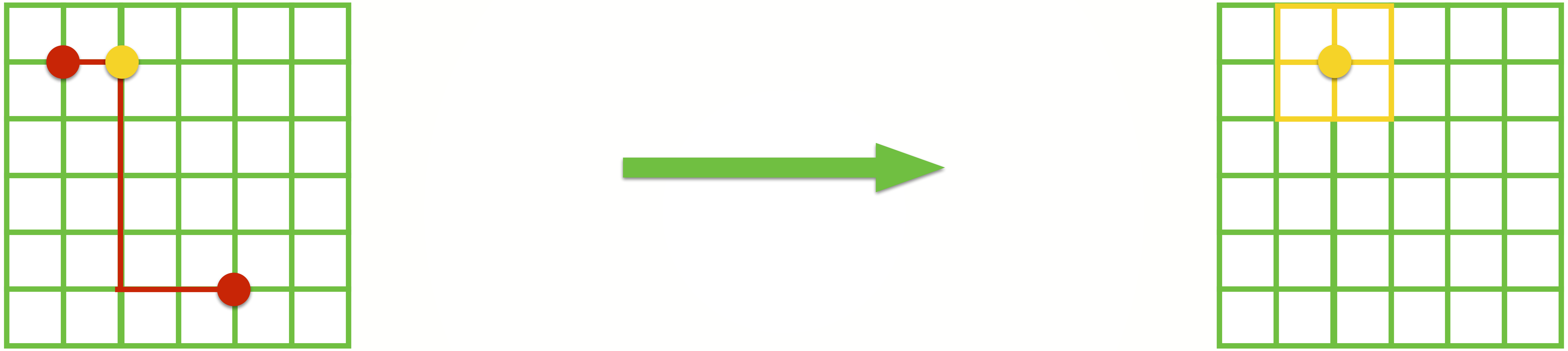






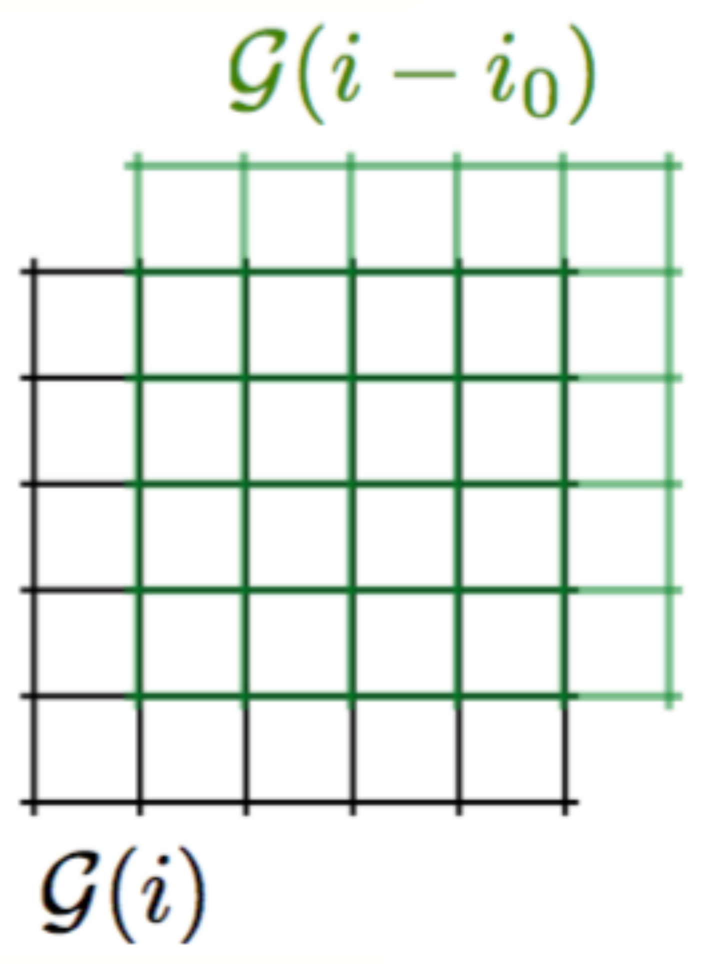
CNN nicely exploits the grid structure



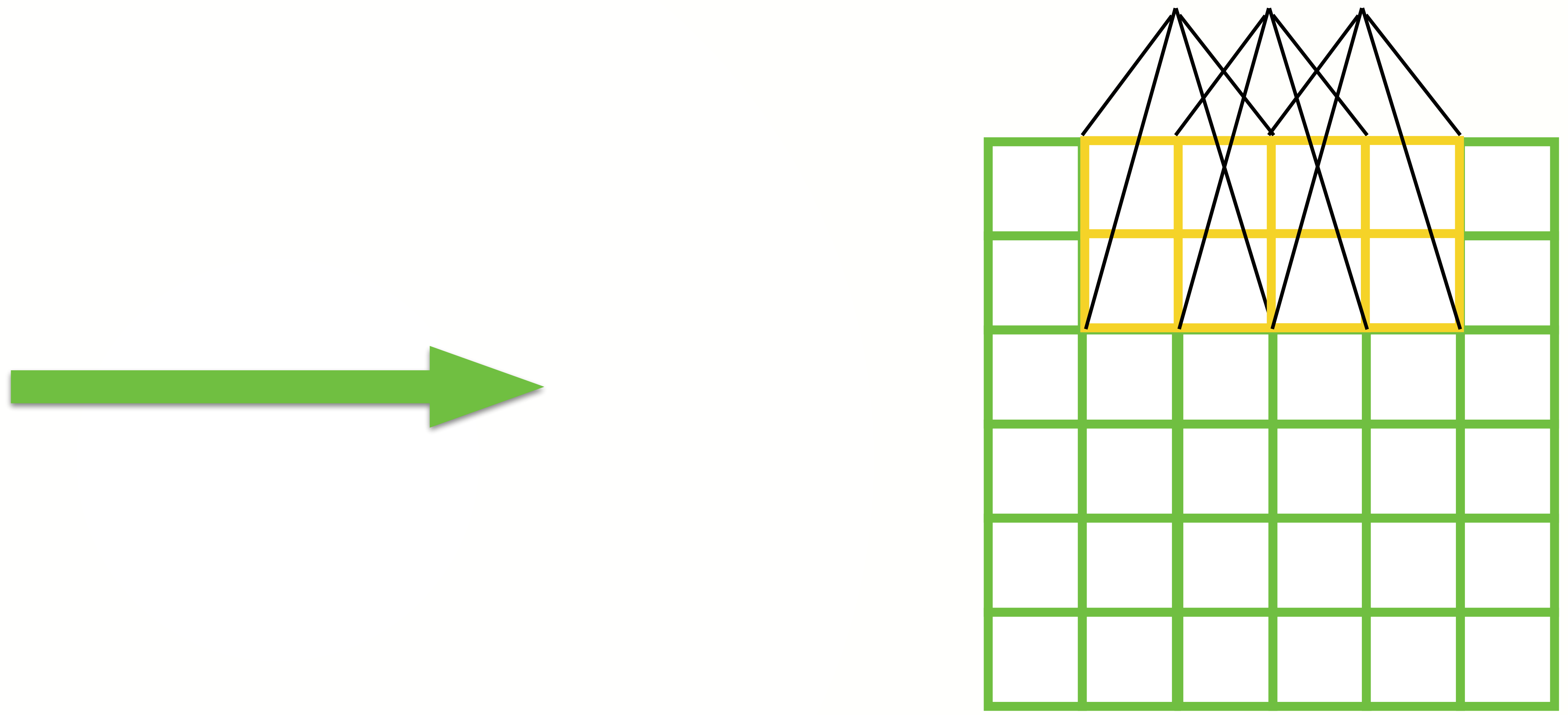
grid metric

locally supported filters

CNN nicely exploits the grid structure

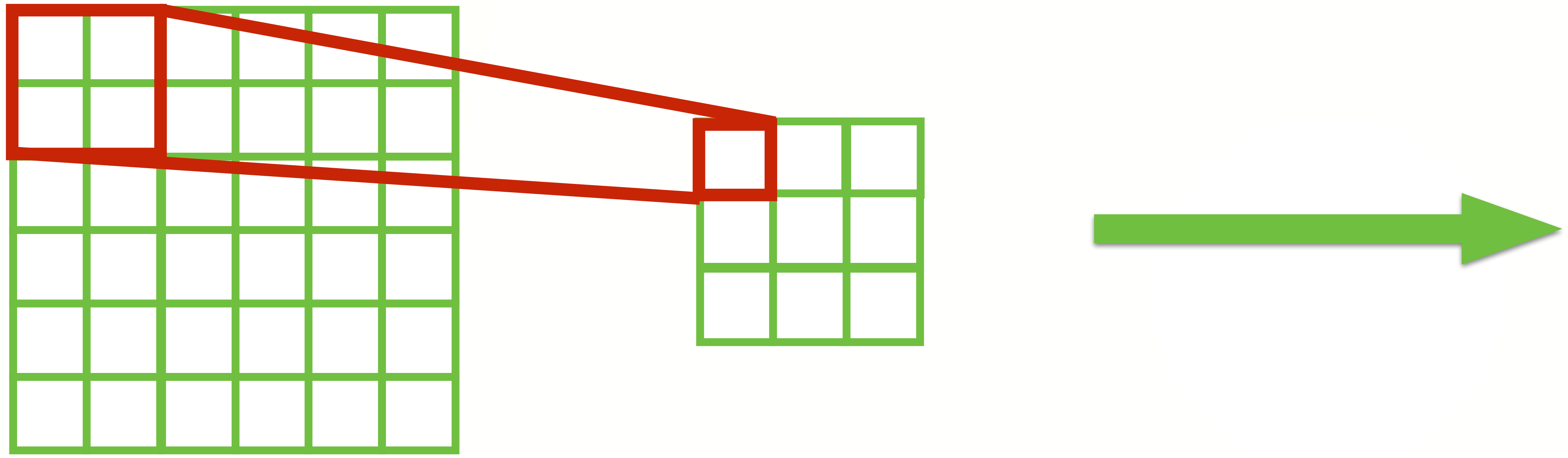


translation structure



allow the use of filters
and weight sharing

CNN nicely exploits the grid structure



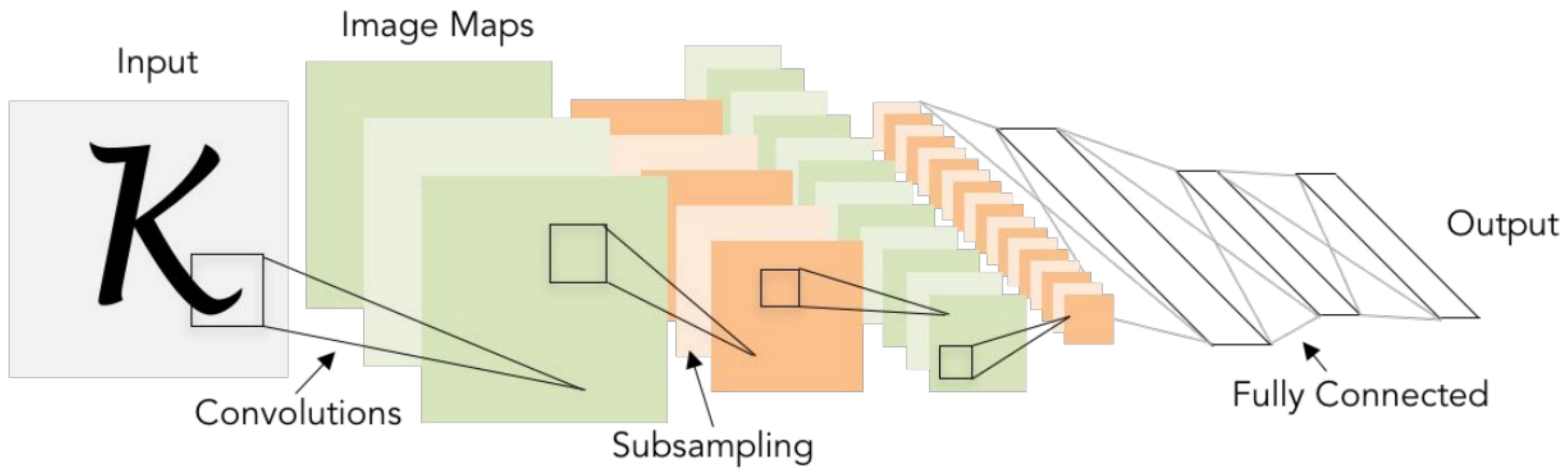
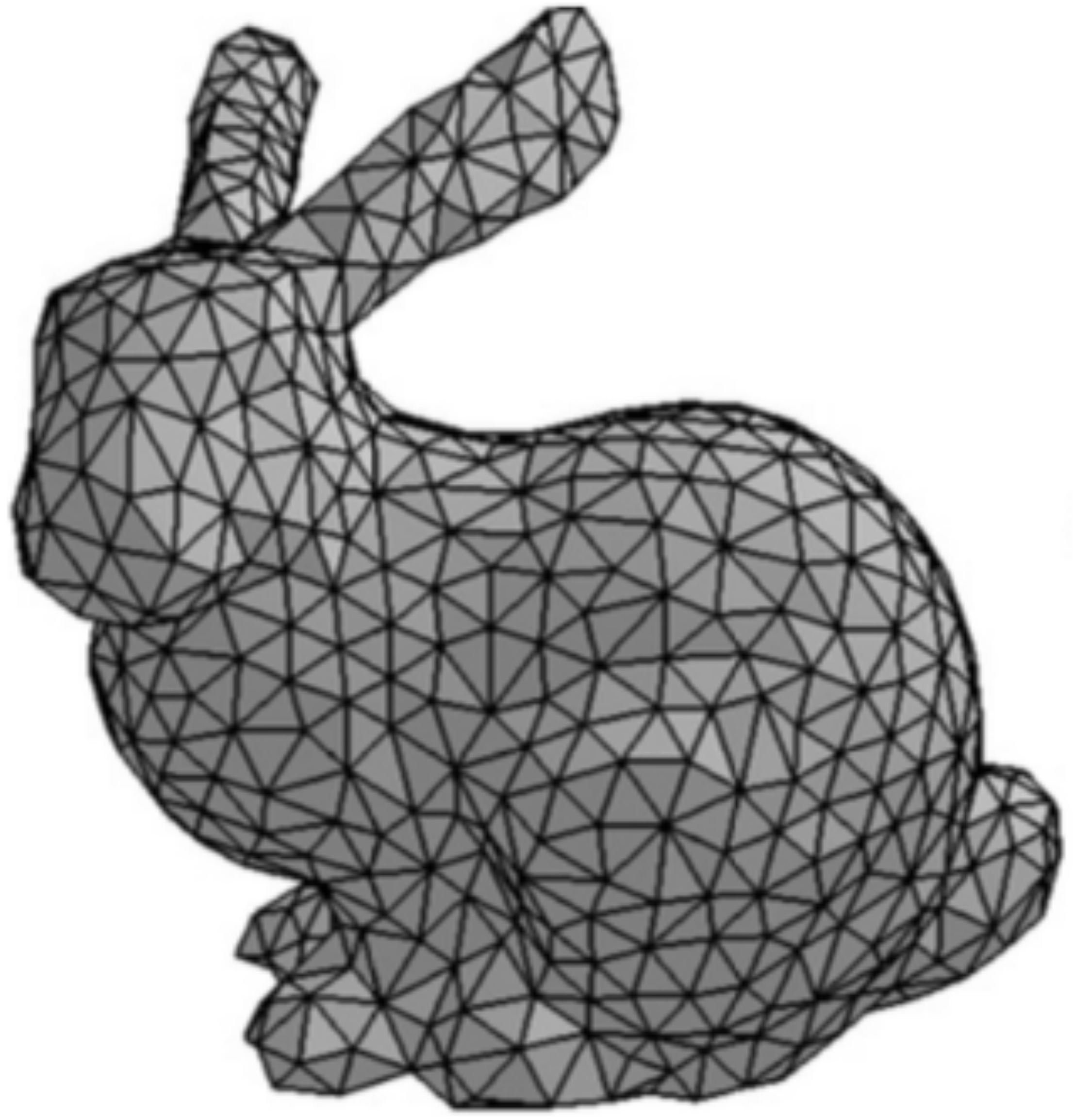


image source: CS231n

natural way to downsample

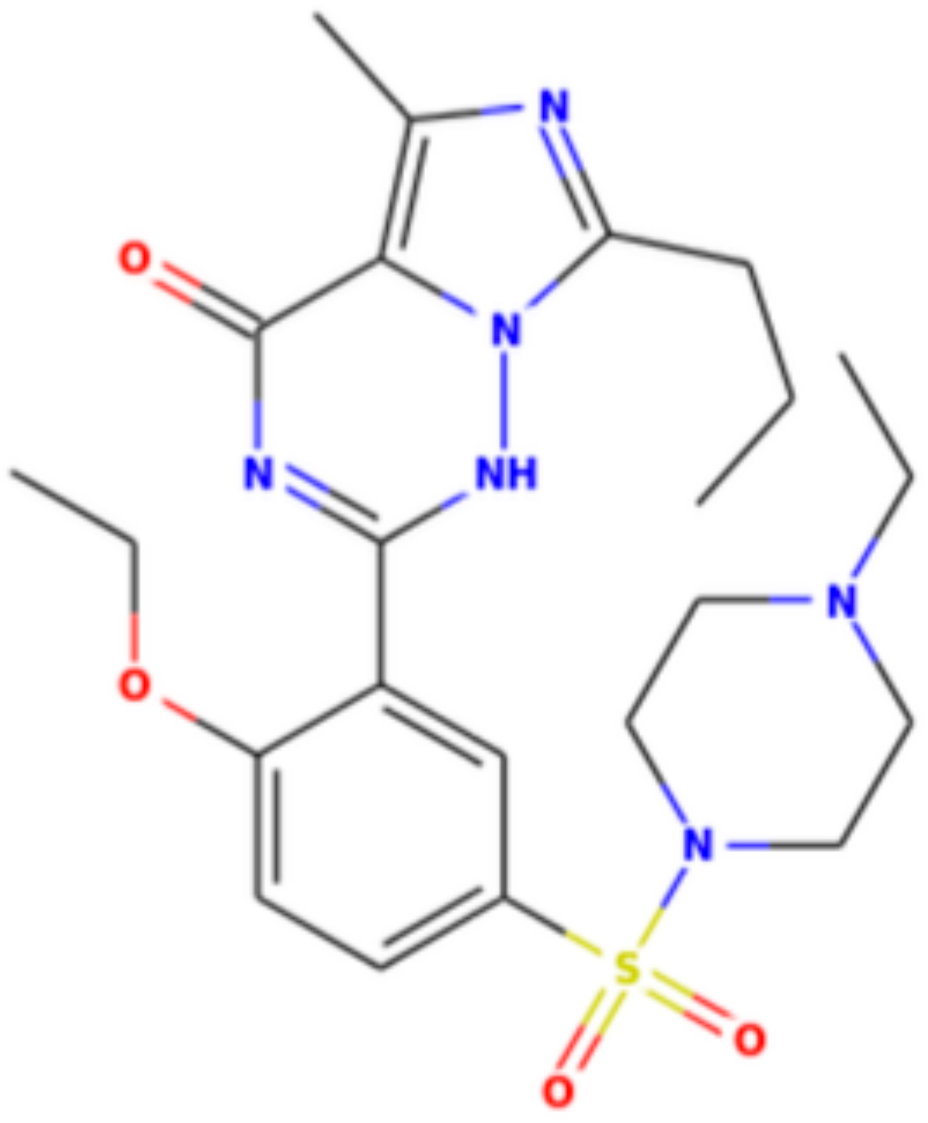
multi-scale analysis

In many cases, data lies on less regular structures (generic graphs)



3D shape graph

social network



molecules

Moreover, conventional CNN doesn't not assume any geometry in feature dimensions

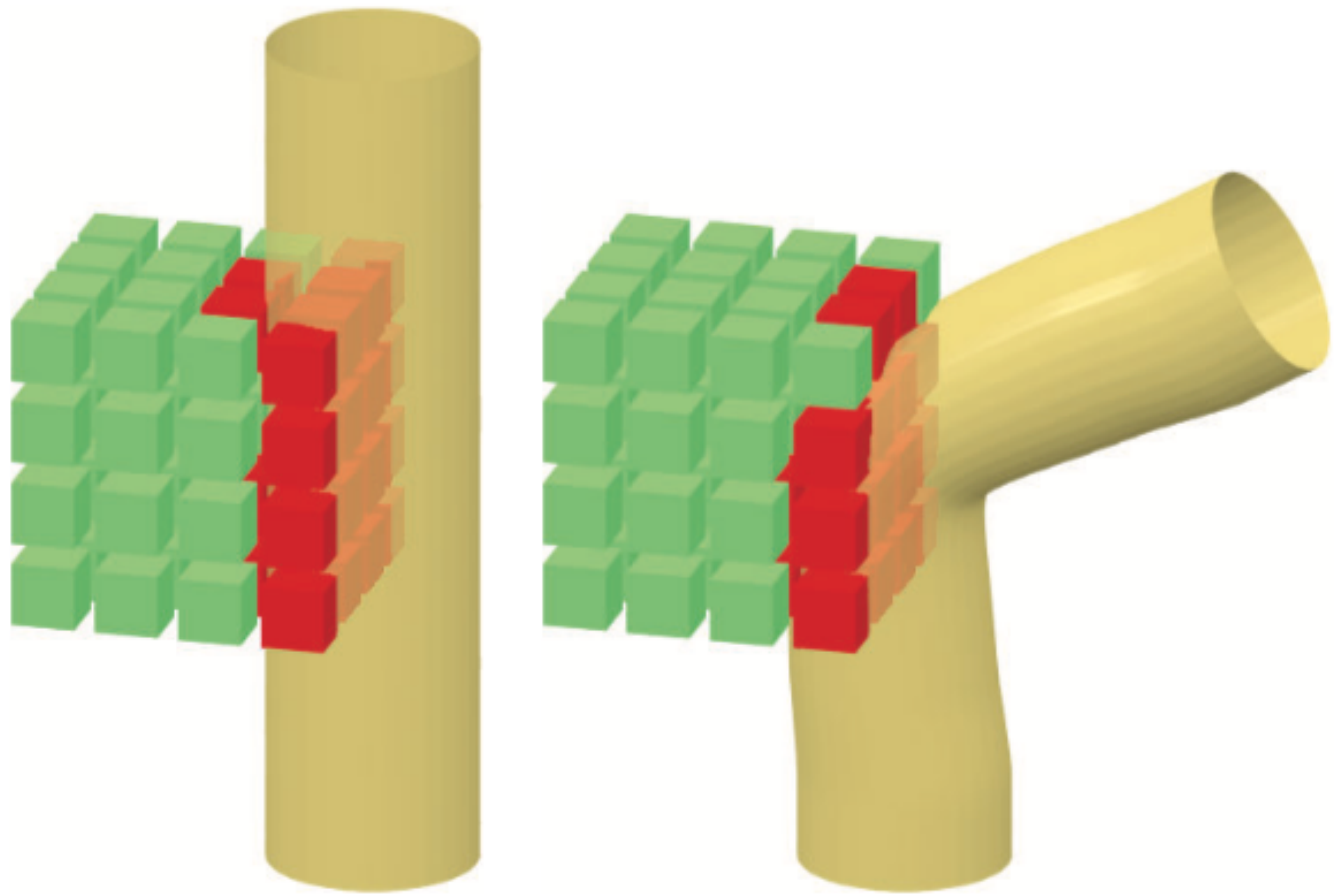
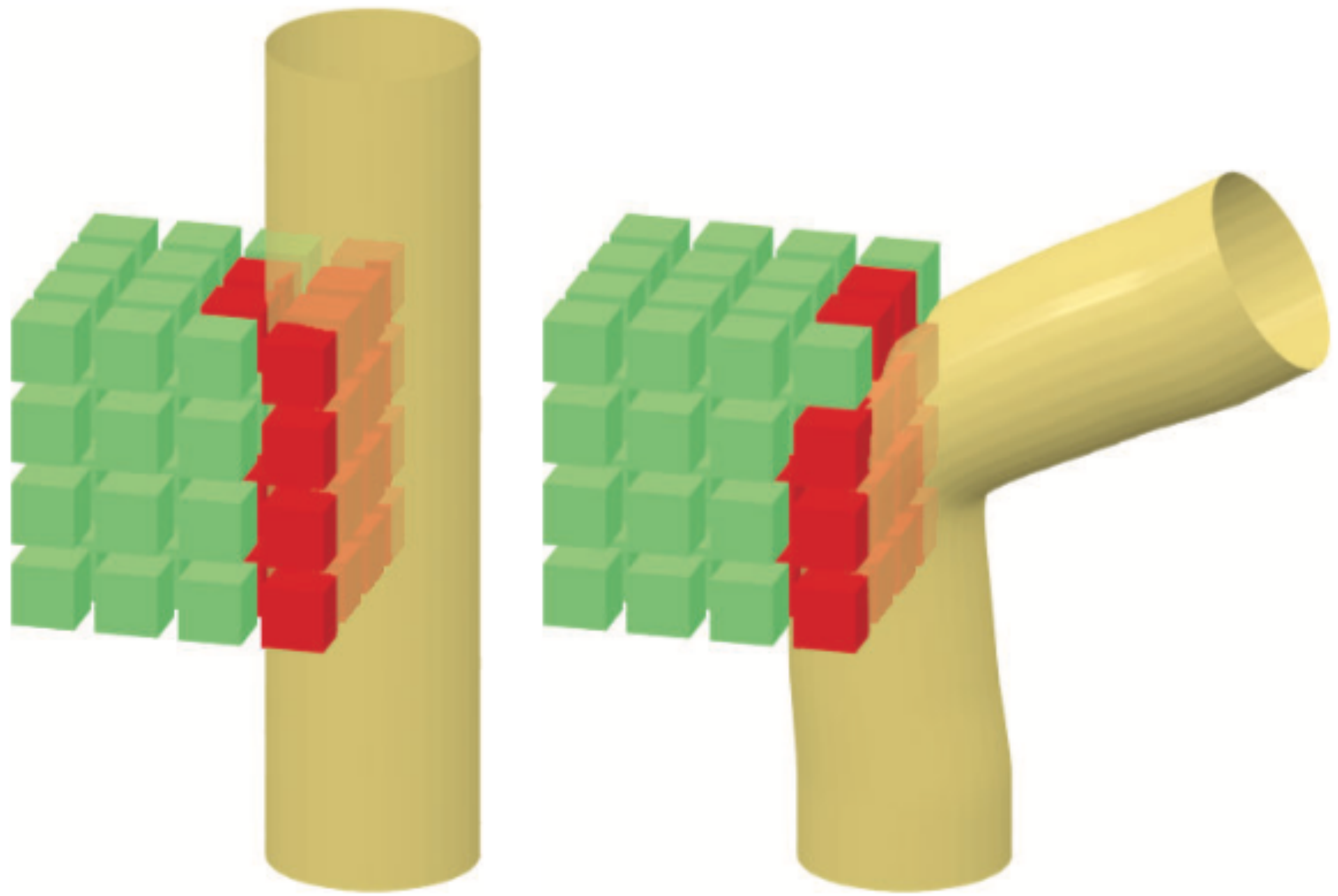


image credit: D. Boscaini, et al.

convolutional along spatial coordinates

Geometry aware convolution can be important



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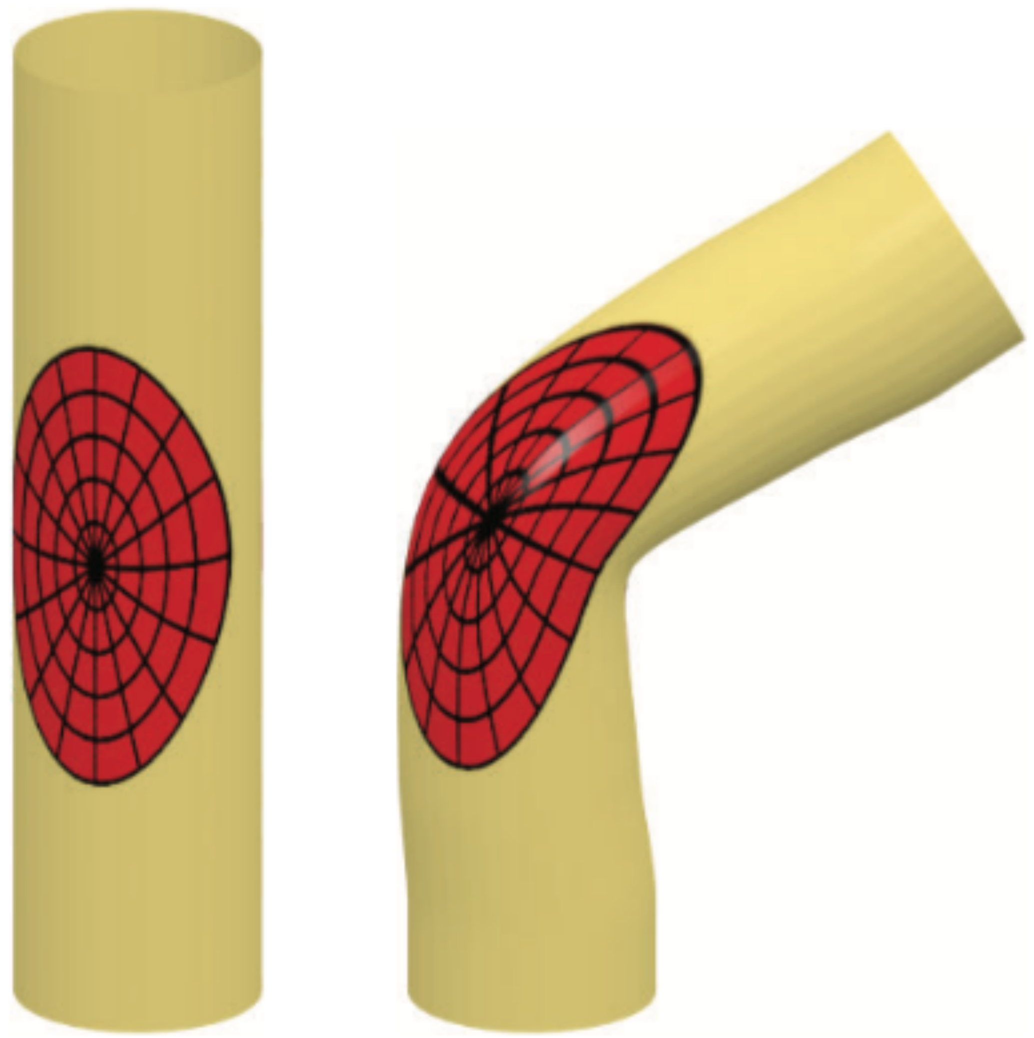

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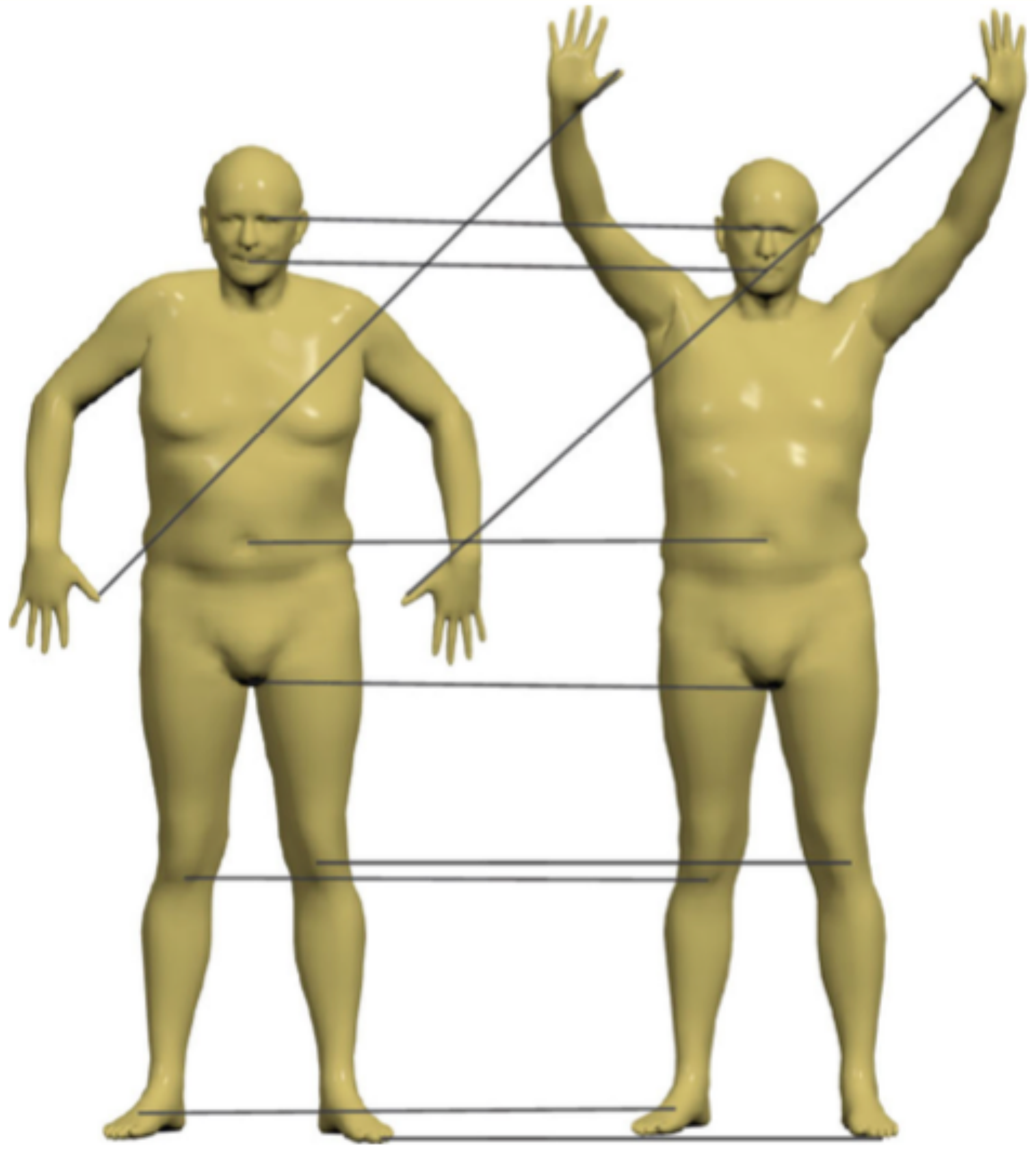
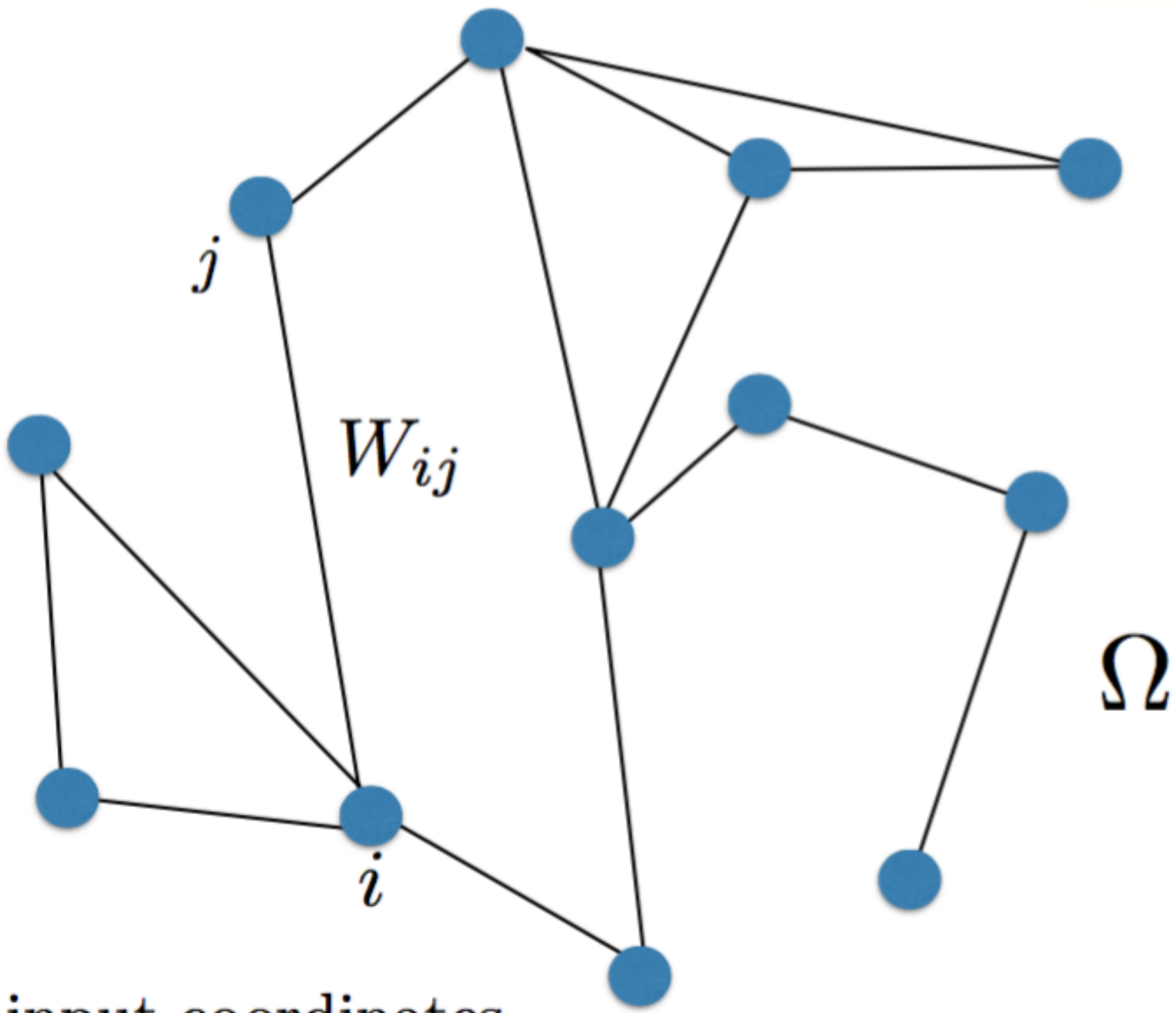
convolutional considering
underlying geometry



Today's topic



Ω: set of input coordinates

$W_{i,j}$: similarity between coordinates i and j

from Joan Bruna's slides

Agenda

- Challenges
- Background knowledge
- Spatial construction
  - Geodesic CNN
- Spectral construction
  - Spectral CNN
  - Anisotropic CNN
  - SyncSpecCNN

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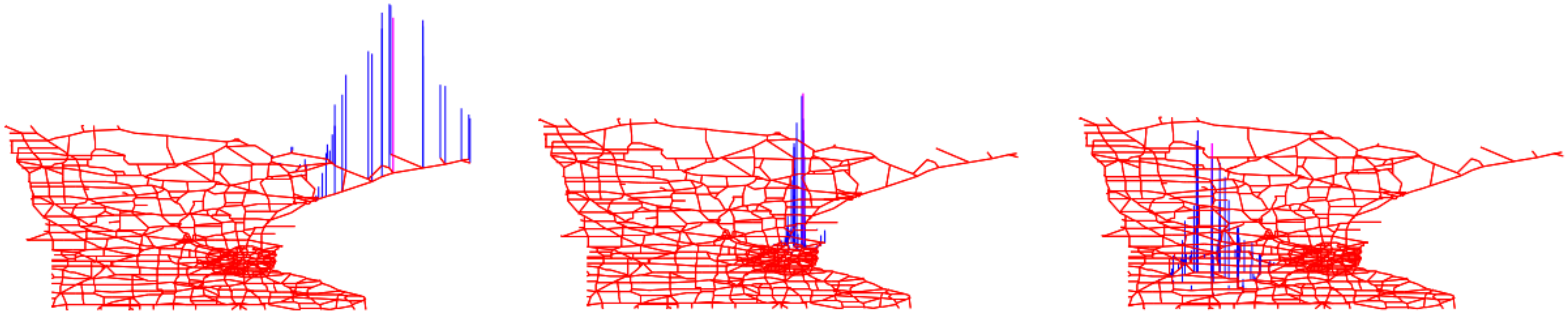
How to define convolution kernel on graphs?

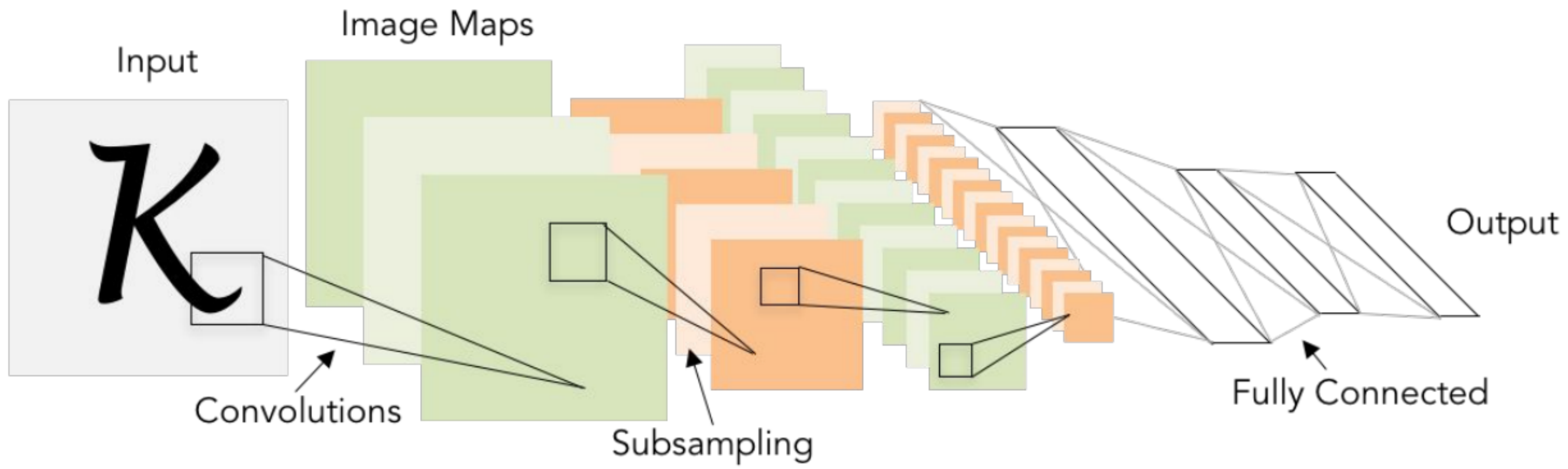
- Desired properties:
  - locally supported (w.r.t graph metric)
  - allowing weight sharing across different coordinates



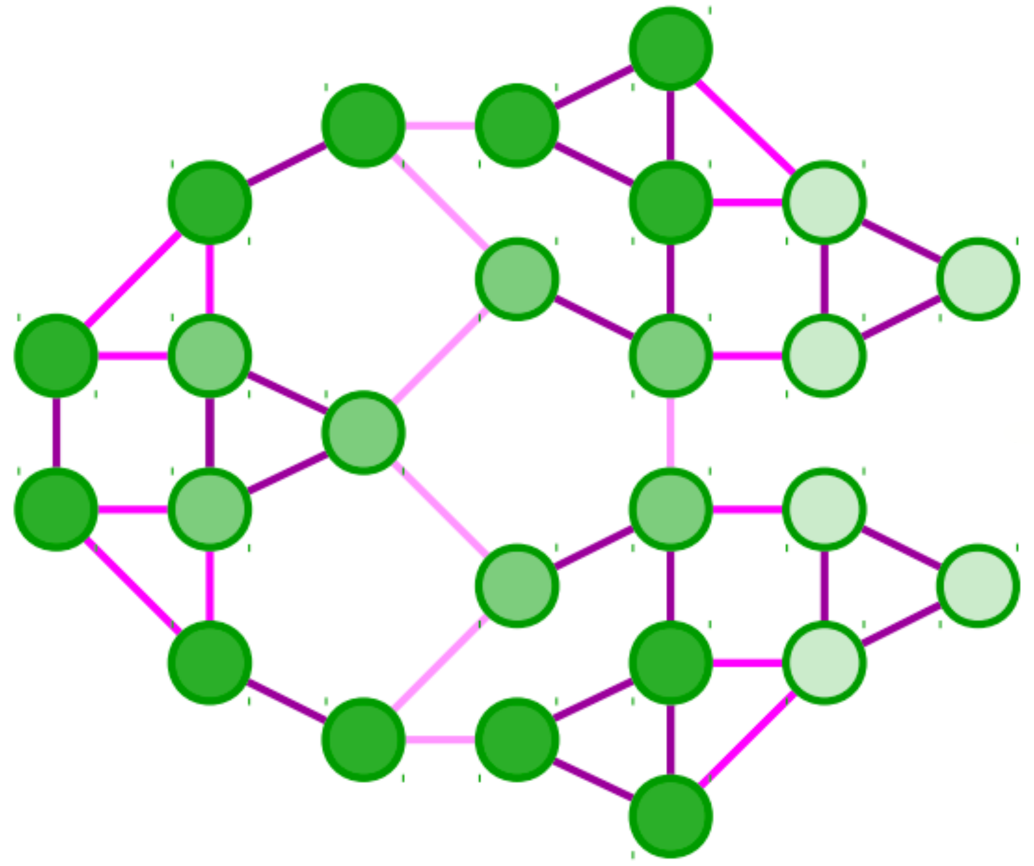
from Shuman et al. 2013

How to allow multi-scale analysis?

grid structure



graph structure

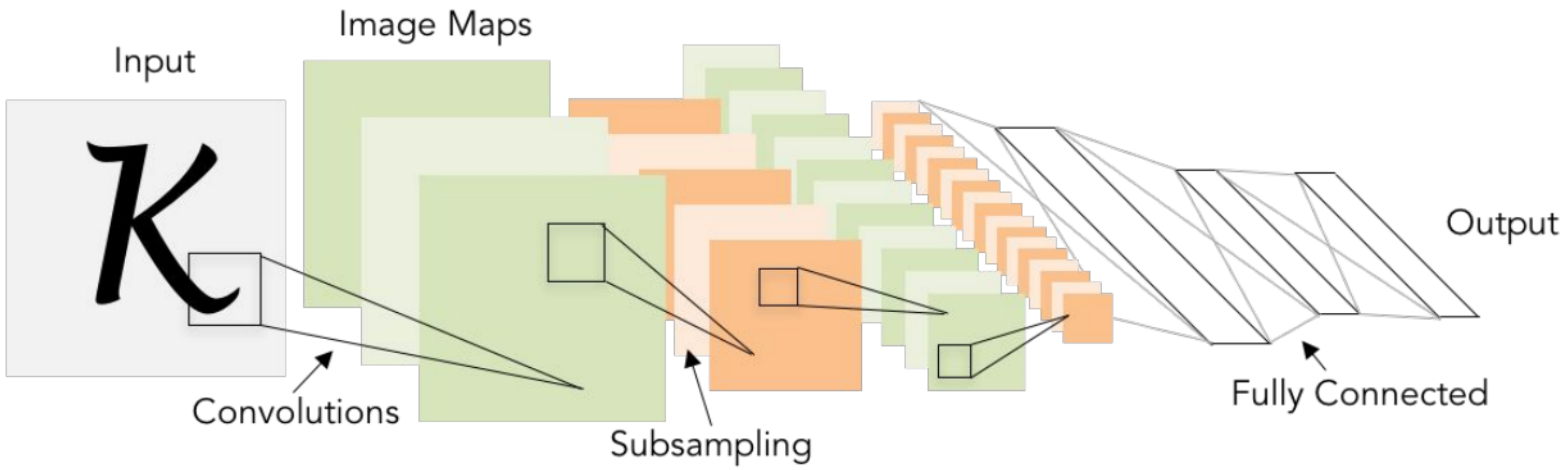


?

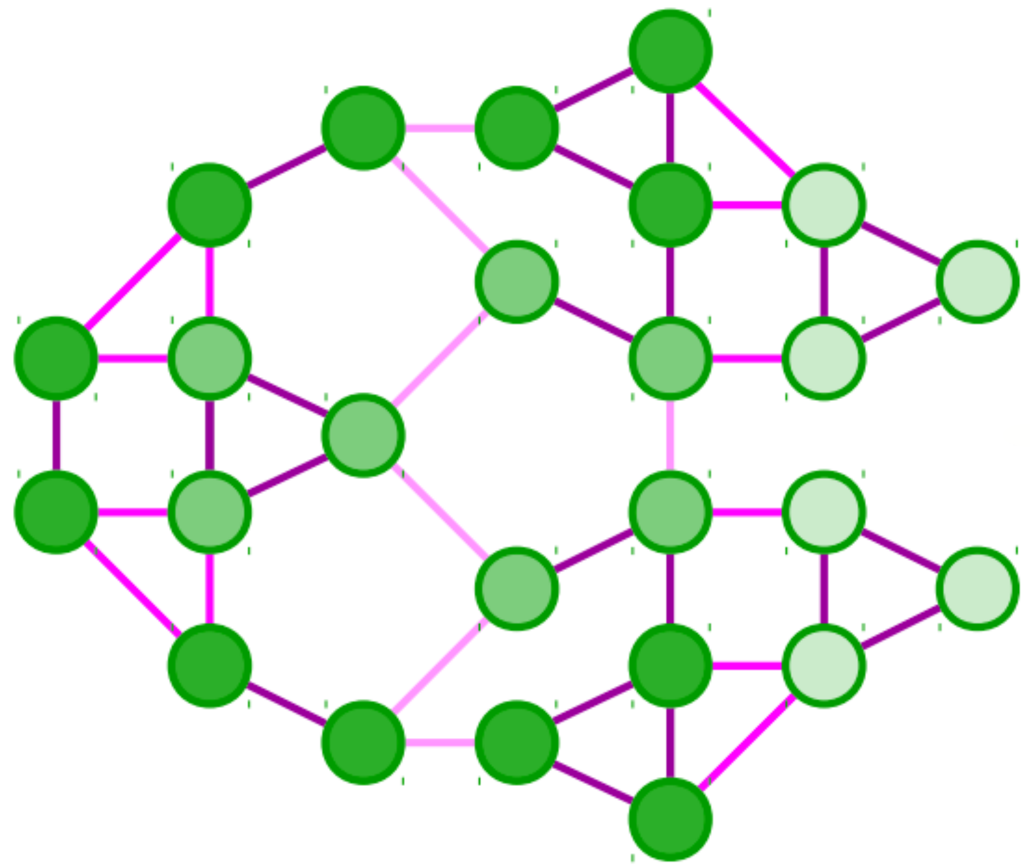
from Michaël Defferrard et al. 2016

How to allow multi-scale analysis?

grid structure



graph structure



from Michaël Defferrard et al. 2016

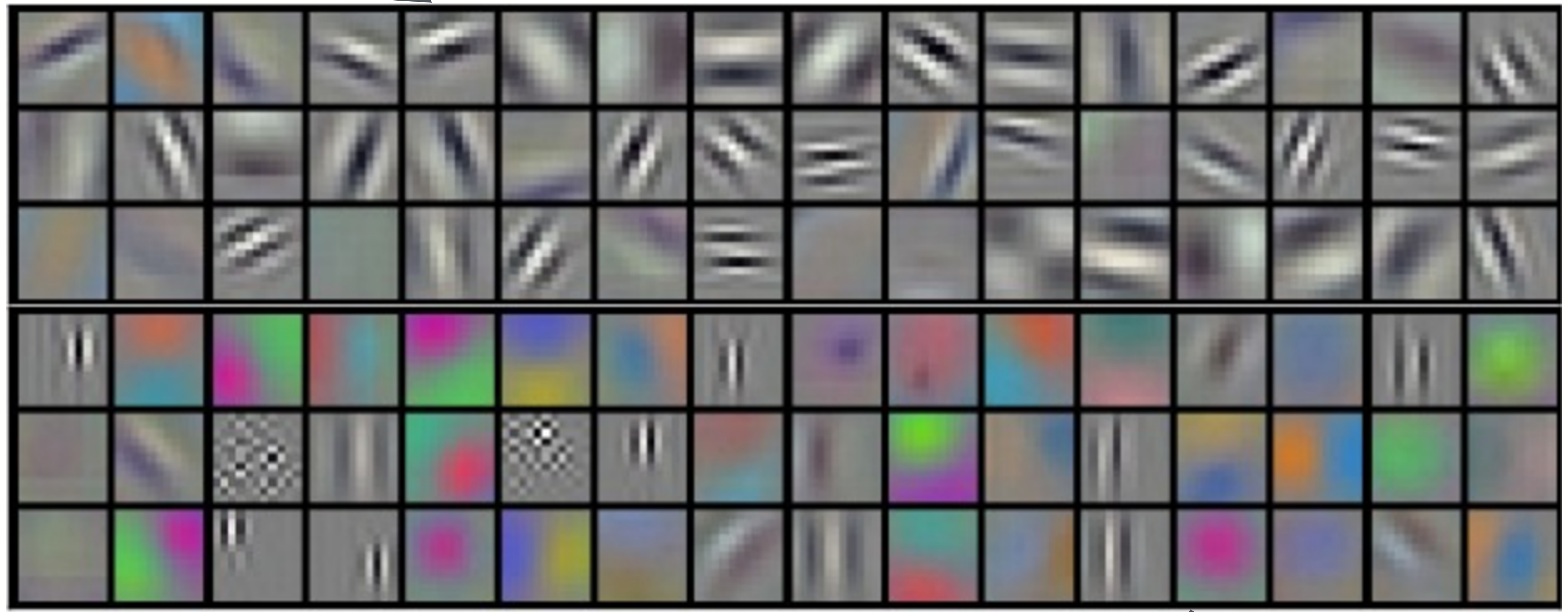
hierarchical graph coarsening

structure aware? efficiency?

can we do more?

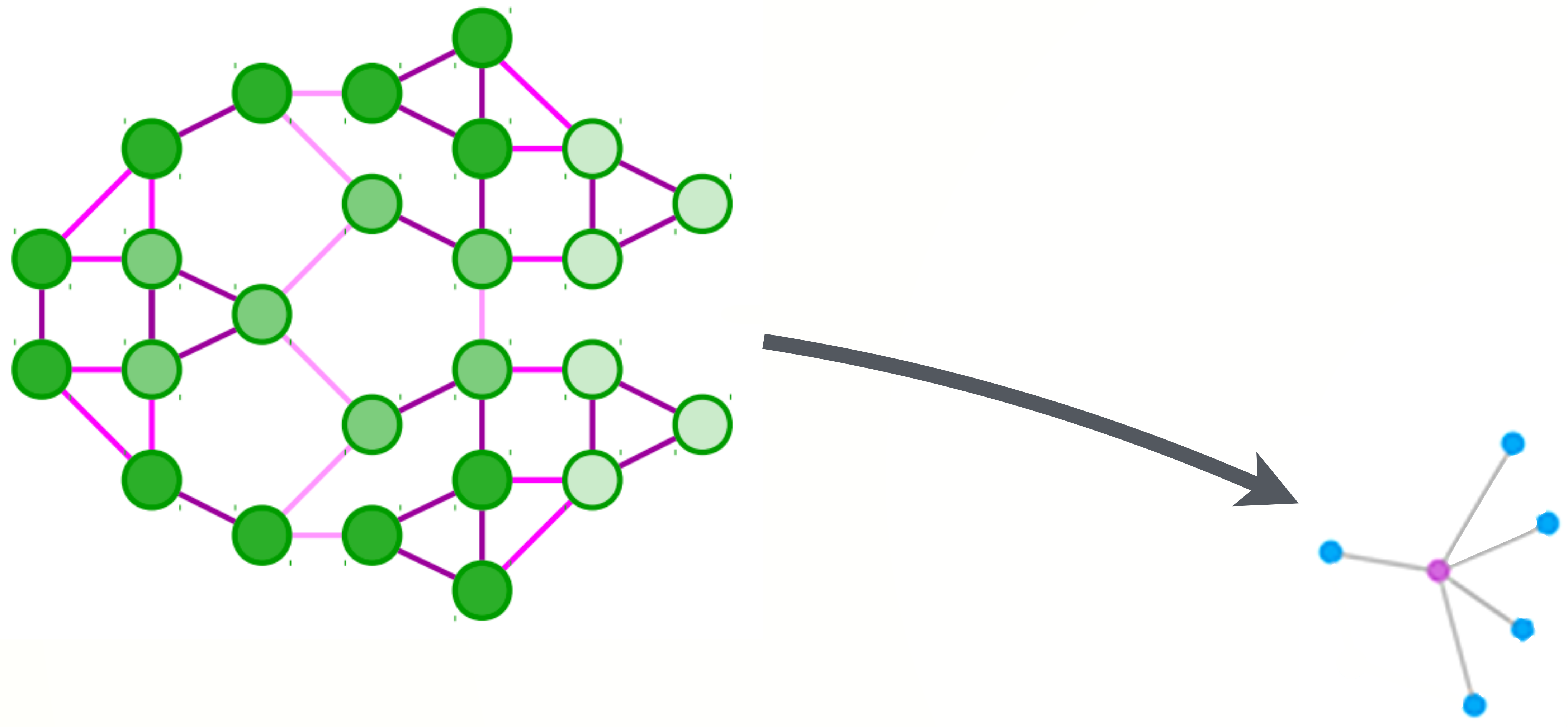
How to ensure generalizability across graphs?

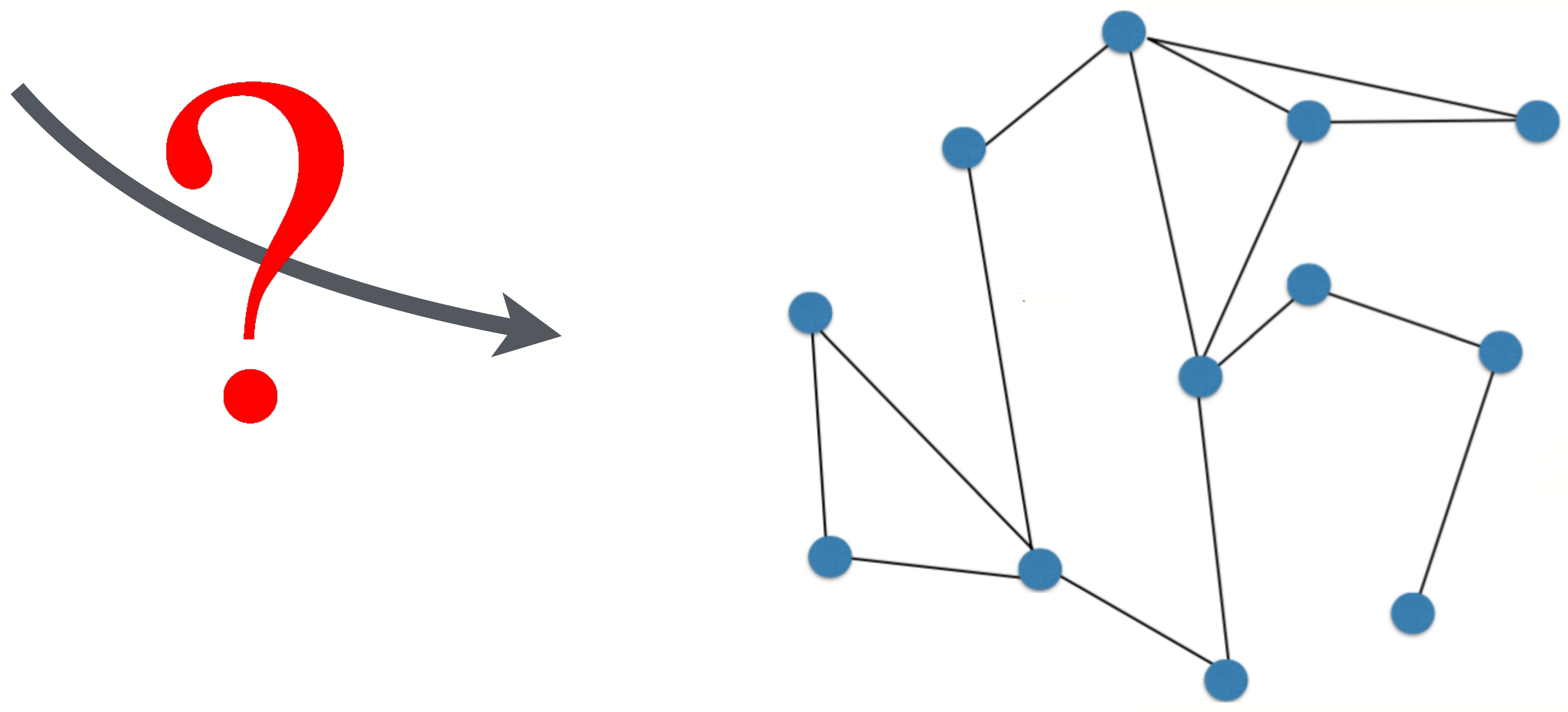
grid structure has a
natural alignment



How to ensure generalizability across graphs?

graph structure does not
has a natural alignment





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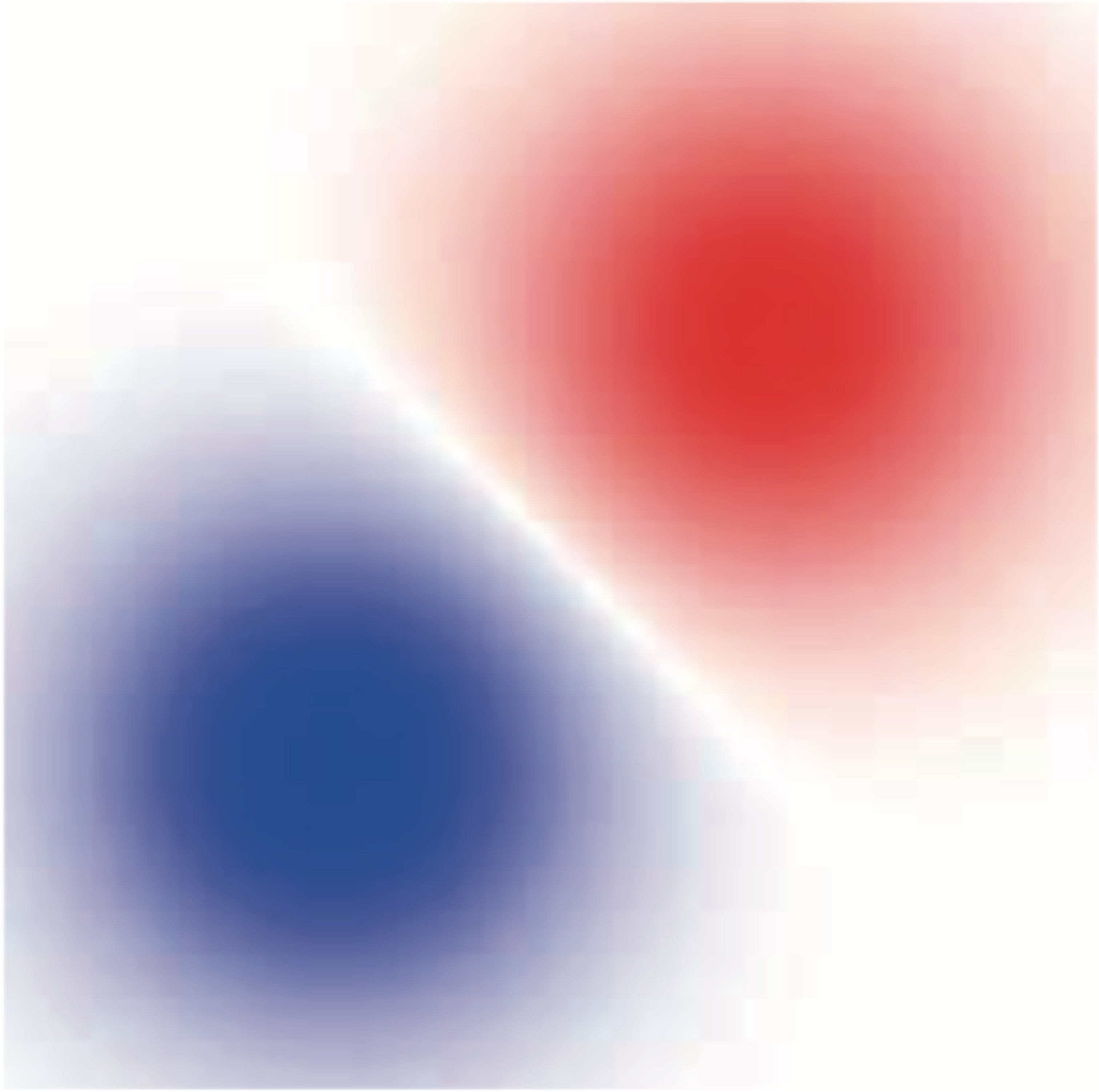
Laplacian

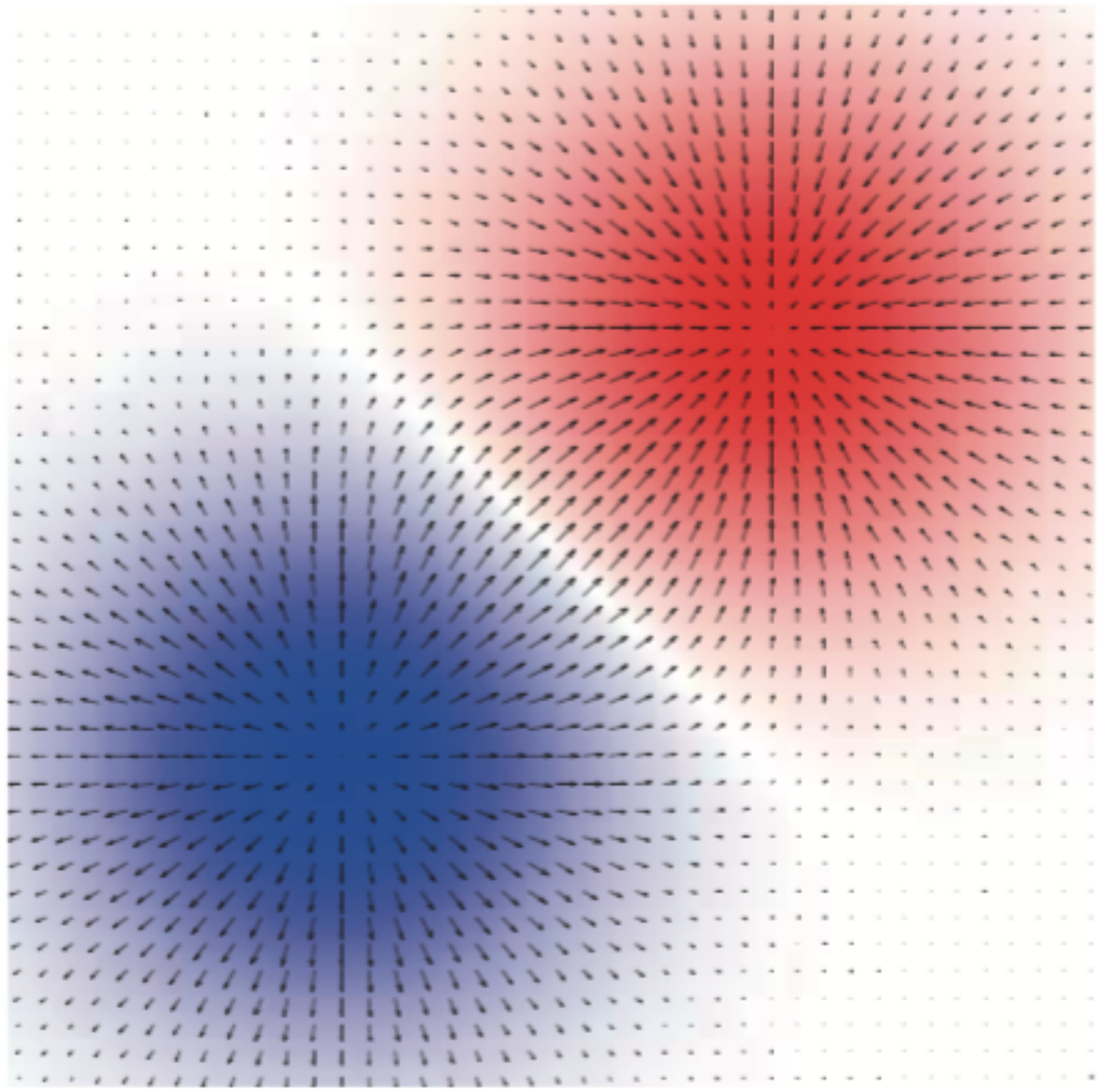


Smooth scalar field f

from Jonathan Masci et al

Laplacian

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



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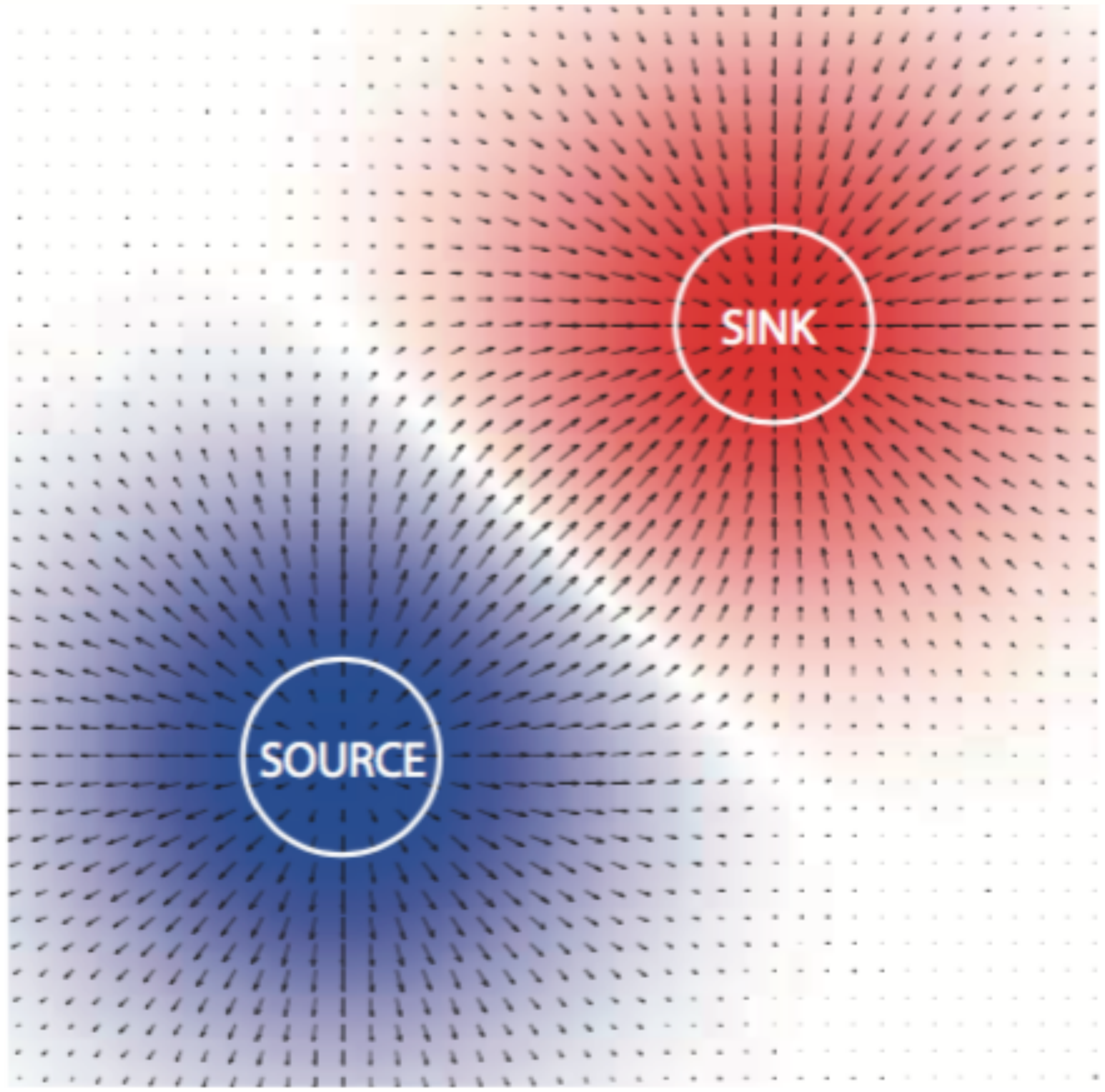
Laplacian

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

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



Smooth vector field F

from Jonathan Masci et al

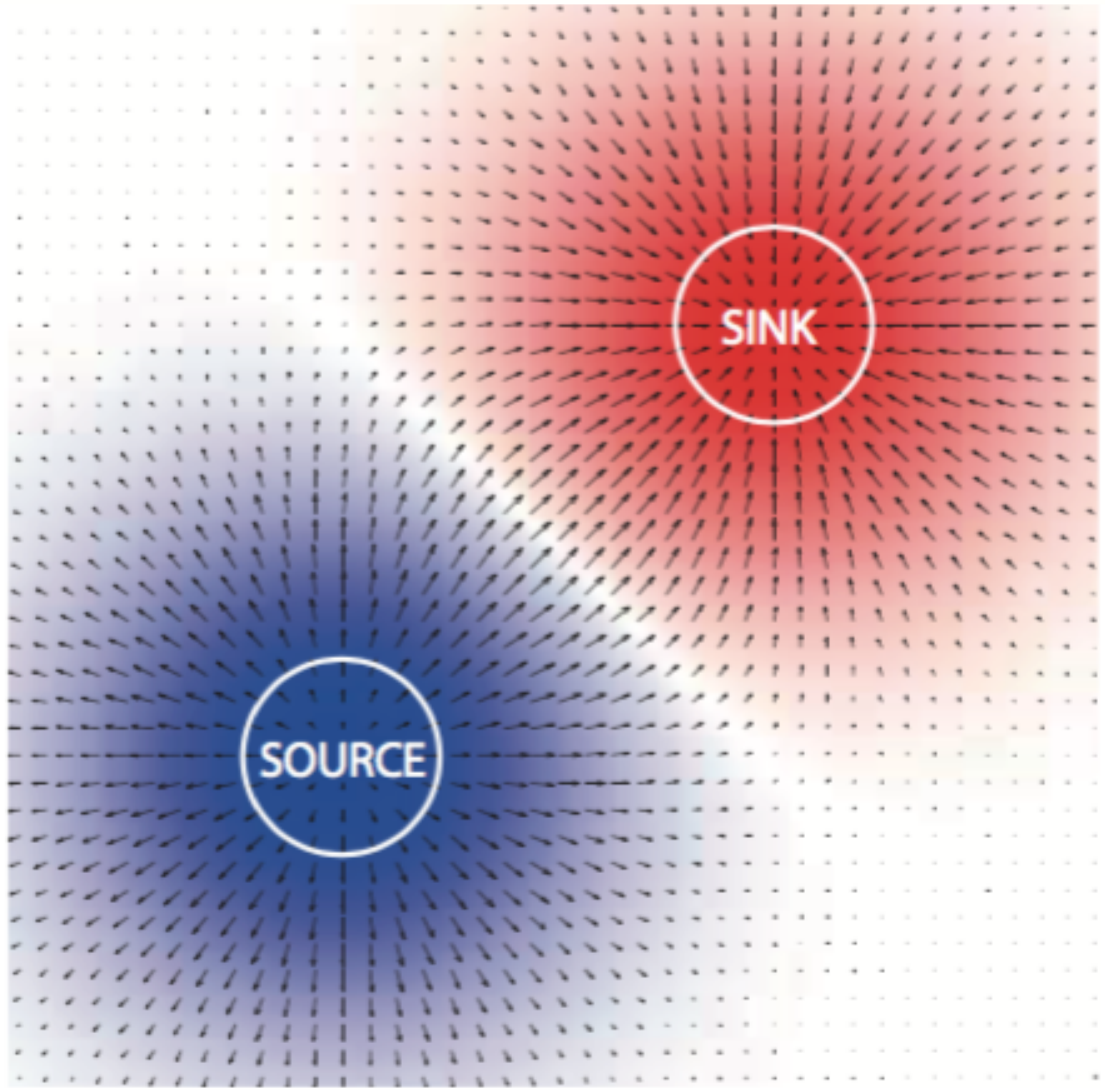
Laplacian

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

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

Divergence theorem:

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



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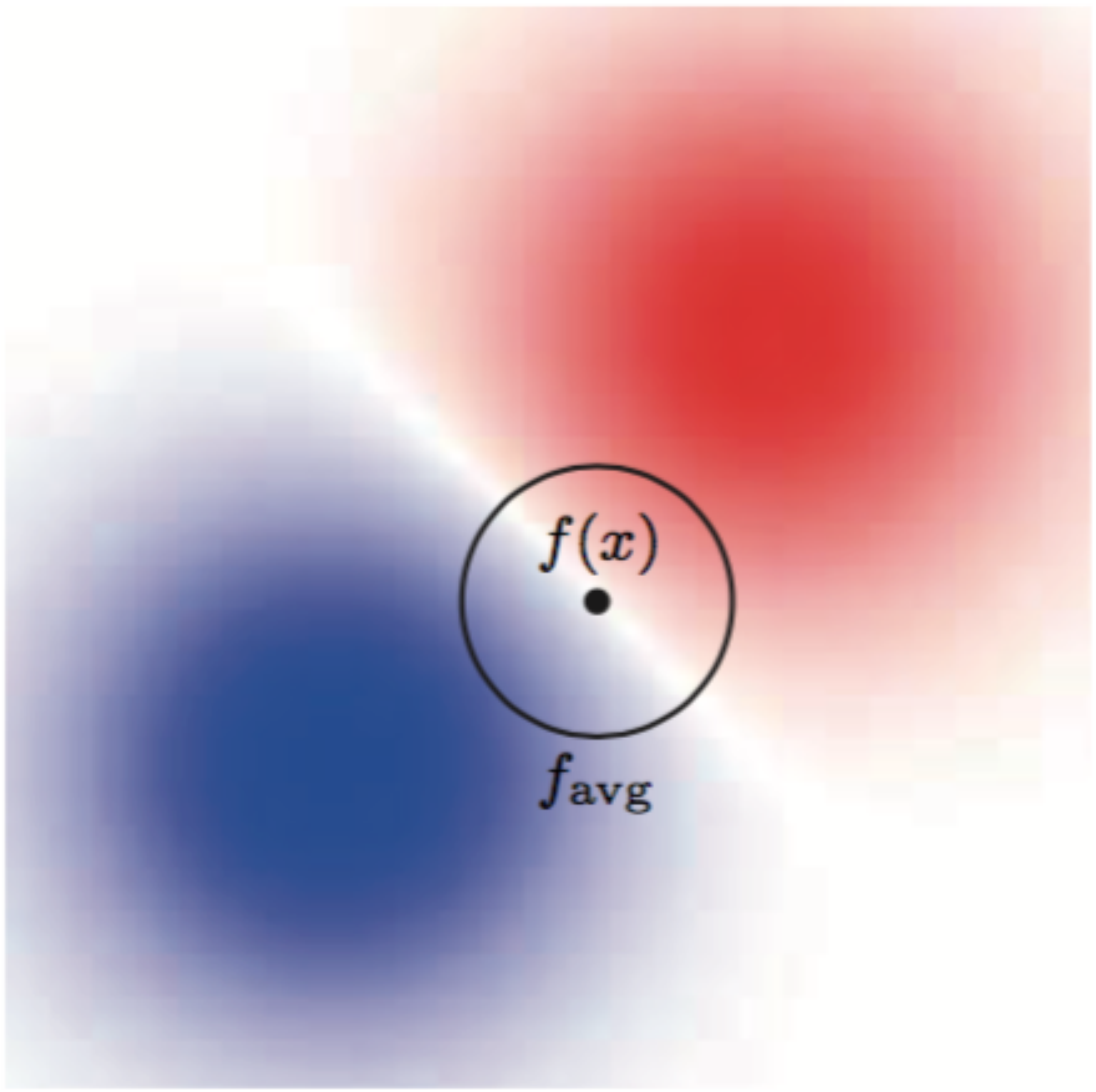
  Divergence theorem:

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

- Laplacian $\Delta f(x) = -\mathrm{div}(\nabla f(x))$
  'difference between $f(x)$ and the average of f on an infinitesimal sphere around x' (consequence of the Divergence theorem)

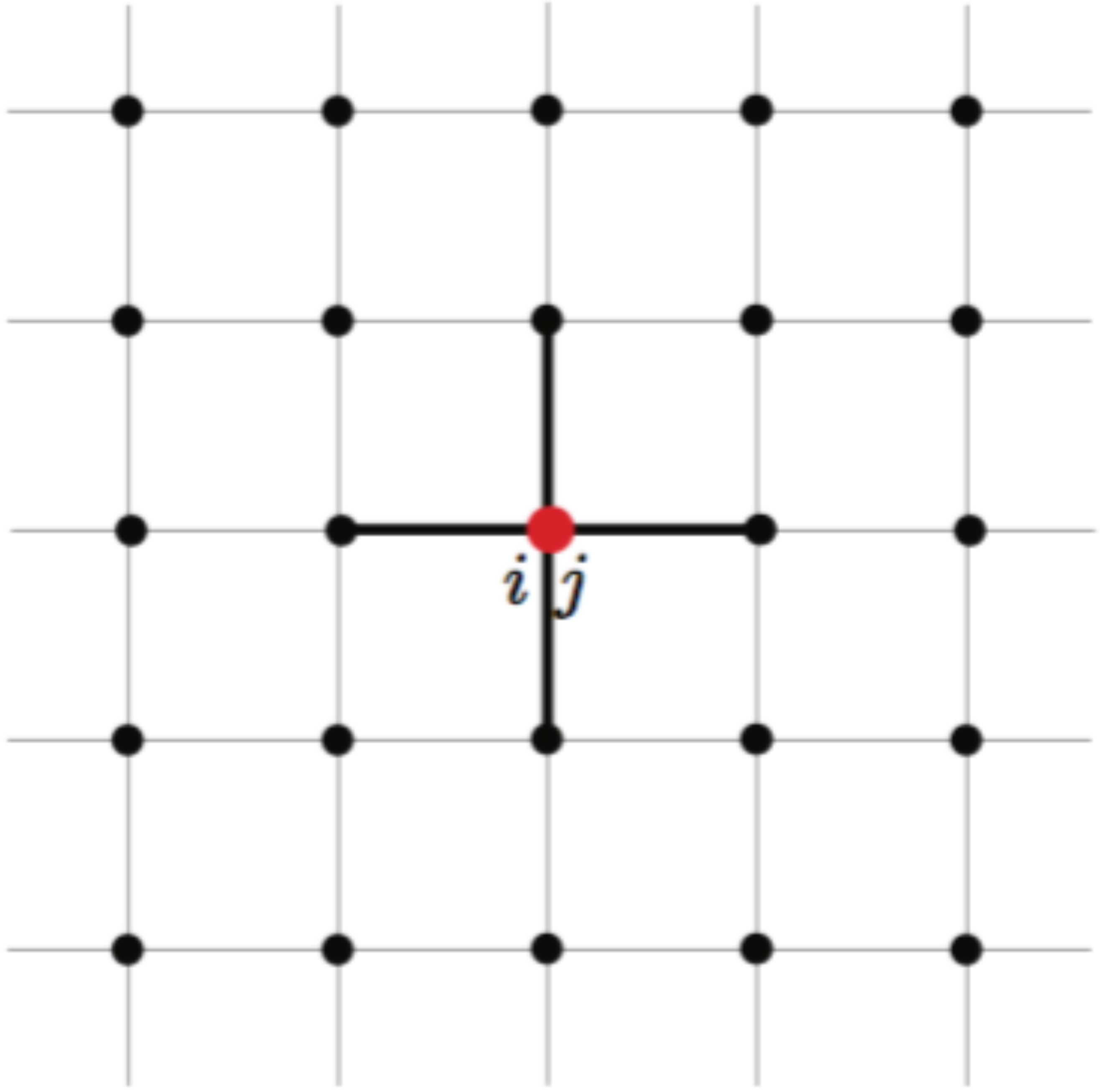


from Jonathan Masci et al

Discrete Laplacian

One-dimensional

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



Two-dimensional

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

from Jonathan Masci et al

Physical application: heat equation

$$f_t = -c\Delta f$$

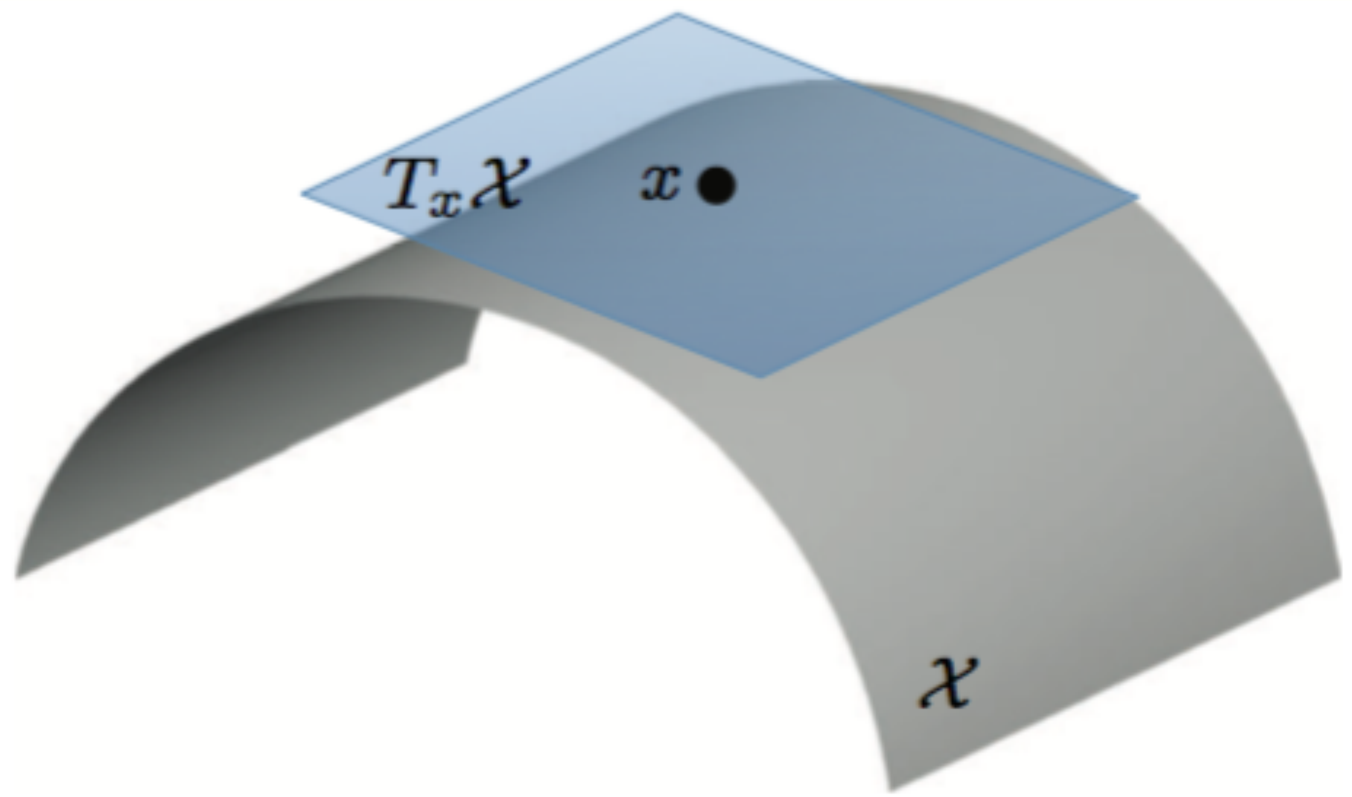
Newton's law of cooling: rate of change of the temperature of an object is proportional to the difference between its own temperature and the temperature of the surrounding

c [m^2/sec] $=$ thermal diffusivity constant (assumed $= 1$)

from Jonathan Masci et al

Riemannian manifold

- Manifold $\mathcal{X}$ = topological space
- No global Euclidean structure
- Tangent plane $T_x\mathcal{X}$ = local Euclidean representation of manifold $\mathcal{X}$ around x



from Jonathan Masci et al

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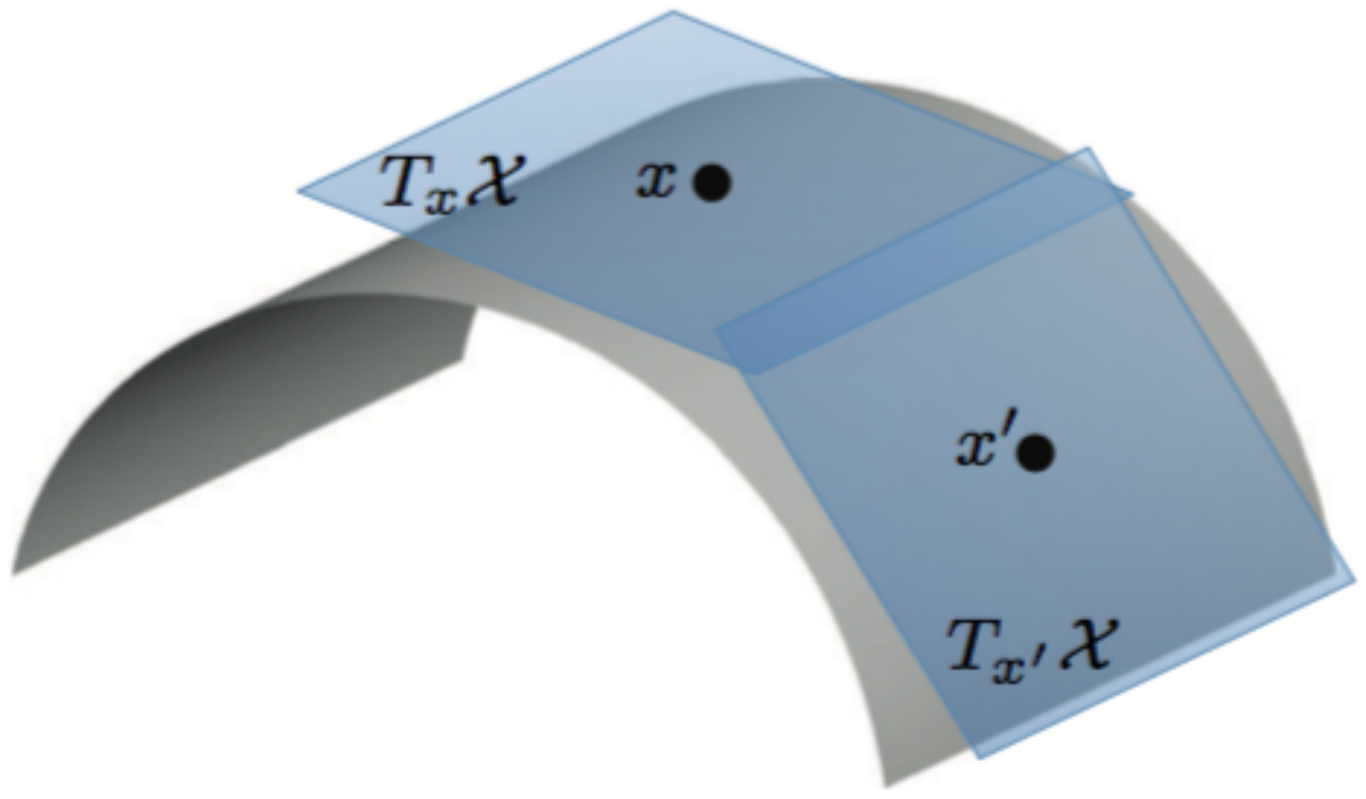
- Riemannian metric

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

depending smoothly on x



from Jonathan Masci et al

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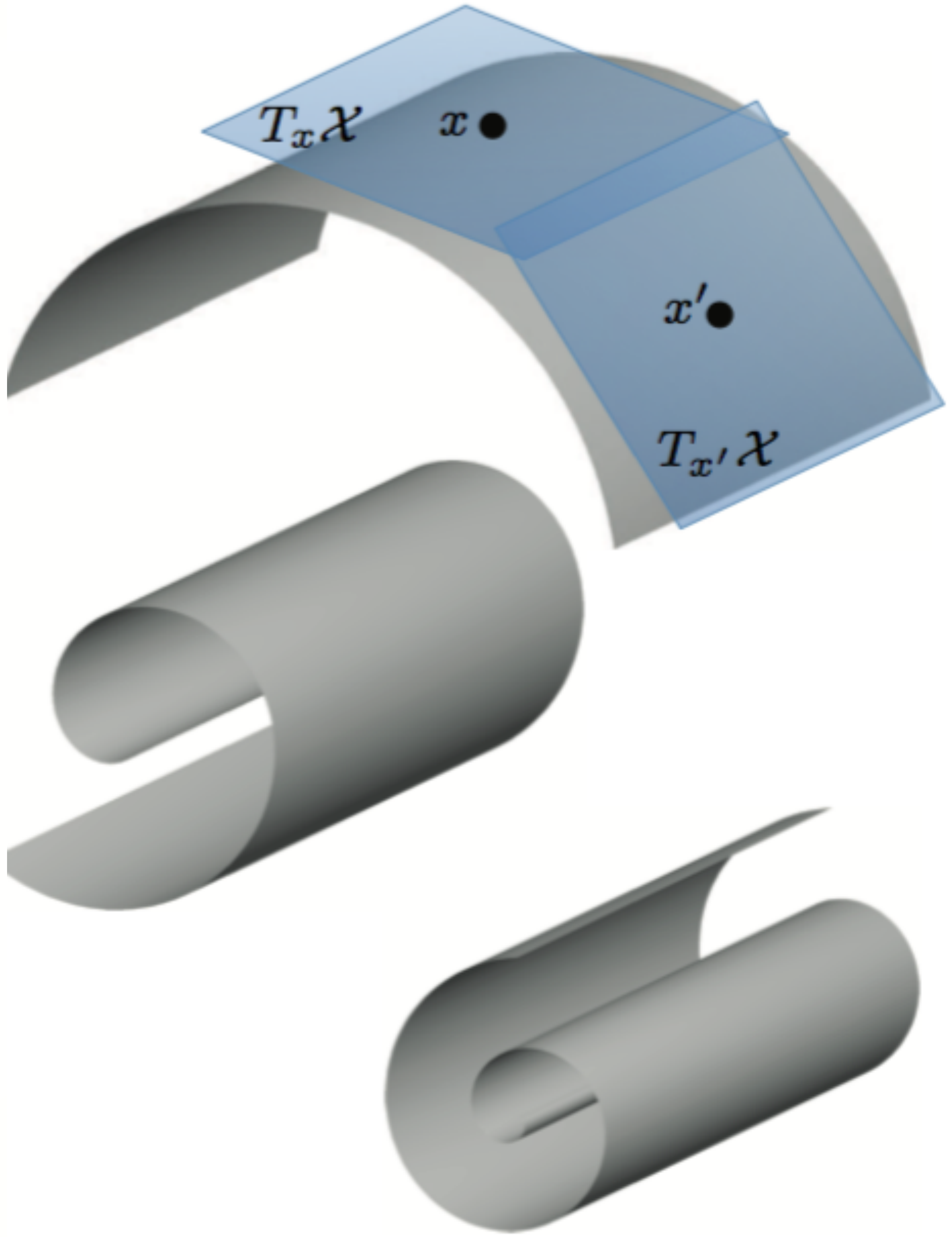
Isometry = metric-preserving shape deformation



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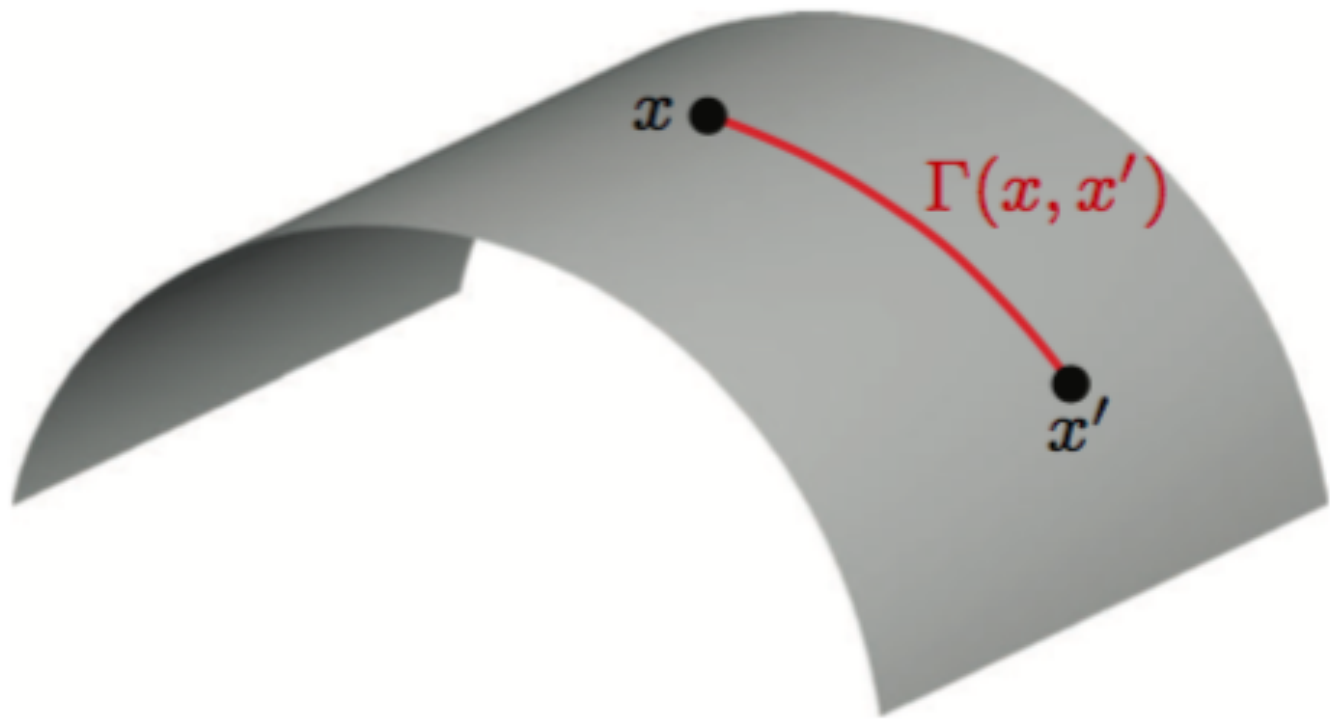
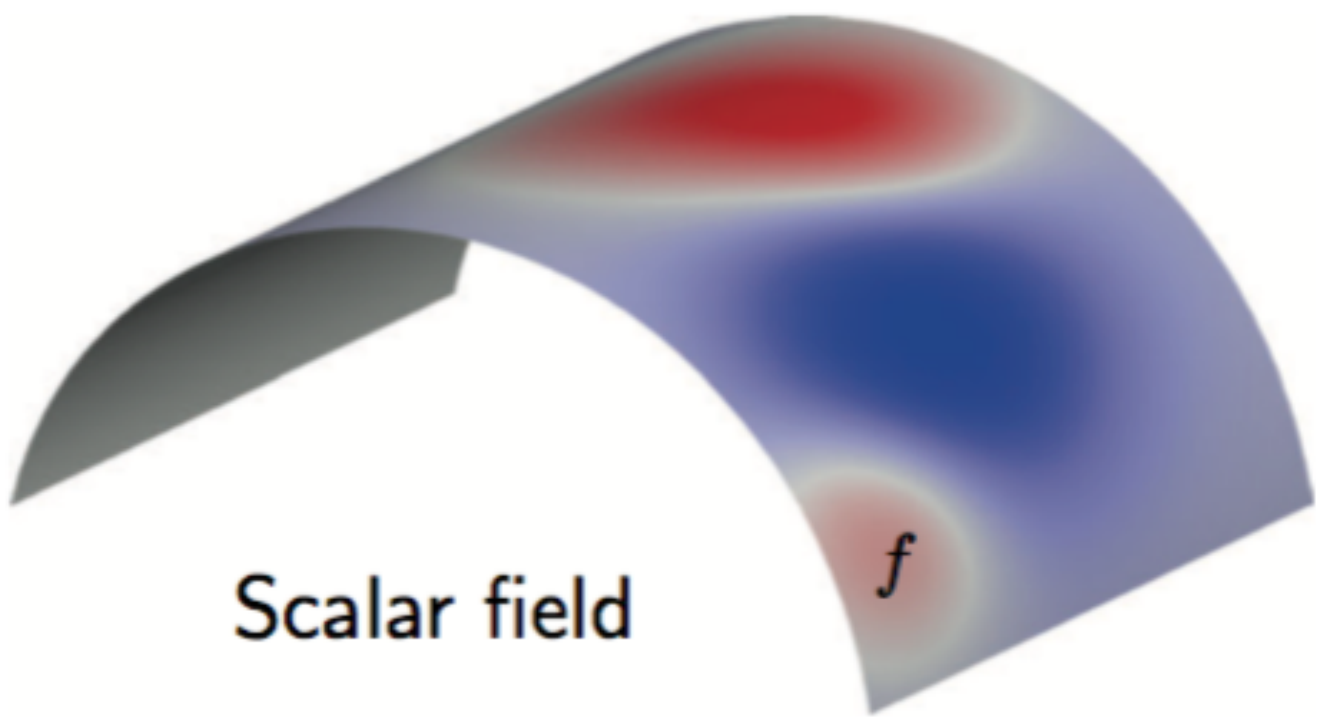


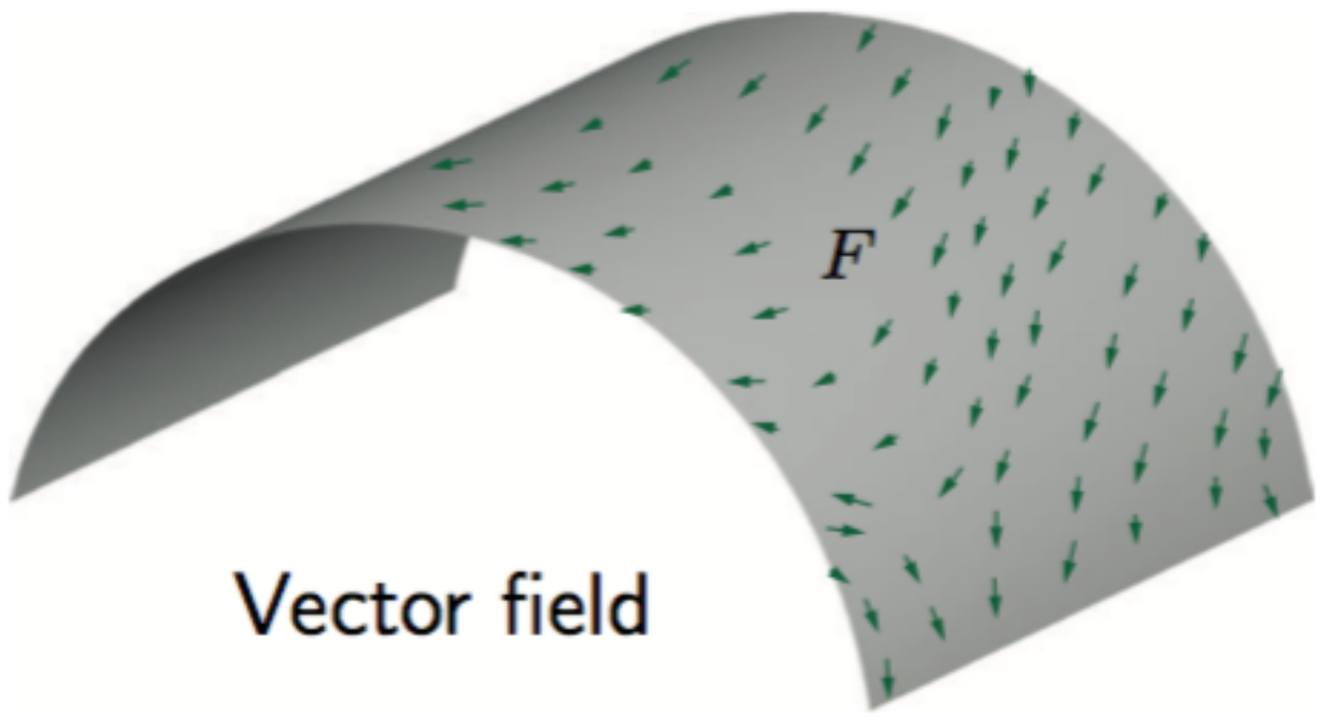
- Geodesic = shortest path on $\mathcal{X}$ between x and x'

from Jonathan Masci et al

Calculus on manifold

- Scalar field $f : \mathcal{X} \to \mathbb{R}$
- Vector field $F : \mathcal{X} \to T\mathcal{X}$





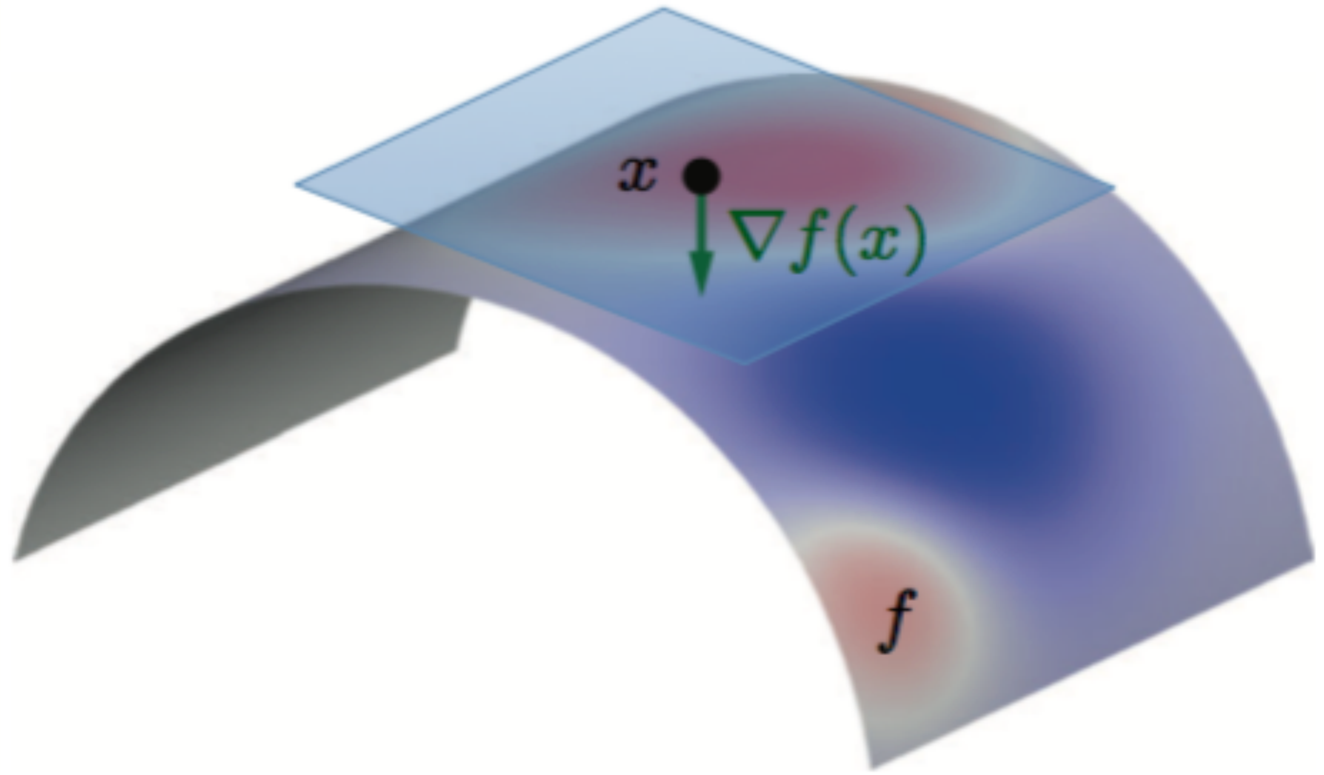
from Jonathan Masci et al

Calculus on manifold

- Intrinsic gradient operator

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

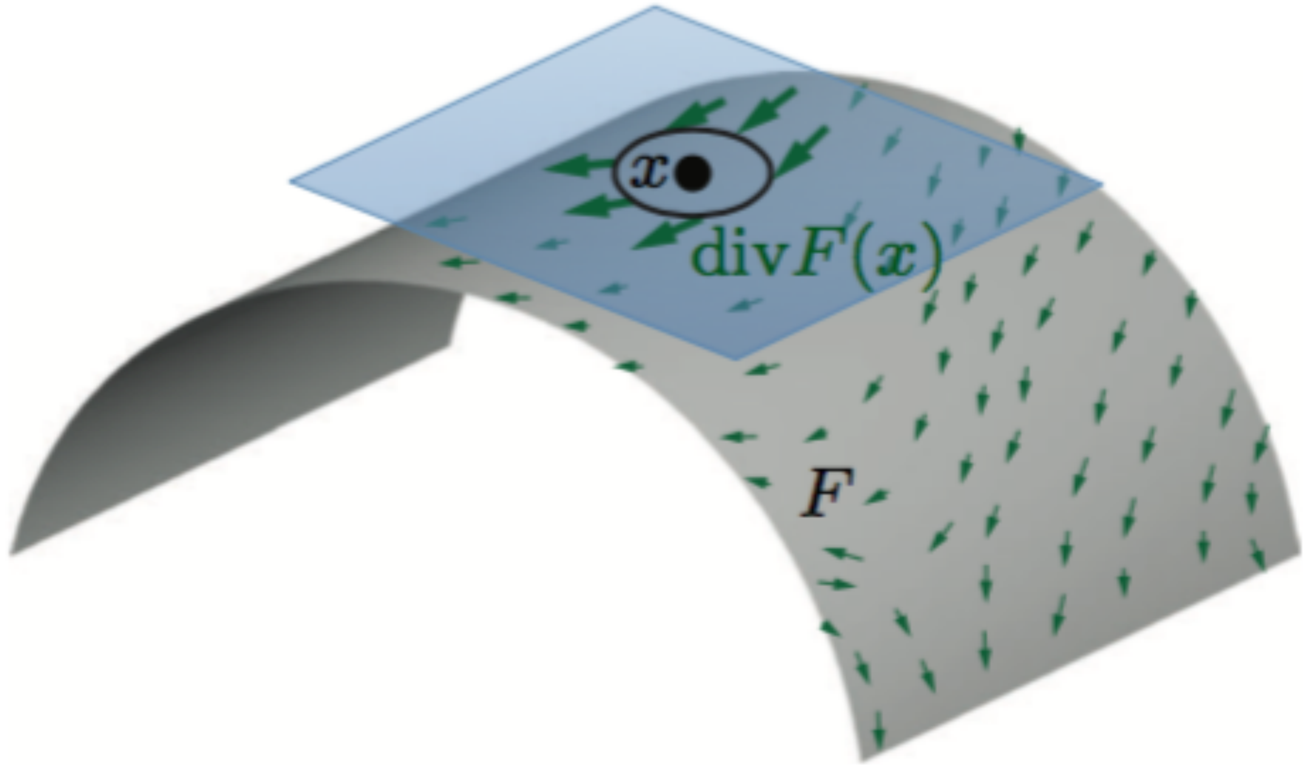
"direction of steepest change of f"



- Intrinsic divergence operator

$$\text{div} : L^2(T\mathcal{X}) \to L^2(\mathcal{X})$$

"net flow of field F at x"



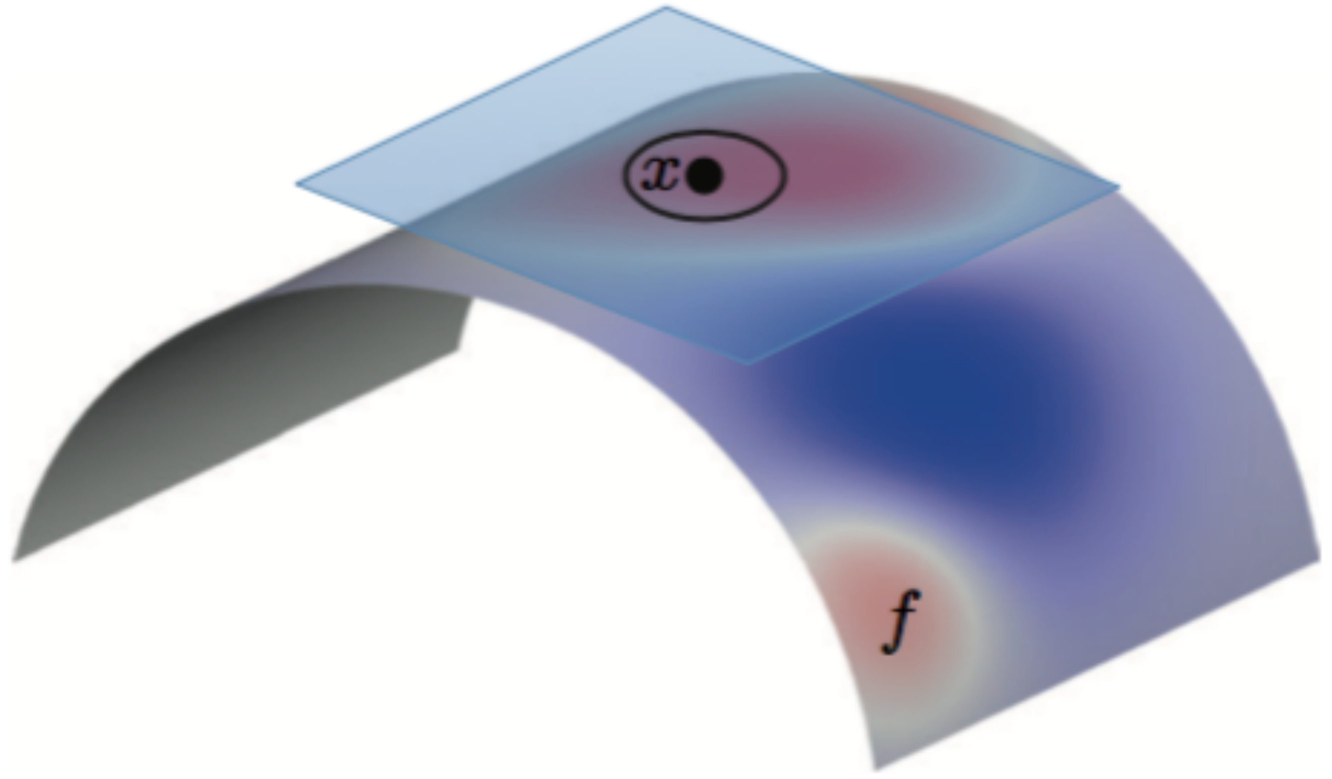
from Jonathan Masci et al

Calculus on manifold

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

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

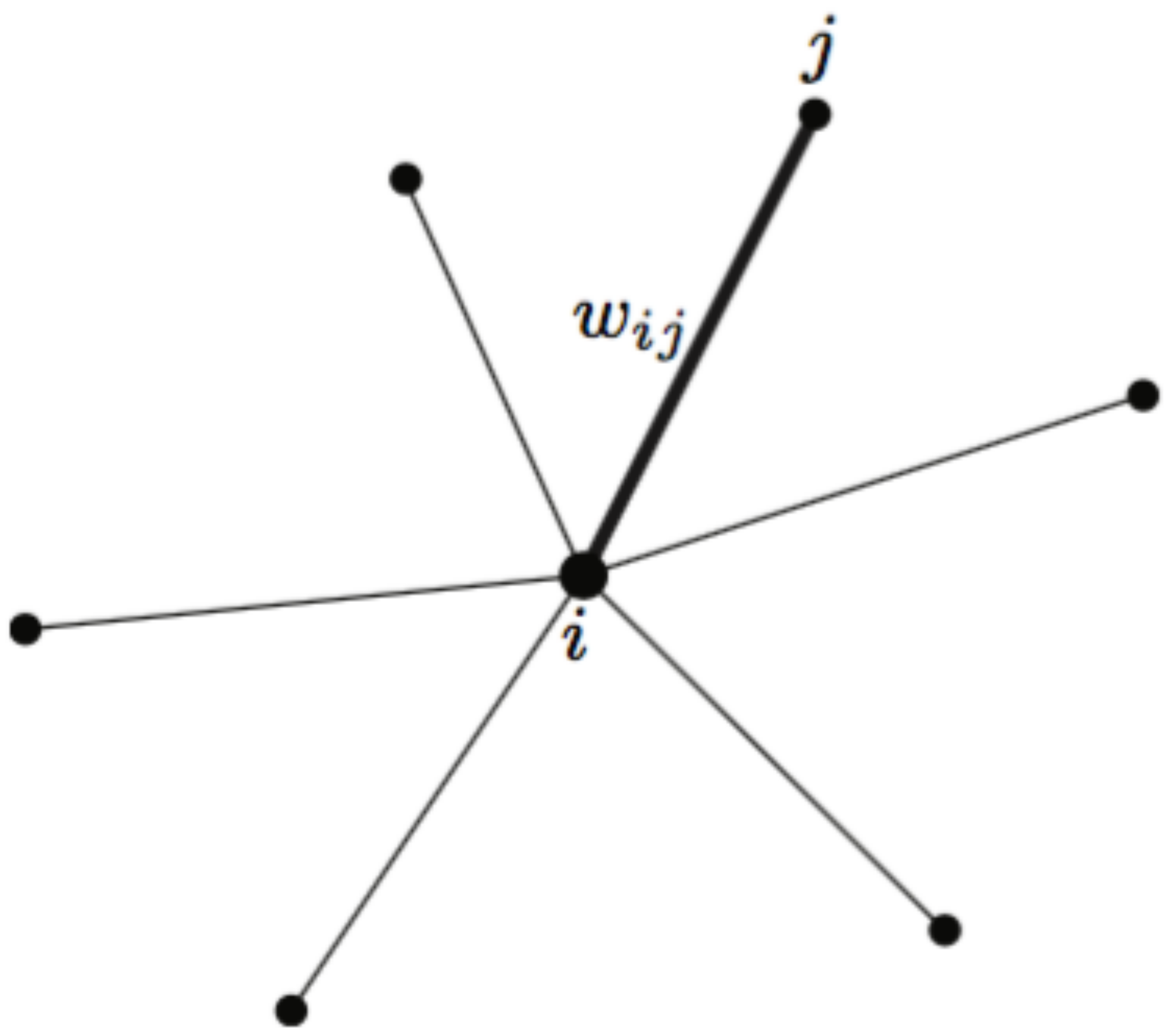
"difference between $f(x)$ and average value of f around x"



- Intrinsic (expressed solely in terms of the Riemannian metric)
- Isometry-invariant
- Positive semidefinite

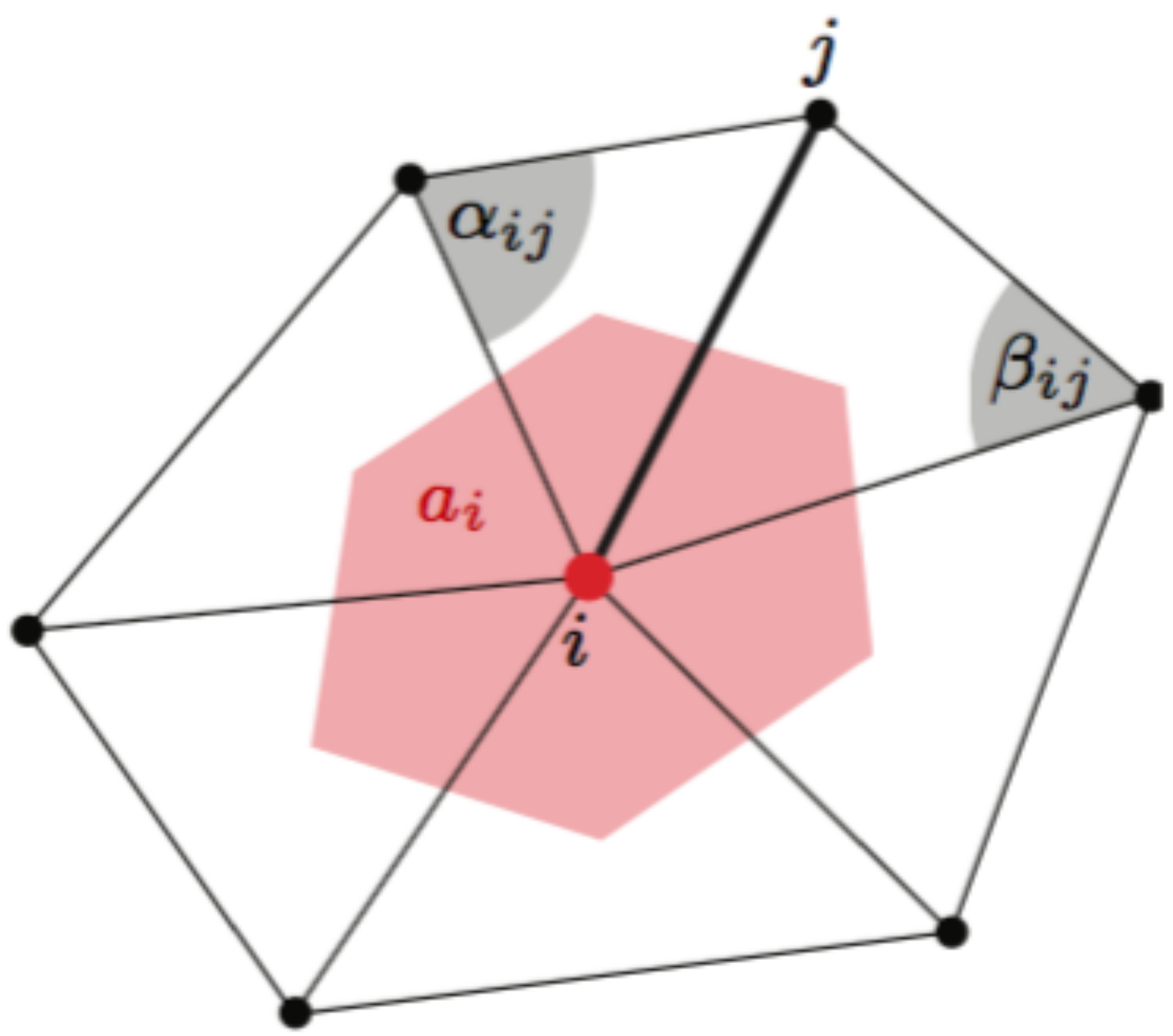
from Jonathan Masci et al

Discrete Laplacian



Undirected graph (V, E)

$$(\Delta f)_i \approx \sum_{(i,j)\in E} w_{ij}(f_i - f_j)$$



Triangular mesh (V, E, F)

$$(\Delta f)_i \approx \frac{1}{a_i} \sum_{(i,j)\in E} \frac{\cot \alpha_{ij} + \cot \beta_{ij}}{2}(f_i - f_j)$$

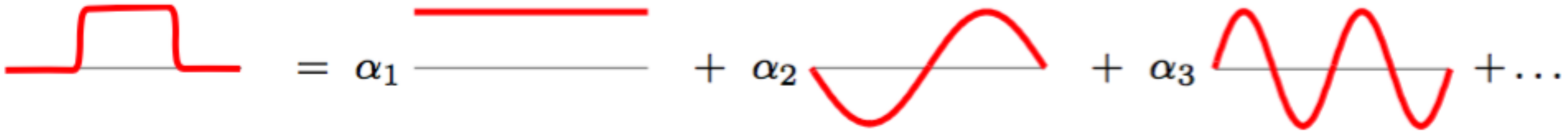
a_i = local area element

from Jonathan Masci et al

Fourier analysis - Euclidean space

A function $f : [-\pi, \pi] \to \mathbb{R}$ can be written as Fourier series

$$f(x) = \sum_{\omega} \frac{1}{2\pi} \int_{-\pi}^{\pi} f(x')e^{i\omega x'} dx' \, e^{-i\omega x}$$



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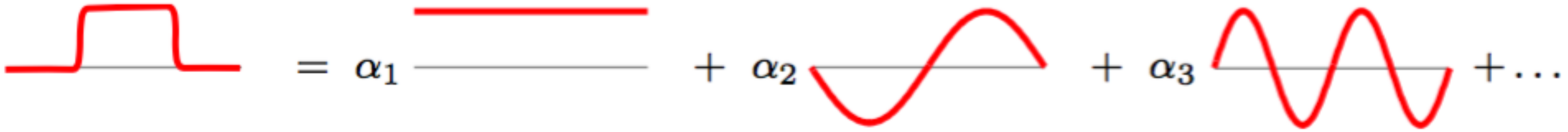
$$f(x) = \sum_{\omega} \underbrace{\frac{1}{2\pi} \int_{-\pi}^{\pi} f(x') e^{i\omega x'} dx'}_{\hat{f}(\omega) = \langle f, e^{-i\omega x} \rangle_{L^2([-\pi,\pi])}} e^{-i\omega x}$$



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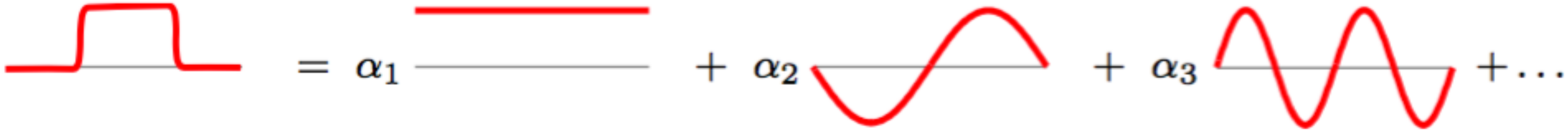


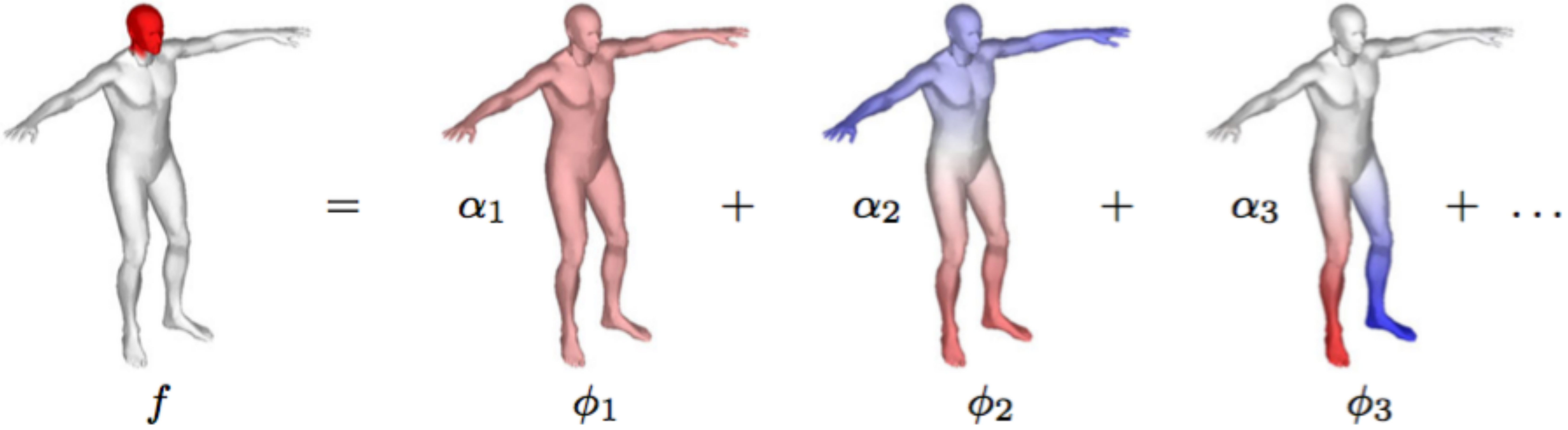
Fourier basis = Laplacian eigenfunctions: $\Delta e^{-i\omega x} = \omega^2 e^{-i\omega x}$

from Jonathan Masci et al

Fourier analysis - non Euclidean space

A function $f : \mathcal{X} \to \mathbb{R}$ can be written as Fourier series

$$f(x) = \sum_{k \geq 0} \underbrace{\int_{\mathcal{X}} f(x')\phi_k(x')dx'}_{\hat{f}_k = \langle f, \phi_k \rangle_{L^2(\mathcal{X})}} \; \phi_k(x)$$



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

from Jonathan Masci et al

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How to define convolution kernel on graphs?

from Shuman et al. 2013

How to allow multi-scale analysis?

How to ensure generalizability across graphs?

Geodesic CNN

- Constructing convolution kernels:
  - Local system of geodesic polar coordinate
  - Extract a small patch at each point x
  - Radial coordinate ρ - geodesic distance (truncated)
  - Angular coordinate θ - direction of geodesics (origin choice)

Jonathan Masci et al 2015

Geodesic CNN

- Local chart: bijective map

$$\Omega(x) : B_{\rho_0}(x) \to [0, \rho_0] \times [0, 2\pi)$$

from manifold to local coordinates
(ρ, θ) around x

Jonathan Masci et al 2015

Geodesic CNN

- Local chart: bijective map

$$\Omega(x) : B_{\rho_0}(x) \to [0, \rho_0] \times [0, 2\pi)$$

from manifold to local coordinates (ρ, θ) around x

- Patch operator applied to $f \in L^2(X)$

interpolate f in the local coordinate

Jonathan Masci et al 2015

Geodesic CNN

$$(D(x)f)(\rho,\theta) = \frac{\int_X v_\rho(x,\xi) v_\theta(x,\xi) f(\xi) d\xi}{\int_X v_\rho(x,\xi) v_\theta(x,\xi) d\xi}$$

Radial weight

$$v_\rho(x,\xi) \propto e^{-(d_X(x,\xi)-\rho)^2/\sigma_\rho^2}$$

Angular weight

$$v_\theta(x,\xi) \propto e^{-d_X^2(\Gamma(x,\theta),\xi)/\sigma_\theta^2}$$

Jonathan Masci et al 2015

Geodesic CNN

- Geodesic convolution = apply filter a to patches extracted from $f \in L^2(X)$ in local geodesic polar coordinates

$$(f \star a)(x) = \sum_{\theta, r} (D(x)f)(r, \theta)\ a(\theta, r)$$

Jonathan Masci et al 2015

Geodesic CNN

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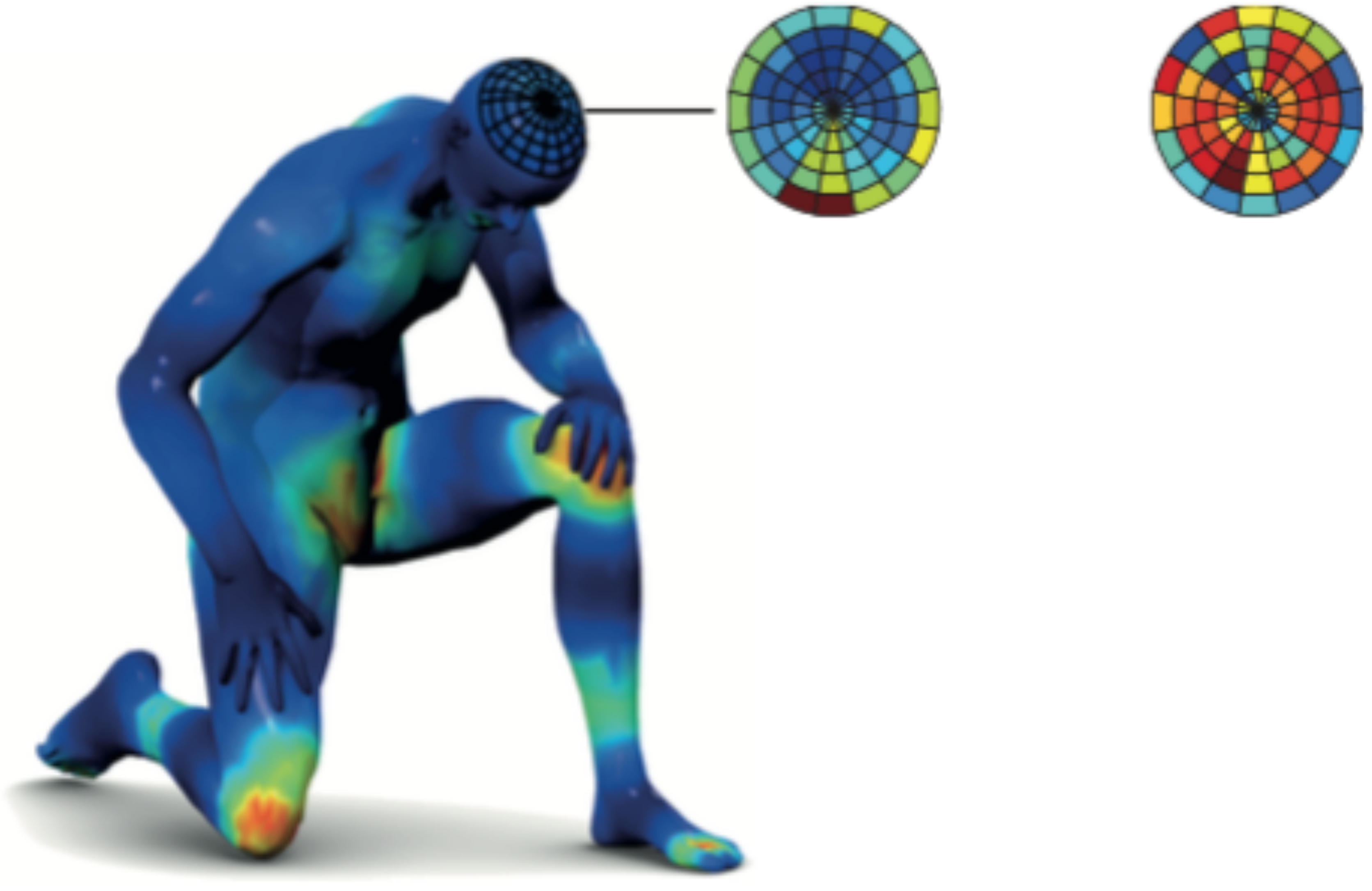

Jonathan Masci et al 2015

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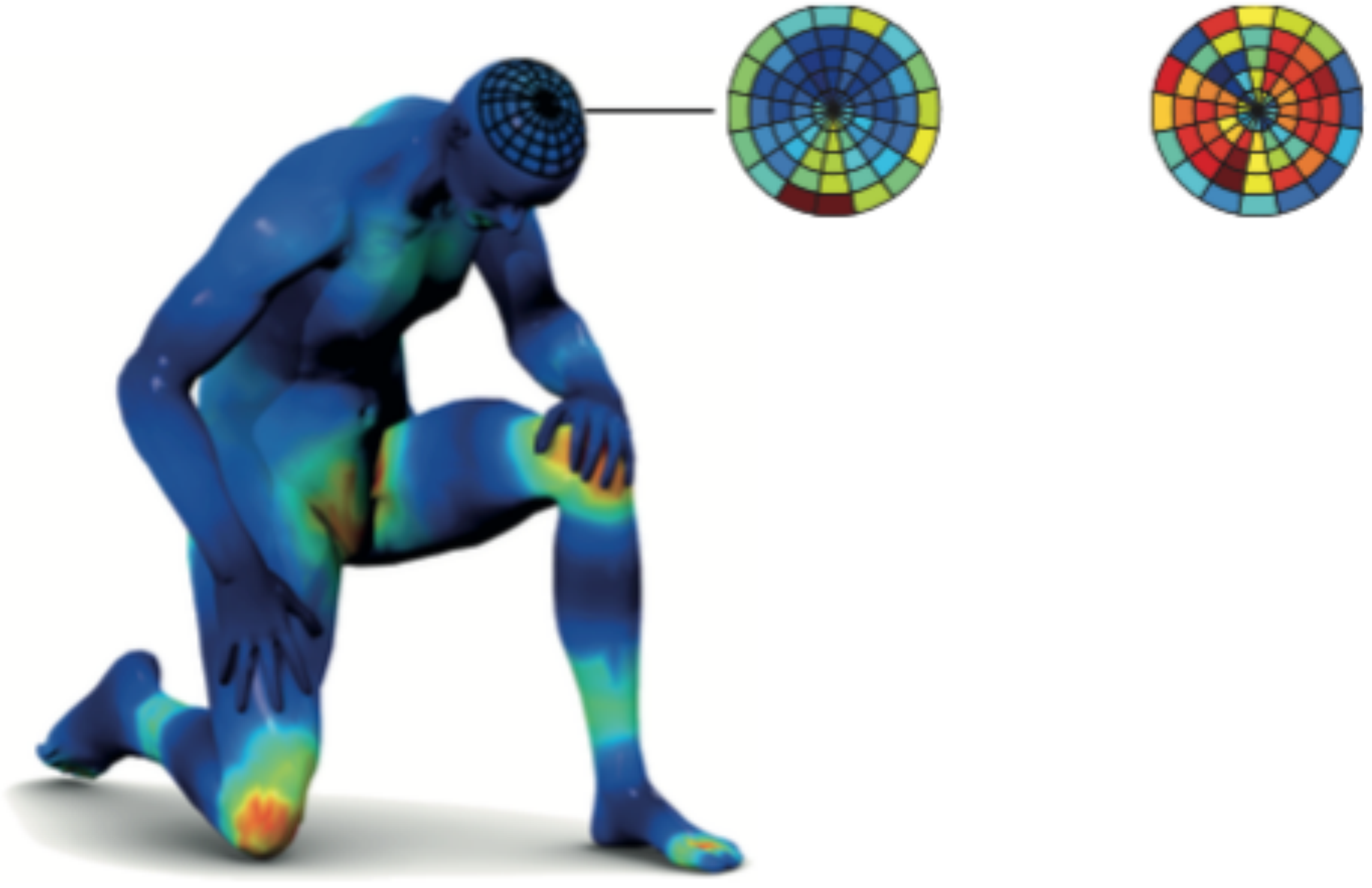

rotation ambiguity

Jonathan Masci et al 2015

Geodesic CNN

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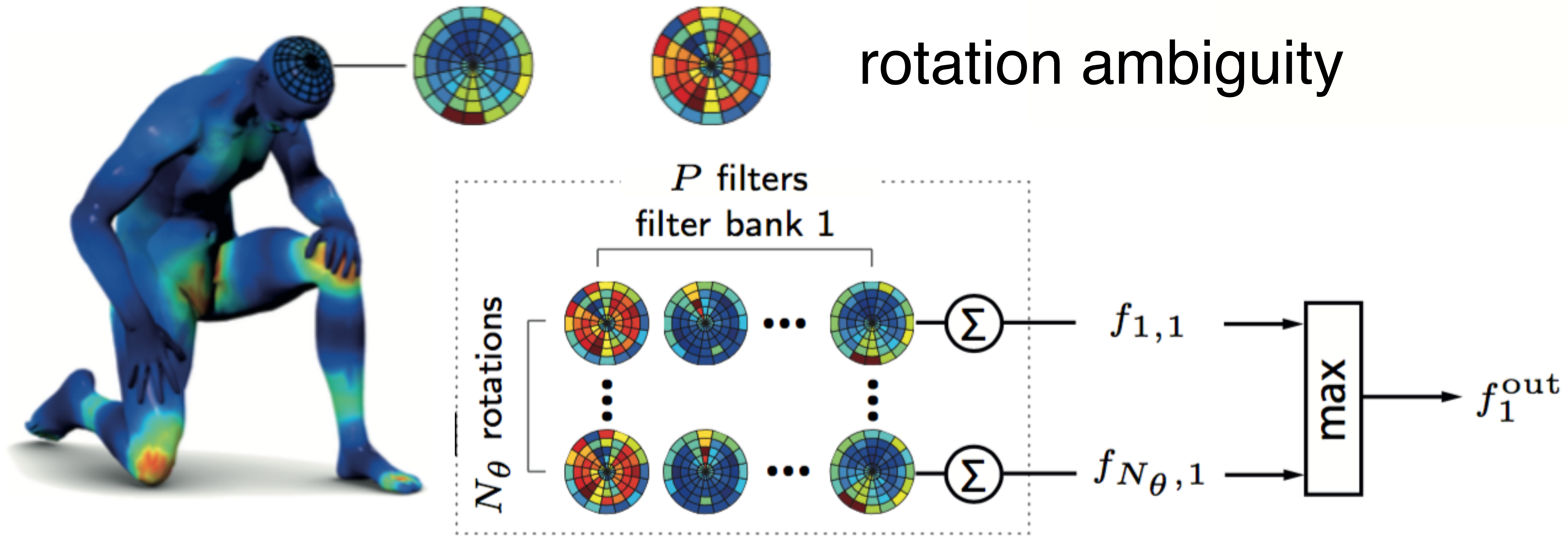
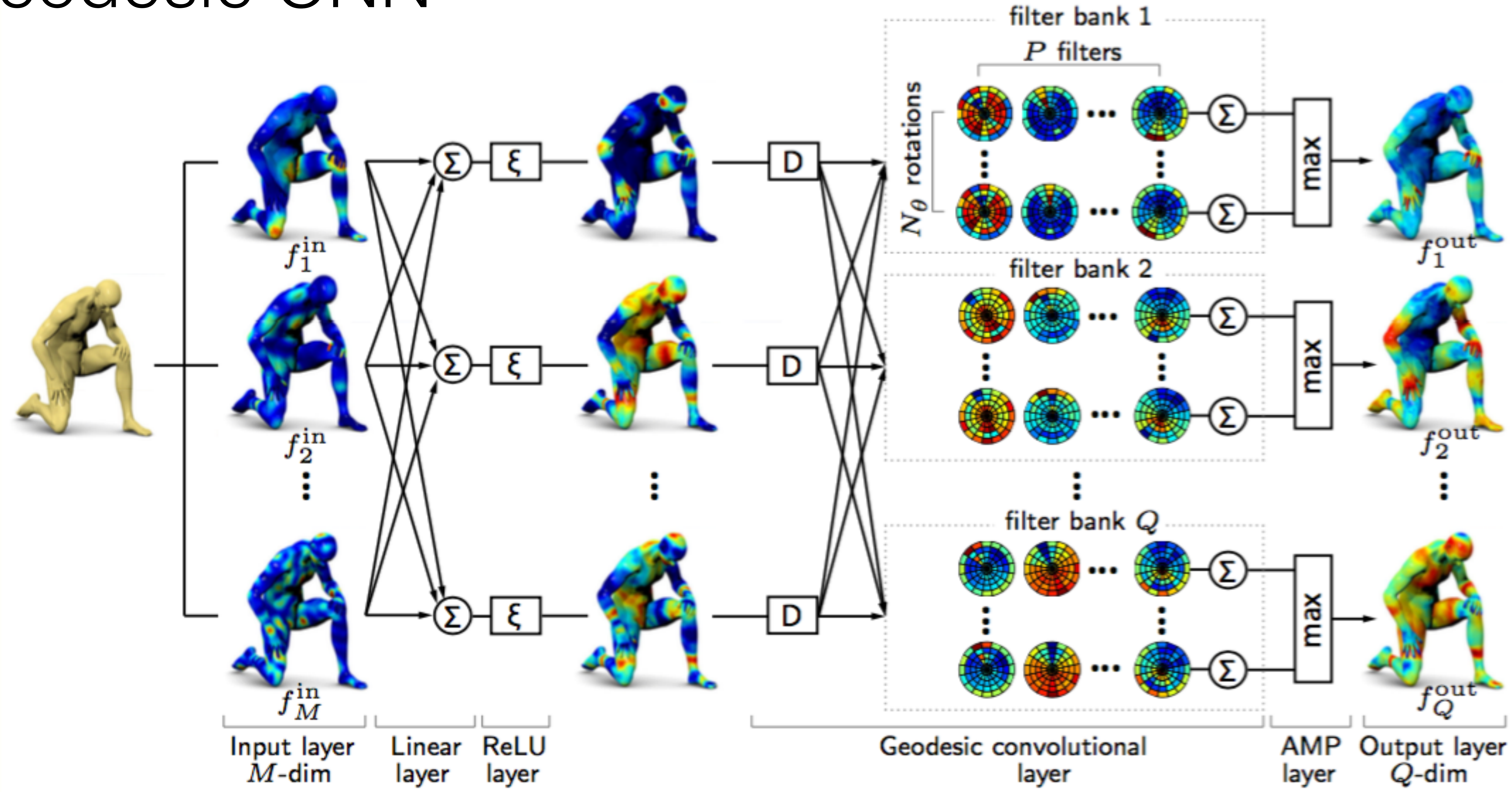


Jonathan Masci et al 2015

Geodesic CNN



Jonathan Masci et al 2015

Geodesic CNN

- Issues:
  - The local charting method relies on a fast marching-like procedure requiring a triangular mesh.
  - The radius of the geodesic patches must be sufficiently small to acquire a topological disk.
  - No effective pooling, purely relying on convolutions to increase receptive field.

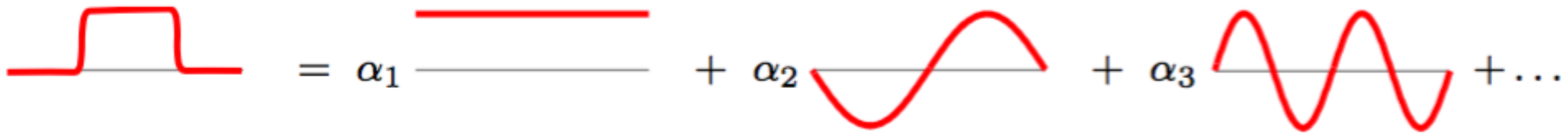
Agenda

- Challenges
- Background knowledge
- Spatial construction
  - Geodesic CNN
- Spectral construction
  - Spectral CNN
  - Anisotropic CNN
  - SyncSpecCNN

Fourier analysis

A function $f : [-\pi, \pi] \to \mathbb{R}$ can be written as Fourier series

$$f(x) = \sum_{\omega} \underbrace{\frac{1}{2\pi} \int_{-\pi}^{\pi} f(x') e^{i\omega x'} dx'}_{\hat{f}(\omega) = \langle f, e^{-i\omega x} \rangle_{L^2([-\pi,\pi])}} \, e^{-i\omega x}$$

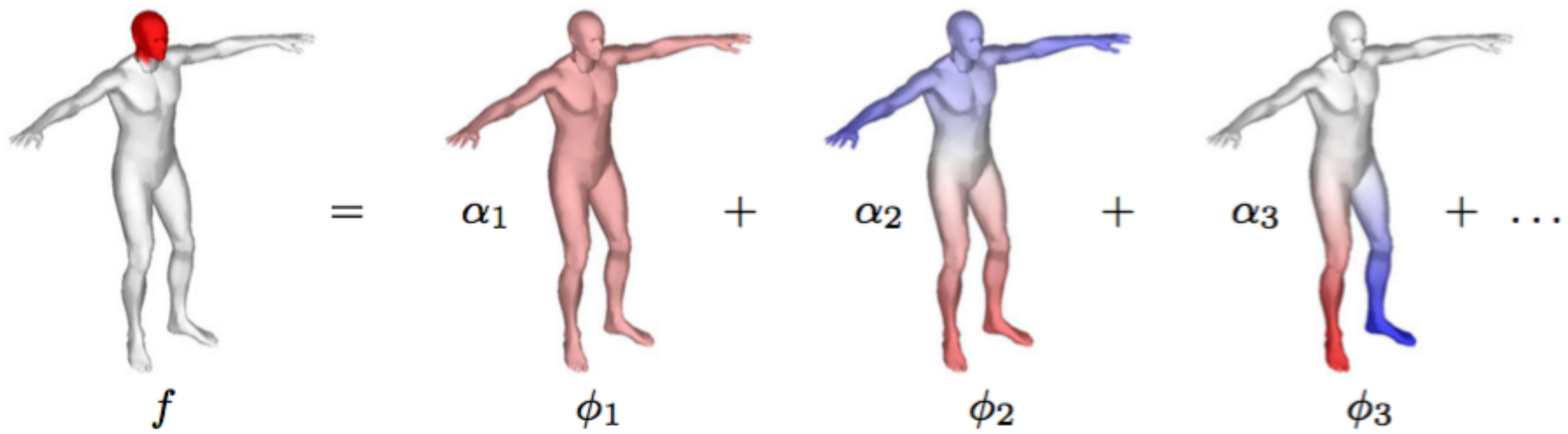


Fourier basis = Laplacian eigenfunctions: $\Delta e^{-i\omega x} = \omega^2 e^{-i\omega x}$

Euclidean domain

A function $f : \mathcal{X} \to \mathbb{R}$ can be written as Fourier series

$$f(x) = \sum_{k \geq 0} \underbrace{\int_{\mathcal{X}} f(x') \phi_k(x') dx'}_{\hat{f}_k = \langle f, \phi_k \rangle_{L^2(\mathcal{X})}} \ \phi_k(x)$$



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

non Euclidean domain

from Jonathan Masci et al

Convolution Theorem in Euclidean domain

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

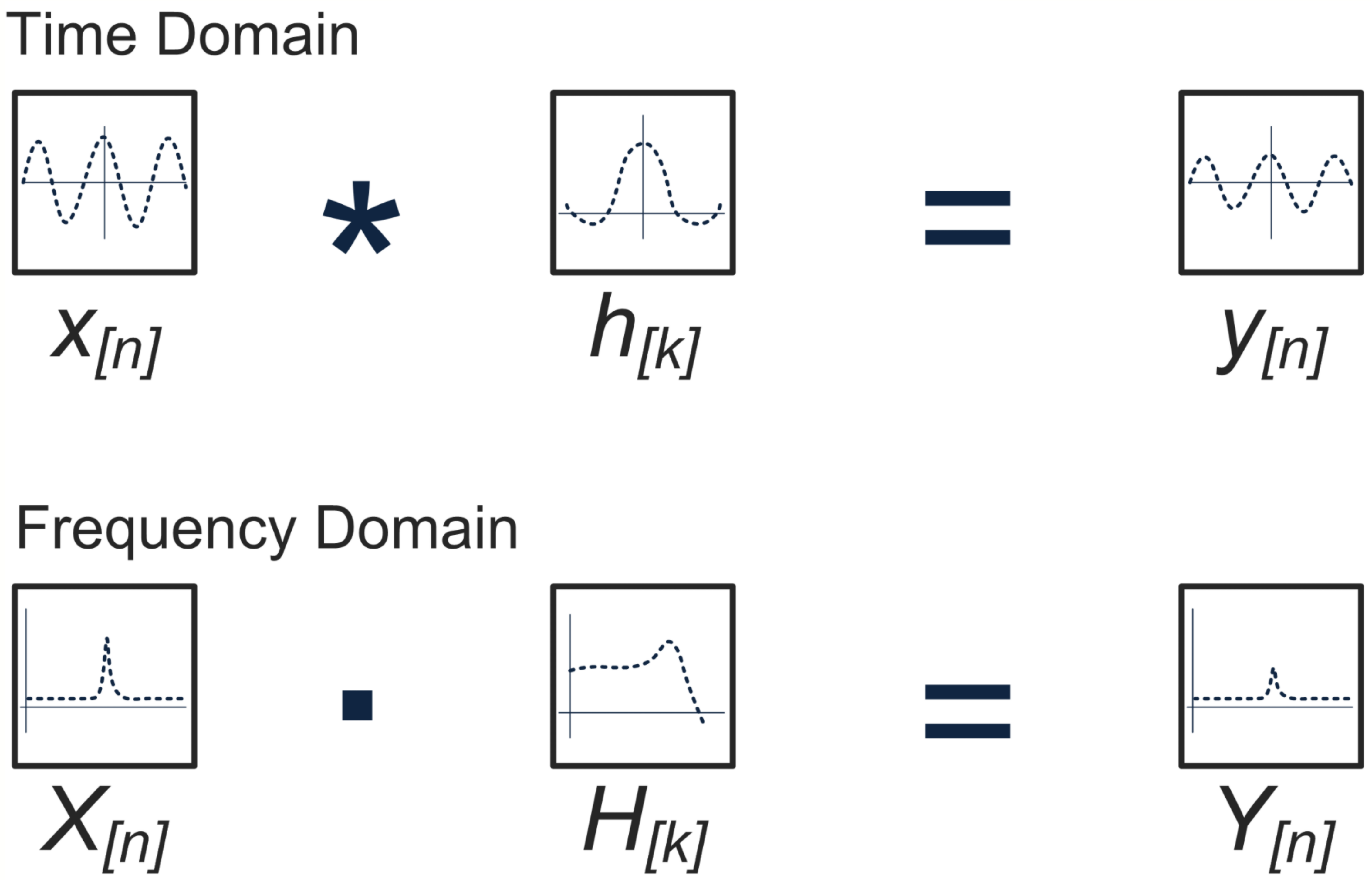
$$(f \star g)(x) = \int_{-\pi}^{\pi} f(\xi) g(x - \xi) d\xi$$

Convolution Theorem: Fourier transform diagonalizes the convolution operator $\Rightarrow$ convolution can be computed in the Fourier domain as

$$f \star g = \mathcal{F}^{-1}(\mathcal{F}f \cdot \mathcal{F}g)$$

from Jonathan Masci et al

Convolution Theorem in Euclidean domain



Convolution Theorem in non Euclidean domain

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

$$(f \star g)(x) = \sum_{k \geq 1} \langle f, \phi_k \rangle_{L^2(X)} \langle g, \phi_k \rangle_{L^2(X)} \phi_k(x)$$

from Jonathan Masci et al

Convolution Theorem in non Euclidean domain

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

from Jonathan Masci et al

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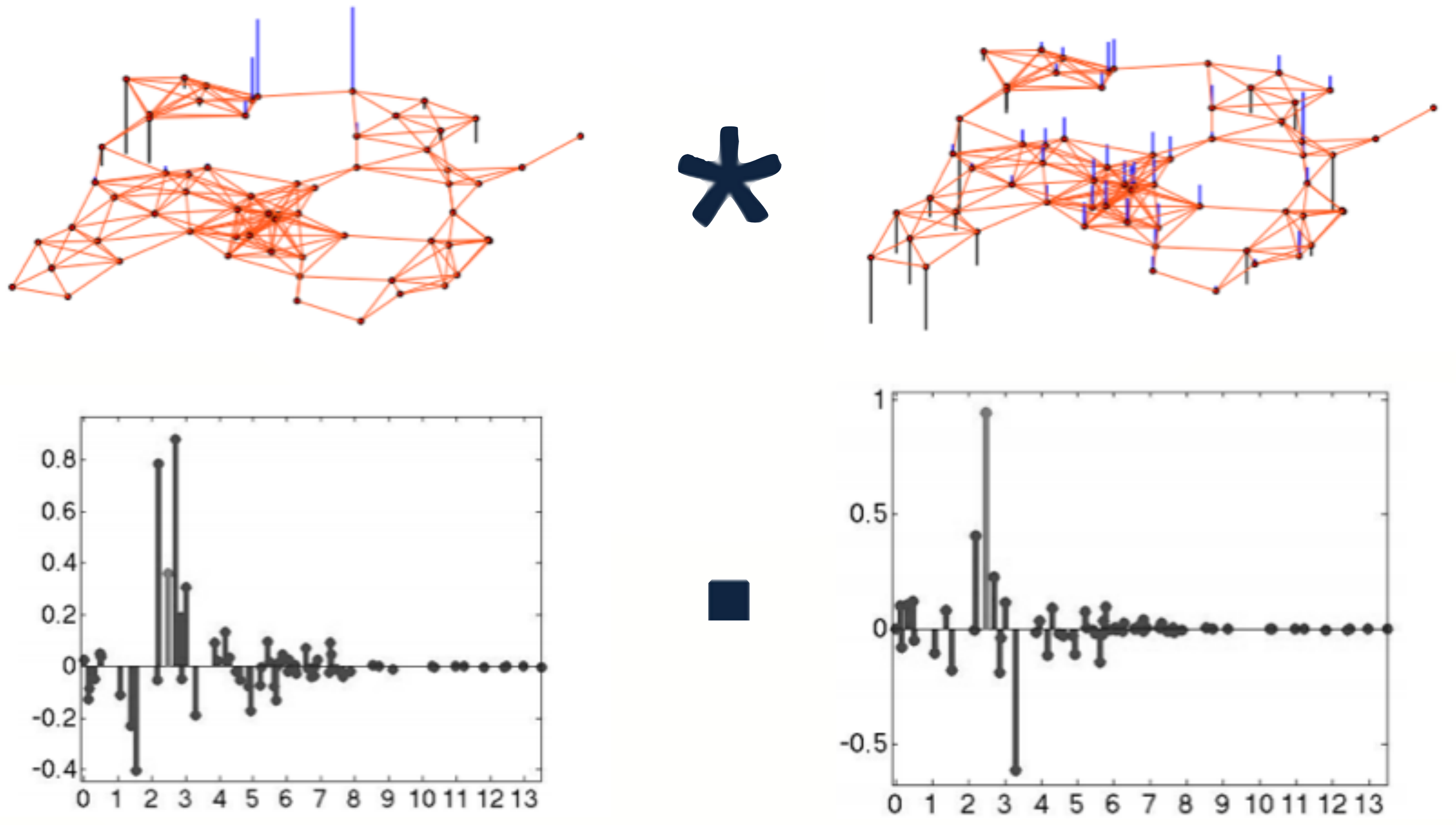

modified from Jonathan Masci et al

Convolution Theorem in non Euclidean domain

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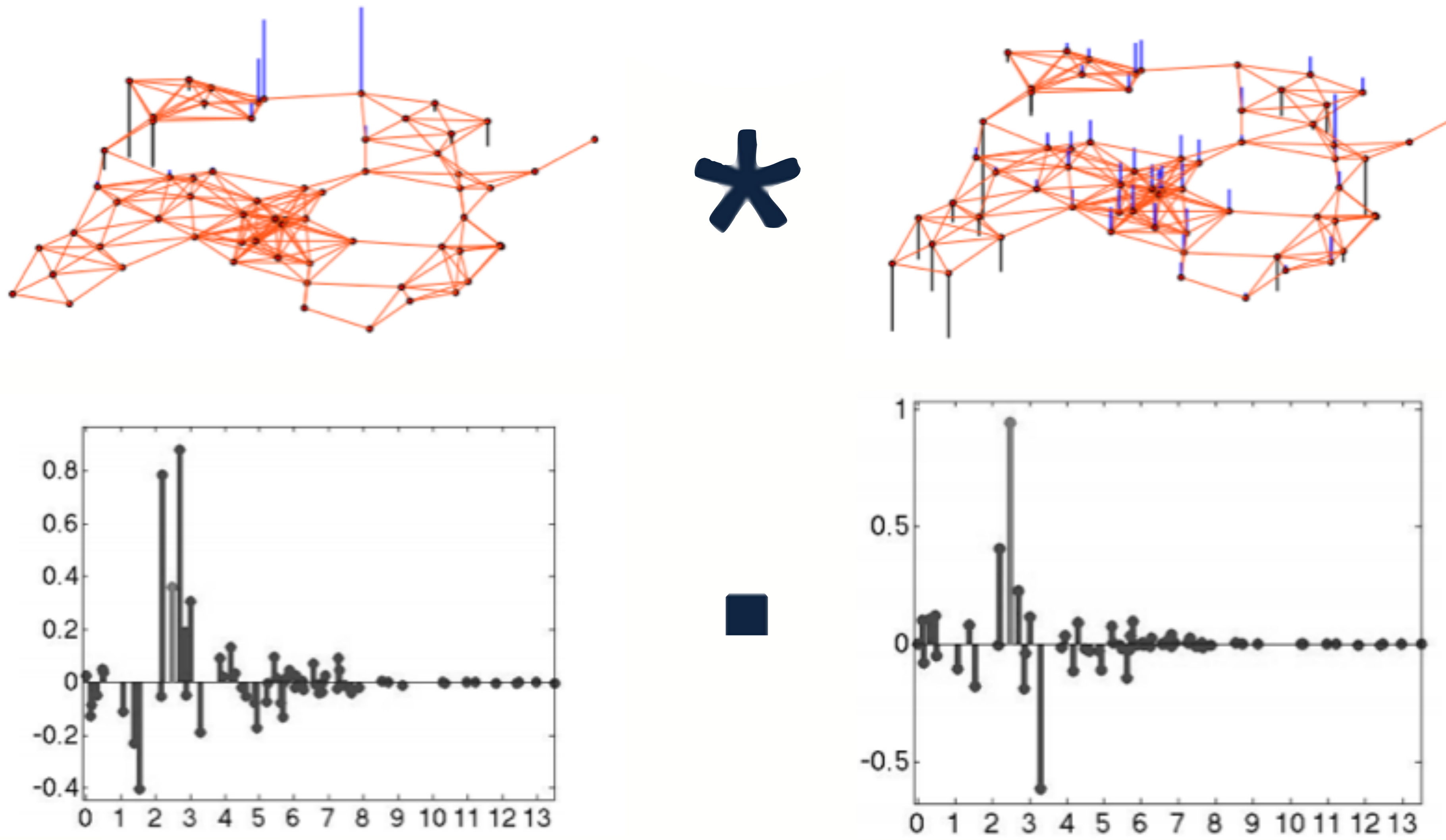
$$(f \star g)(x) = \underbrace{\sum_{k \geq 1} \underbrace{\langle f, \phi_k \rangle_{L^2(X)} \langle g, \phi_k \rangle_{L^2(X)}}_{\text{product in the Fourier domain}} \phi_k(x)}_{\text{inverse Fourier transform}}$$

directly design convolution kernel in the spectral domain



modified from Jonathan Masci et al

Spectral CNN

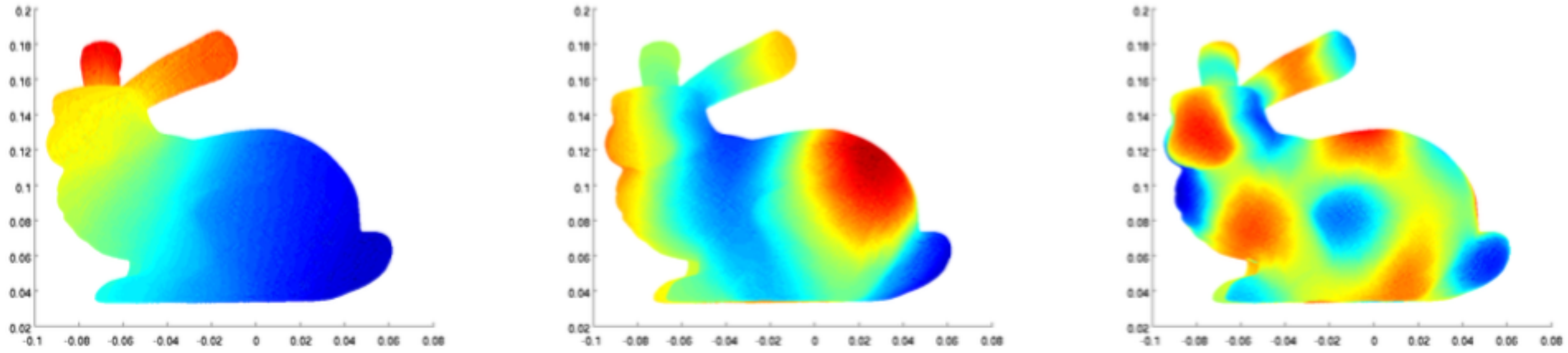
- We can define the Laplacian on an undirected graph:

  $\Delta = (I - \tilde{W})$, $\tilde{W} = D^{-1/2} W D^{-1/2}$, $D = \mathrm{diag}(W\mathbf{1})$

  $(\Delta x)_k = x_k - \sum_j \tilde{w}_{kj} x_j$ measures smoothness in the graph

- Δ is positive definite and symmetric. $\Delta = V \mathrm{diag}(\lambda) V^T$

- "Fourier basis" of the graph: V : Eigenvectors of Δ



v_2 v_{10} v_{30}

Joan Bruna et al. 2013

Spectral CNN

- "Convolution" on a graph: Linear Operator commuting with Δ:

$$x *_G h := V \text{diag}(h) V^T x$$

  - Filter coefficients *h* are specified in the spectral domain.

- Spectral Network: filter bank $(x *_G h_k)_{k \leq K}$

Joan Bruna et al. 2013

Spectral CNN

- "Convolution" on a graph: Linear Operator commuting with Δ:

$$x *_G h := V \text{diag}(h) V^T x$$

  – Filter coefficients *h* are specified in the spectral domain.

- Spectral Network: filter bank $(x *_G h_k)_{k \leq K}$

Needs O(n) parameters per filter

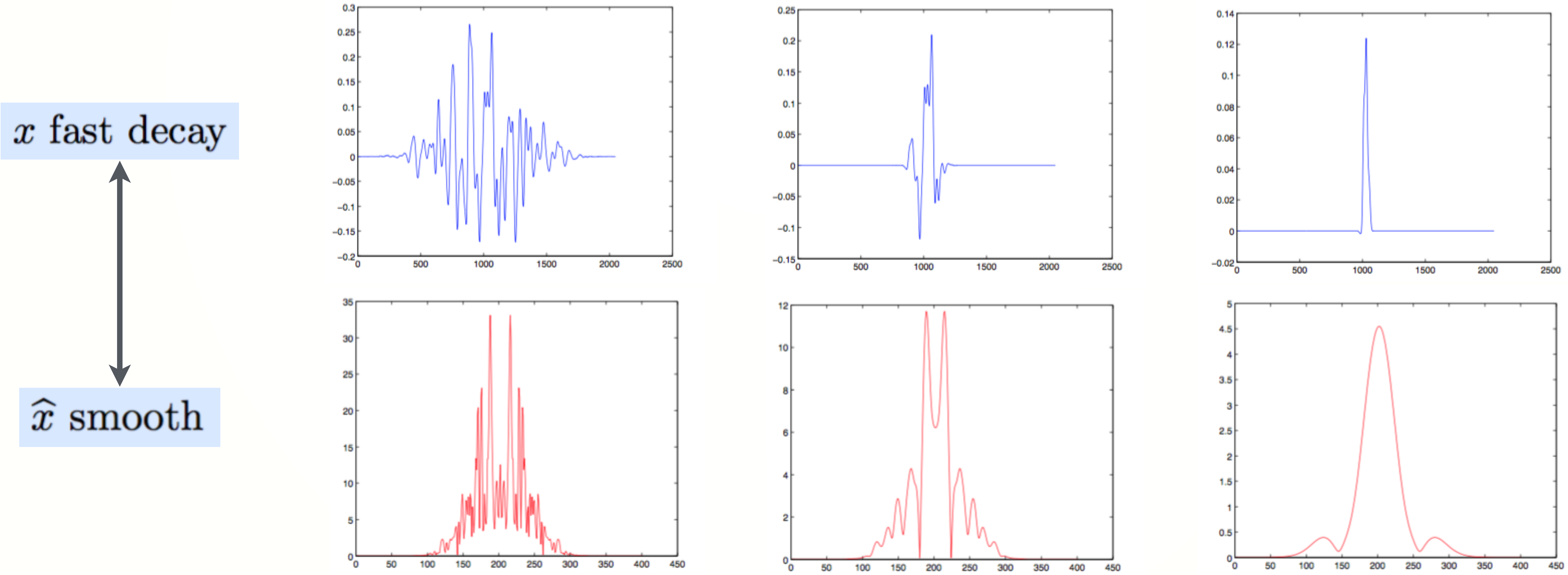
There's no guarantee the filter will have local support on the graph

Joan Bruna et al. 2013

Spectral CNN

- Observation:

In Fourier analysis, smoothness and sparsity are dual notions



Joan Bruna et al. 2013

Spectral CNN

- Use smooth interpolation kernels (spline, polynomial, heat kernel, etc.) to parameterize the filters

Joan Bruna et al. 2013

Spectral CNN

- Use smooth interpolation kernels (spline, polynomial, heat kernel, etc.) to parameterize the filters

spatially locally concentrated

Joan Bruna et al. 2013

Spectral CNN

- Use smooth interpolation kernels (spline, polynomial, heat kernel, etc.) to parameterize the filters

control #parameter

spatially locally concentrated

Spectral CNN

- Issues:
  - Convolution kernels are not shift-invariant.

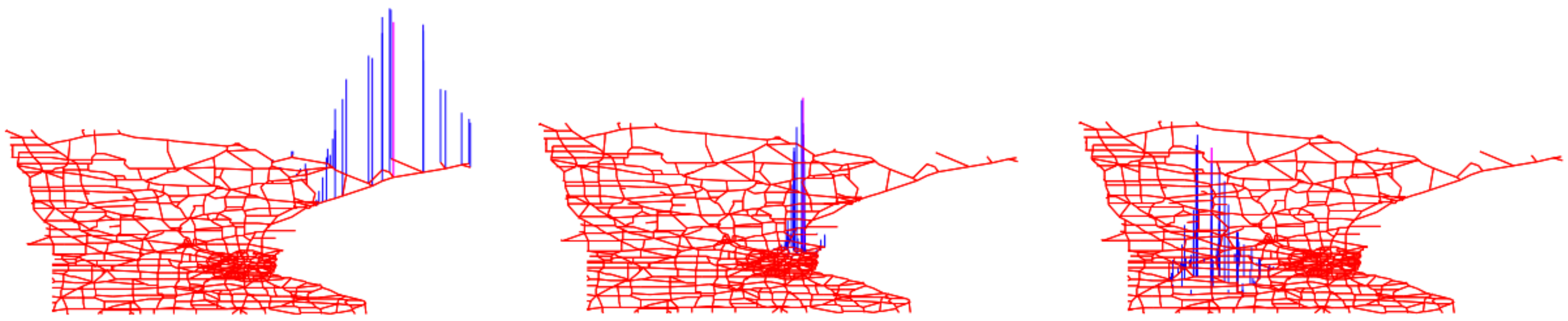


image from David I Shuman et al. 2016

A heat kernel translated to different vertices

Spectral CNN

- Issues:
    - Convolution kernels are not shift-invariant.
    - No effective pooling
    - Filter weights depend on Fourier basis, does not generalize well to new domains

Spectral CNN

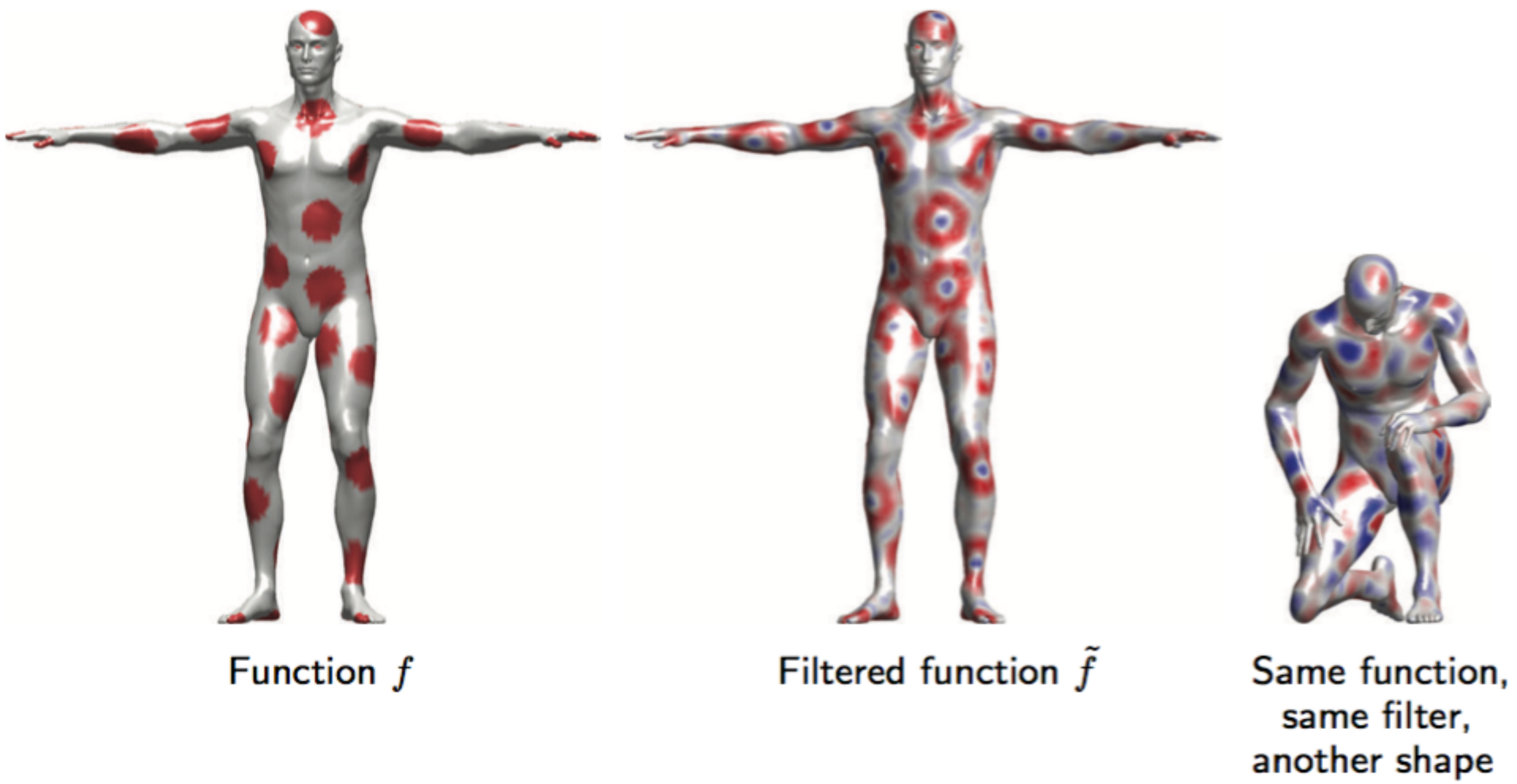


image from Jonathan Masci et al

Agenda

- Challenges
- Background knowledge
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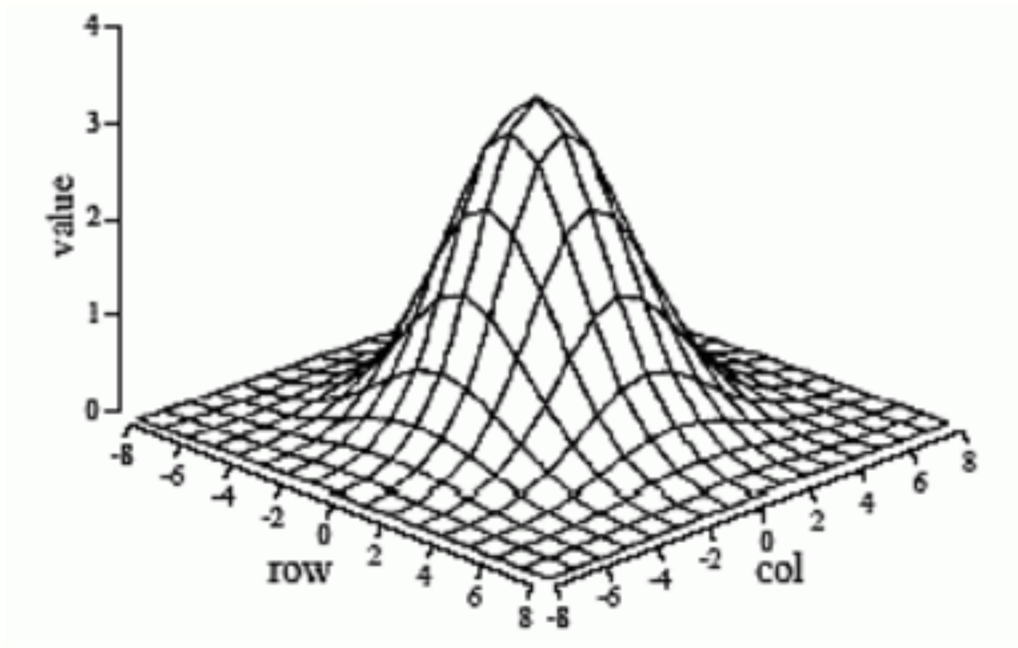
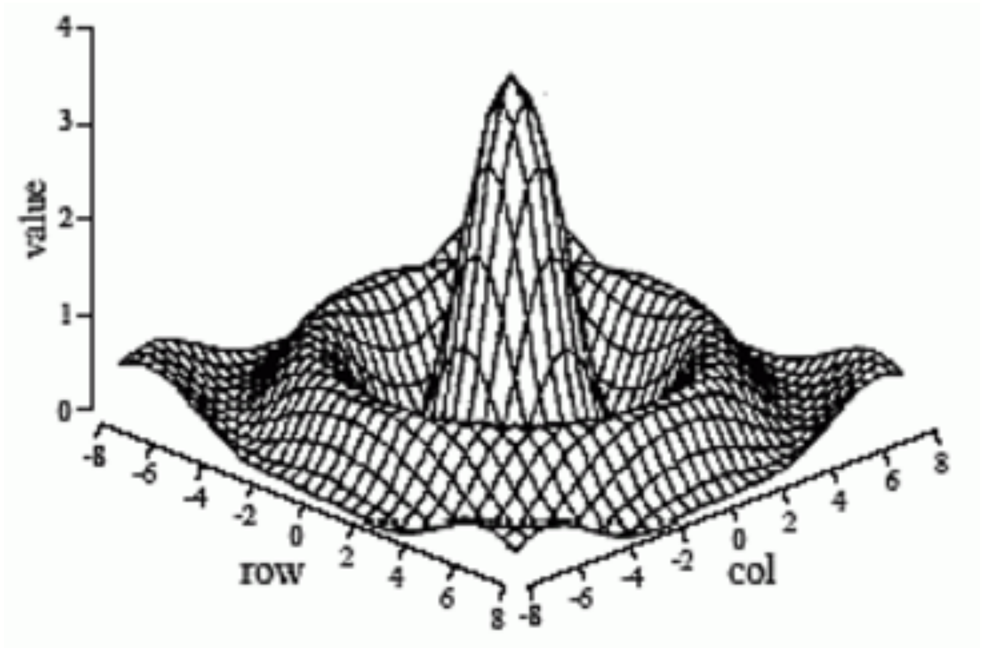
    - SyncSpecCNN

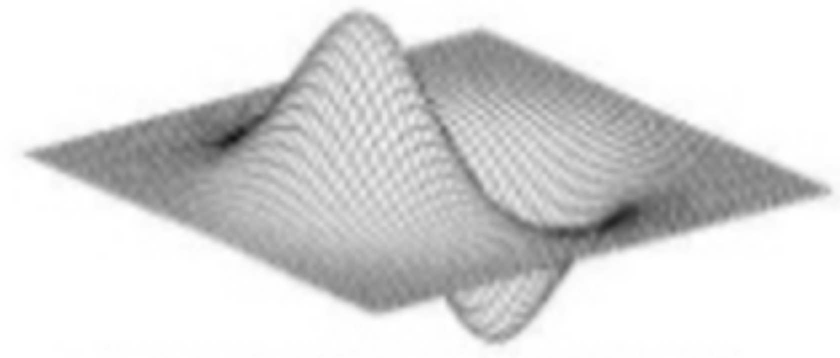
By far, we are using isotropic filters

- Less descriptive, in analogy to circular filters in image CNN





circular filters

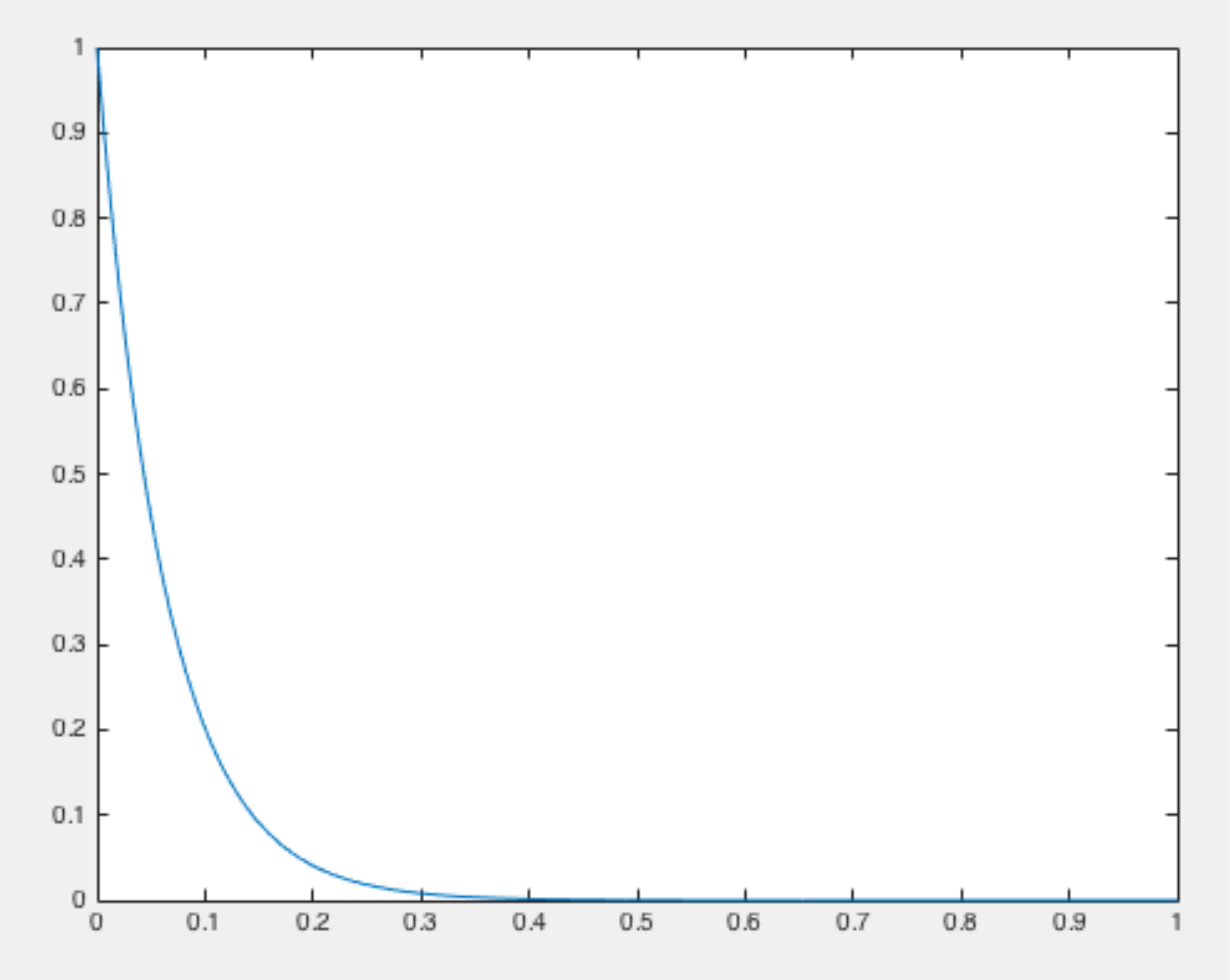


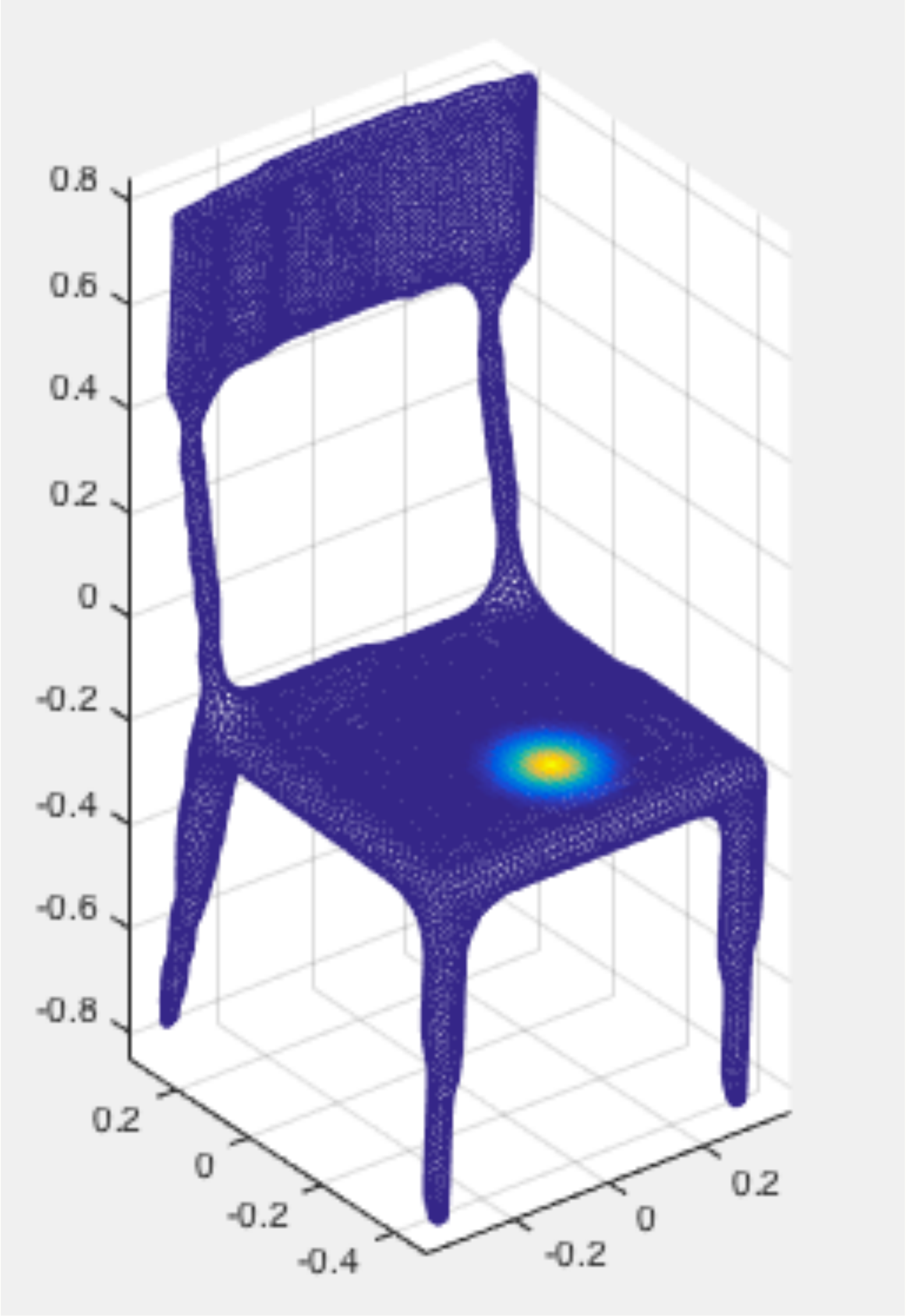
edge filters

Consider a specific type of interpolation kernels

- Heat kernel

$$h_t(x,\xi) = \sum_{k\geq 0} e^{-t\lambda_k}\phi_k(x)\phi_k(\xi).$$





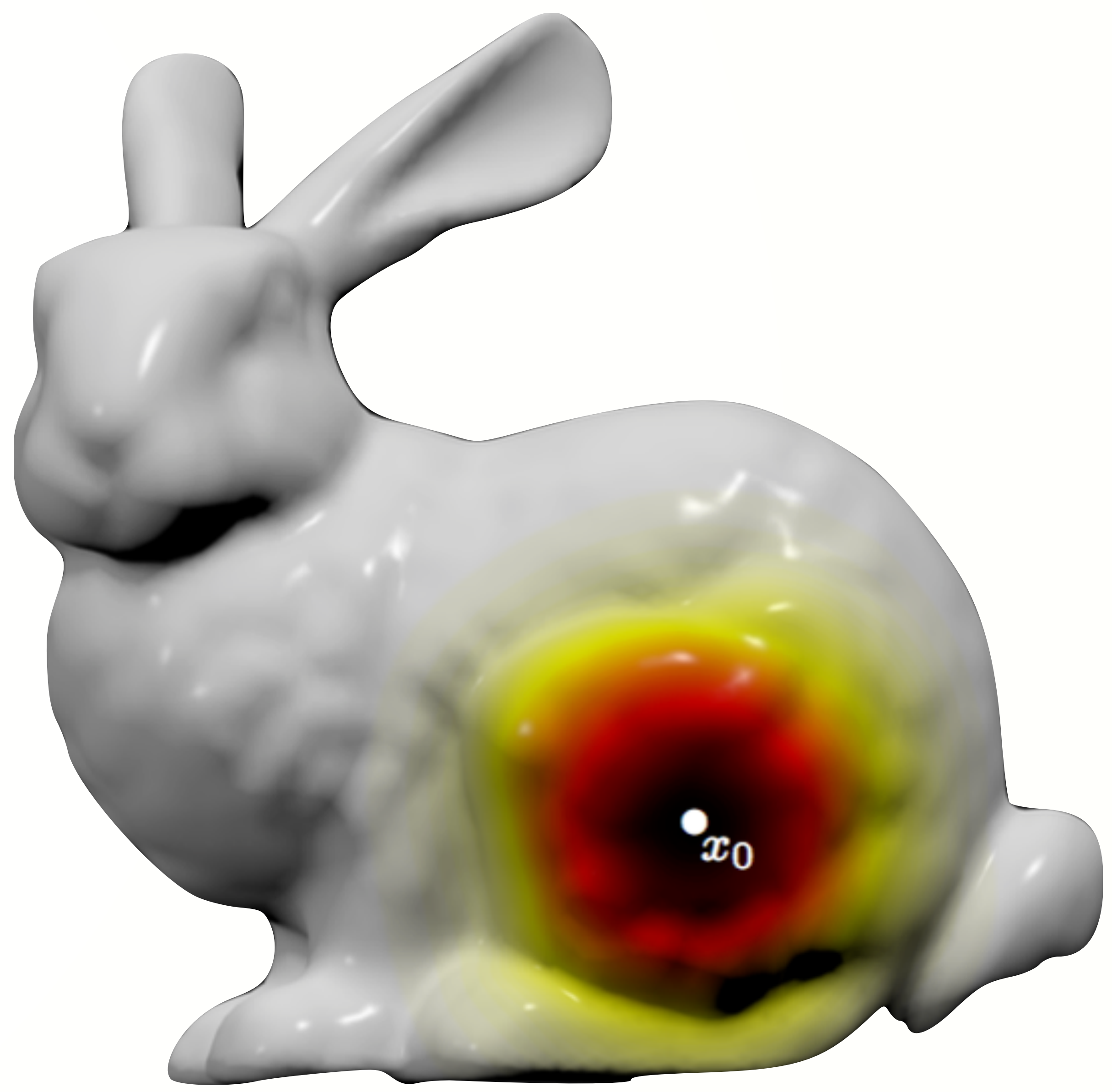
Davide Boscaini et al. 2016

Consider a specific type of interpolation kernels

- Heat kernel - isotropic diffusion

$$f_t(x) = -\mathrm{div}_X(c\nabla_X f(x))$$

$c =$ **thermal diffusivity constant** describing heat conduction properties of the material (diffusion speed is equal everywhere)



Davide Boscaini et al. 2016

Consider a specific type of interpolation kernels

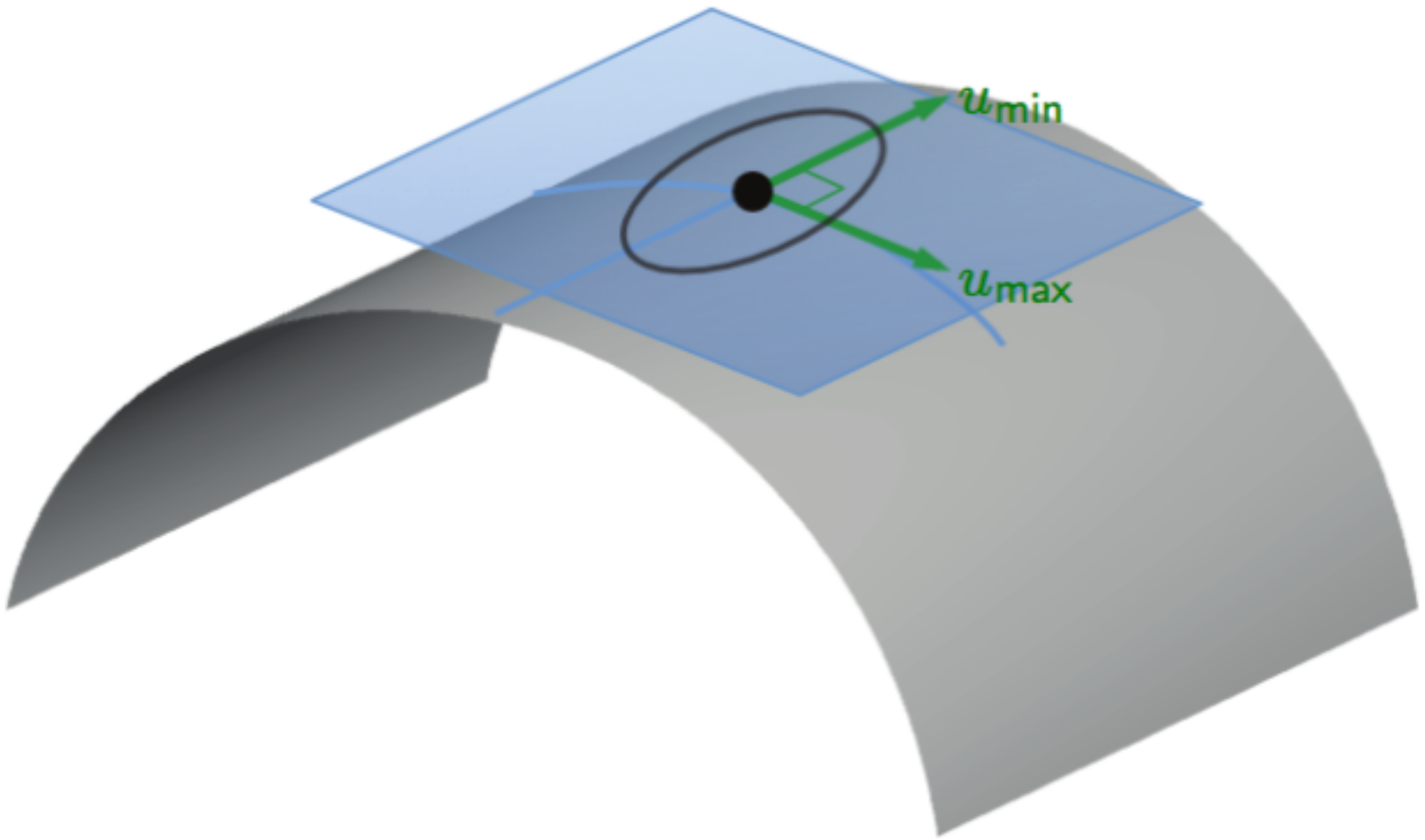
- Heat kernel - anisotropic diffusion

$$f_t(x) = -\mathrm{div}_X(A(x)\nabla_X f(x))$$

$A(x)$ = **heat conductivity tensor** describing heat conduction properties of the material (diffusion speed is position + direction dependent)

Davide Boscaini et al. 2016

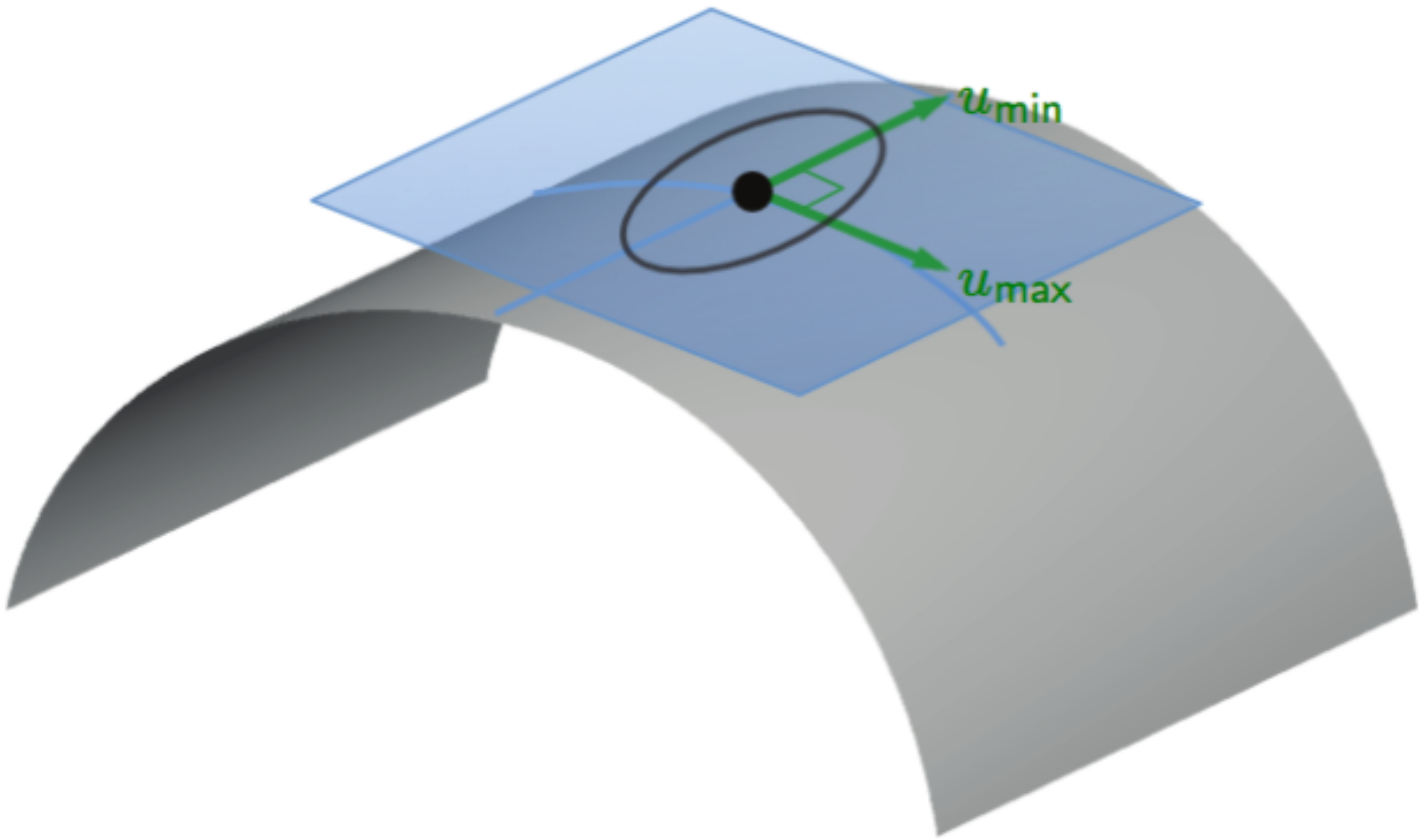
Anisotropic diffusion on manifold

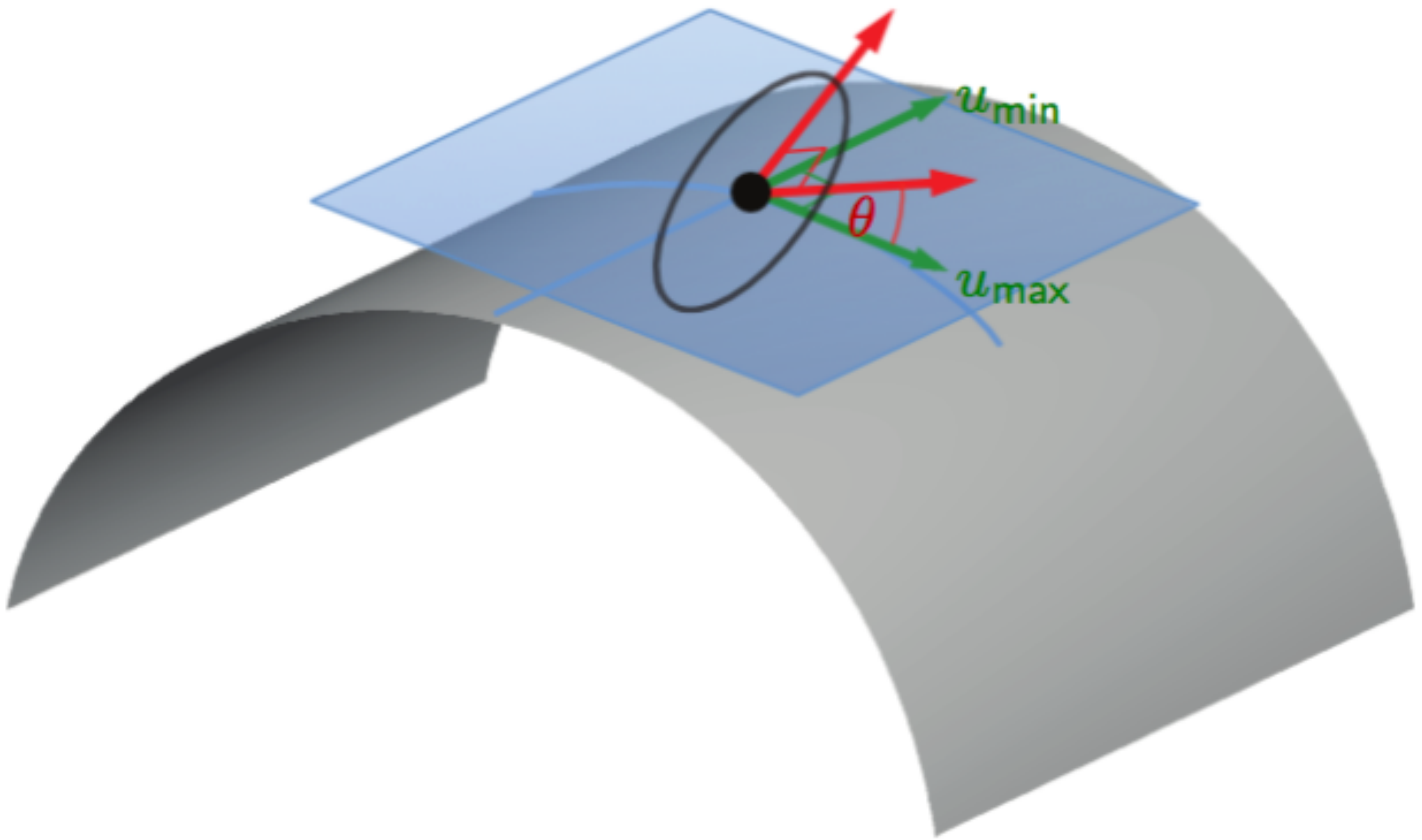


$$f_t(x) = -\text{div}_X \left(\begin{bmatrix} \alpha & \\ & 1 \end{bmatrix} \nabla_X f(x) \right)$$

Davide Boscaini et al. 2016

Anisotropic diffusion on manifold



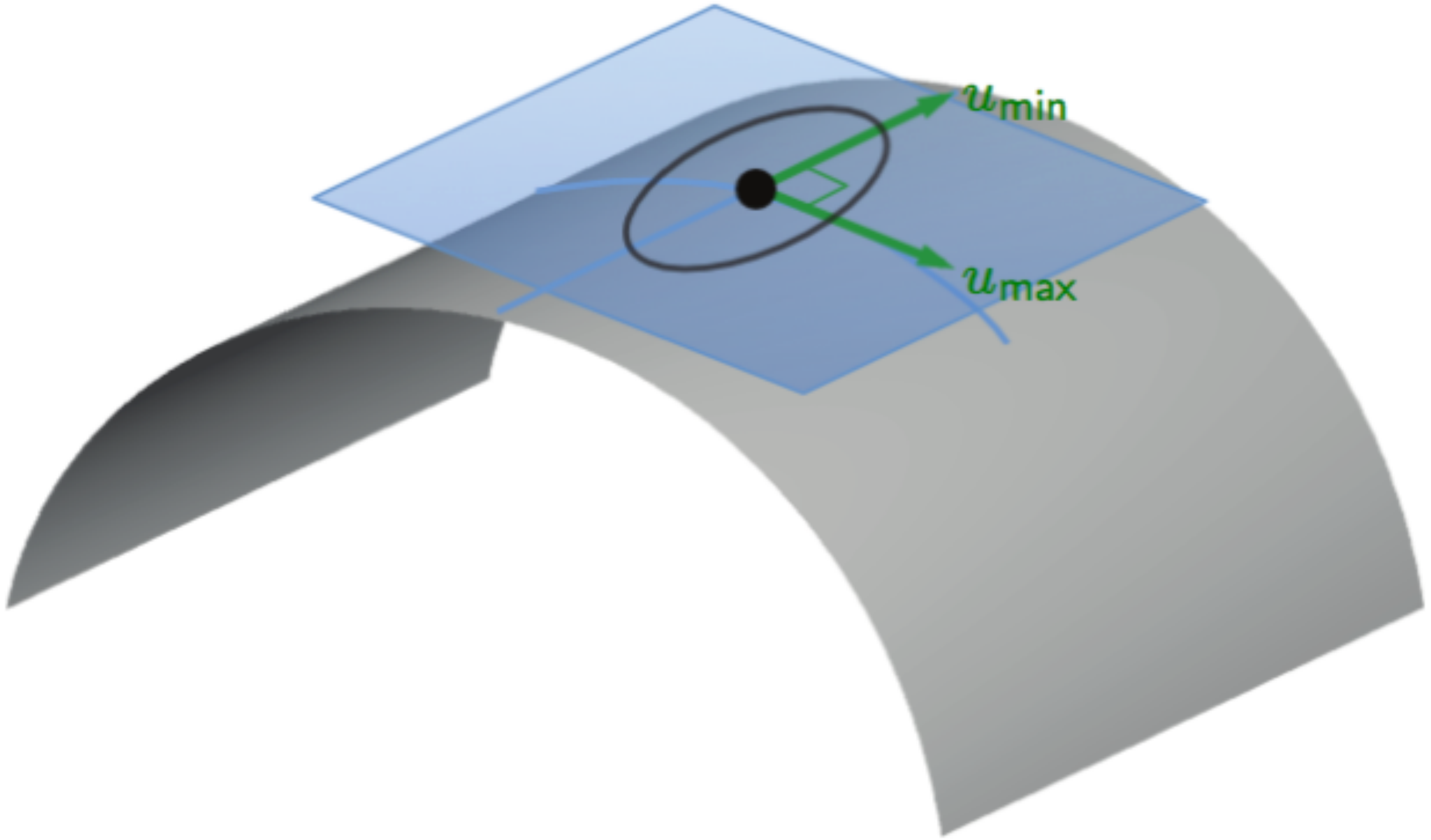


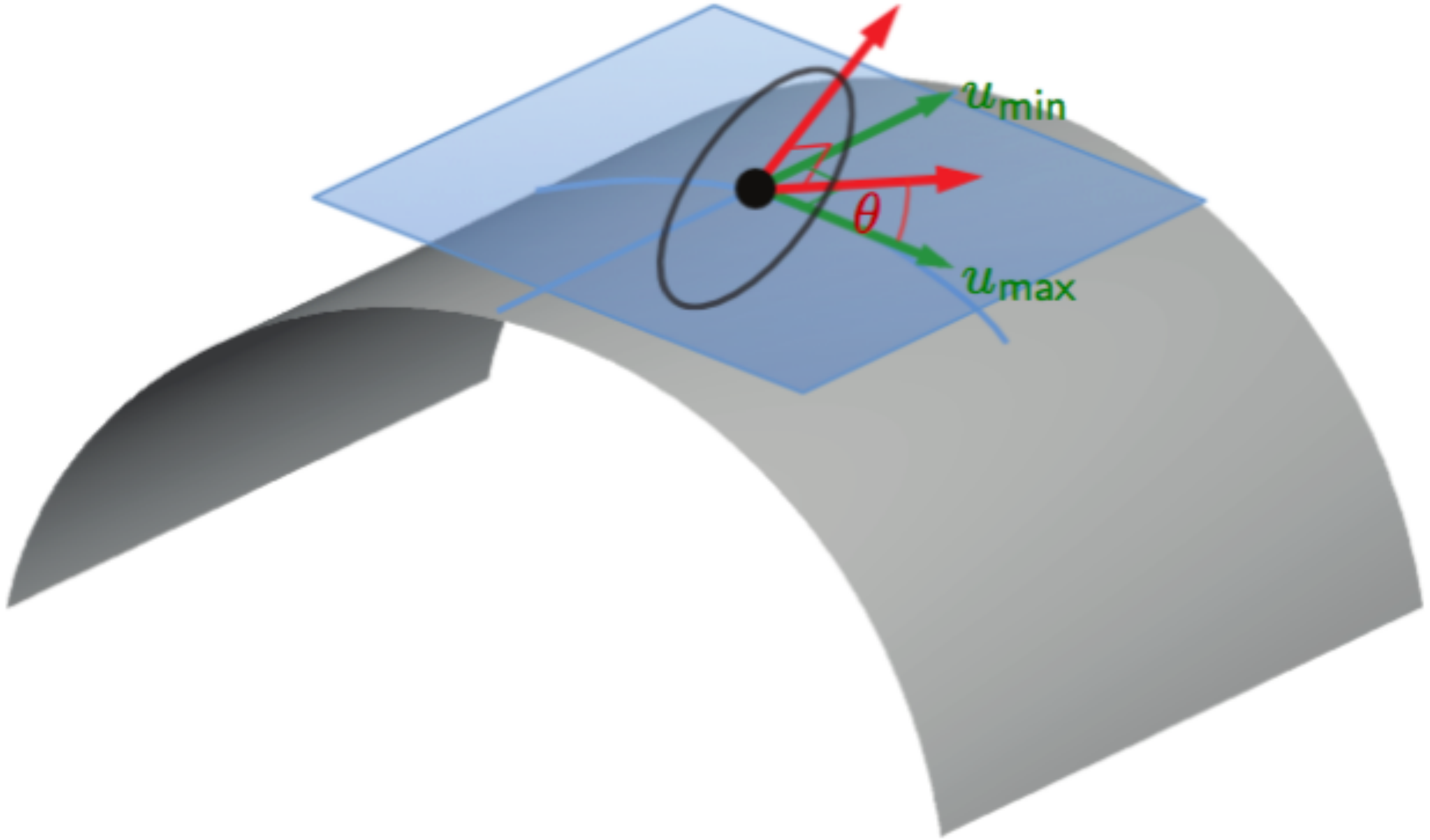
$$f_t(x) = -\mathrm{div}_X \left(\begin{bmatrix} \alpha & \\ & 1 \end{bmatrix} \nabla_X f(x) \right)$$

$$f_t(x) = -\mathrm{div}_X \left(\underbrace{R_\theta \begin{bmatrix} \alpha & \\ & 1 \end{bmatrix} R_\theta^\top}_{A_{\alpha\theta}(x)} \nabla_X f(x) \right)$$

Davide Boscaini et al. 2016

Anisotropic diffusion on manifold





$$f_t(x) = -\mathrm{div}_X \left(\begin{bmatrix} \alpha & \\ & 1 \end{bmatrix} \nabla_X f(x) \right)$$

$$f_t(x) = -\mathrm{div}_X \left(\underbrace{R_\theta \begin{bmatrix} \alpha & \\ & 1 \end{bmatrix} R_\theta^\top}_{A_{\alpha\theta}(x)} \nabla_X f(x) \right)$$

- **Anisotropic Laplacian** $\Delta_{\alpha\theta} f(x) = \mathrm{div}_X \left(A_{\alpha\theta}(x) \nabla_X f(x) \right)$
- $\theta =$ orientation w.r.t. max curvature direction
- $\alpha =$ 'elongation'

Davide Boscaini et al. 2016

Anisotropic heat kernels

Davide Boscaini et al. 2016

Anisotropic heat kernels

- Using anisotropic heat kernels to parameterize spectral filters is more descriptive

Davide Boscaini et al. 2016

Anisotropic heat kernels

- Sensitive to noise (computing the directions of principle curvatures)
- Does not tackle the generalization issue
- No pooling structure

Davide Boscaini et al. 2016

Agenda

- Challenges
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- Spatial construction
  - Geodesic CNN
- Spectral construction
  - Spectral CNN
  - Anisotropic CNN
  - SyncSpecCNN

Spectral CNN

- Issues:
  - Convolution kernels are not shift-invariant.
  - No effective pooling
  - Filter weights depend on Fourier basis, does not generalize well to new domains

SyncSpecCNN

- Introduce spectral counterpart for spatial pooling
- Synchronize Fourier basis for better generalizability

Spectral CNN

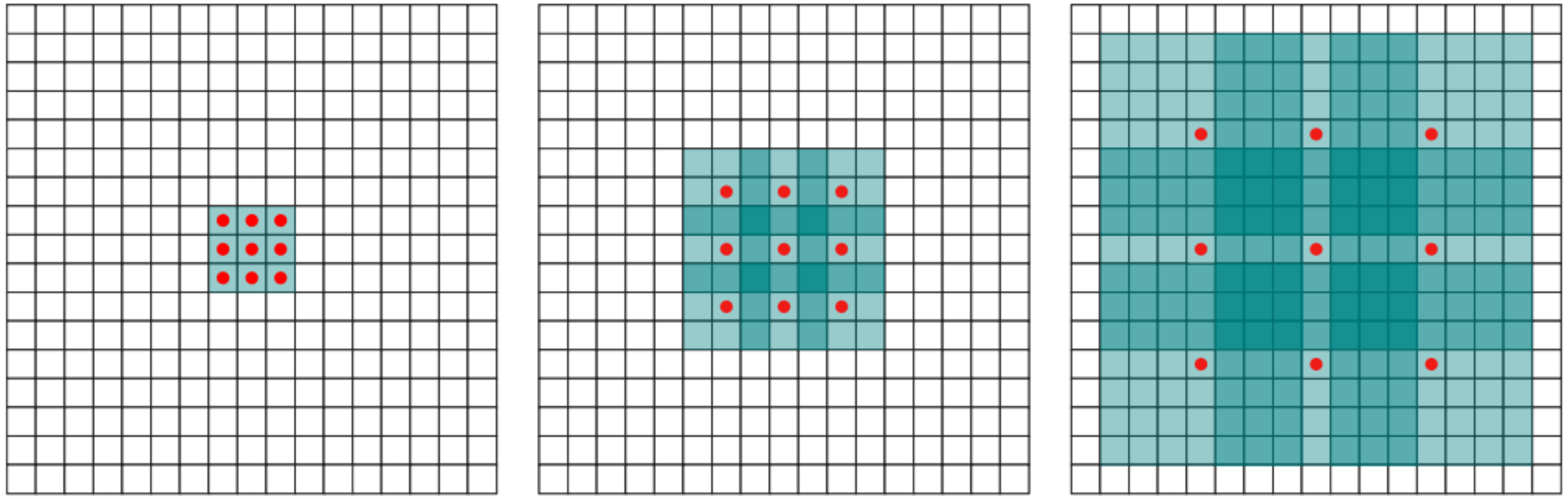
- Issues:
  - Convolution kernels are not shift-invariant.
  - No effective pooling → Introduce spectral counterpart for spatial pooling
  - Filter weights depend on Fourier basis, does not generalize well to new domains → Synchronize Fourier basis for better generalizability

SyncSpecCNN

- Introduce spectral counterpart for spatial pooling
- Synchronize Fourier basis for better generalizability

Dilated convolution

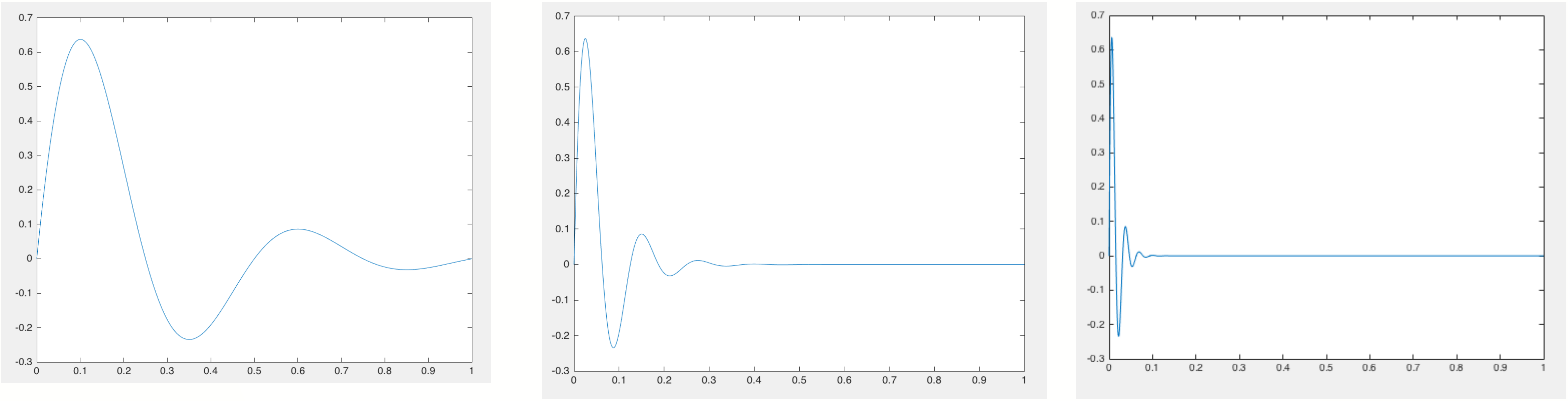
- Achieving large receptive field quickly without pooling

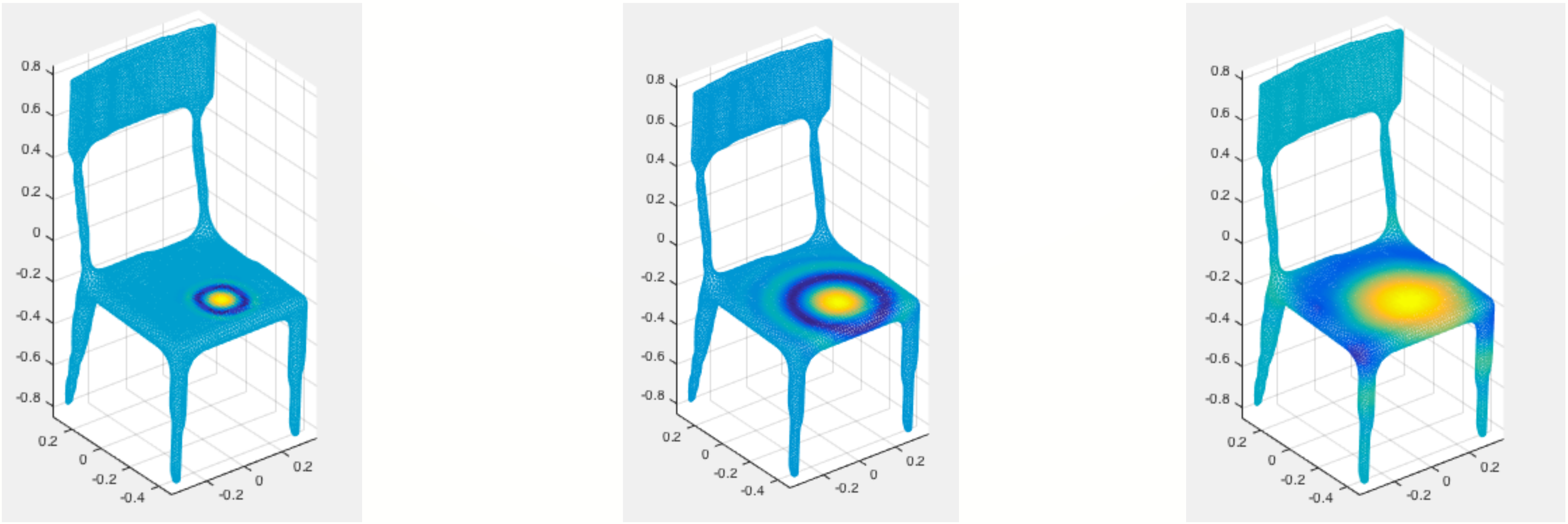


Yu et al. 2016

SyncSpecCNN: spectral dilated convolution

- Parameterize filters with interpolation kernels.
- Shrink kernel bandwidth to increase spatial support of filters





Li Yi et al. 2017

SyncSpecCNN: spectral dilated convolution

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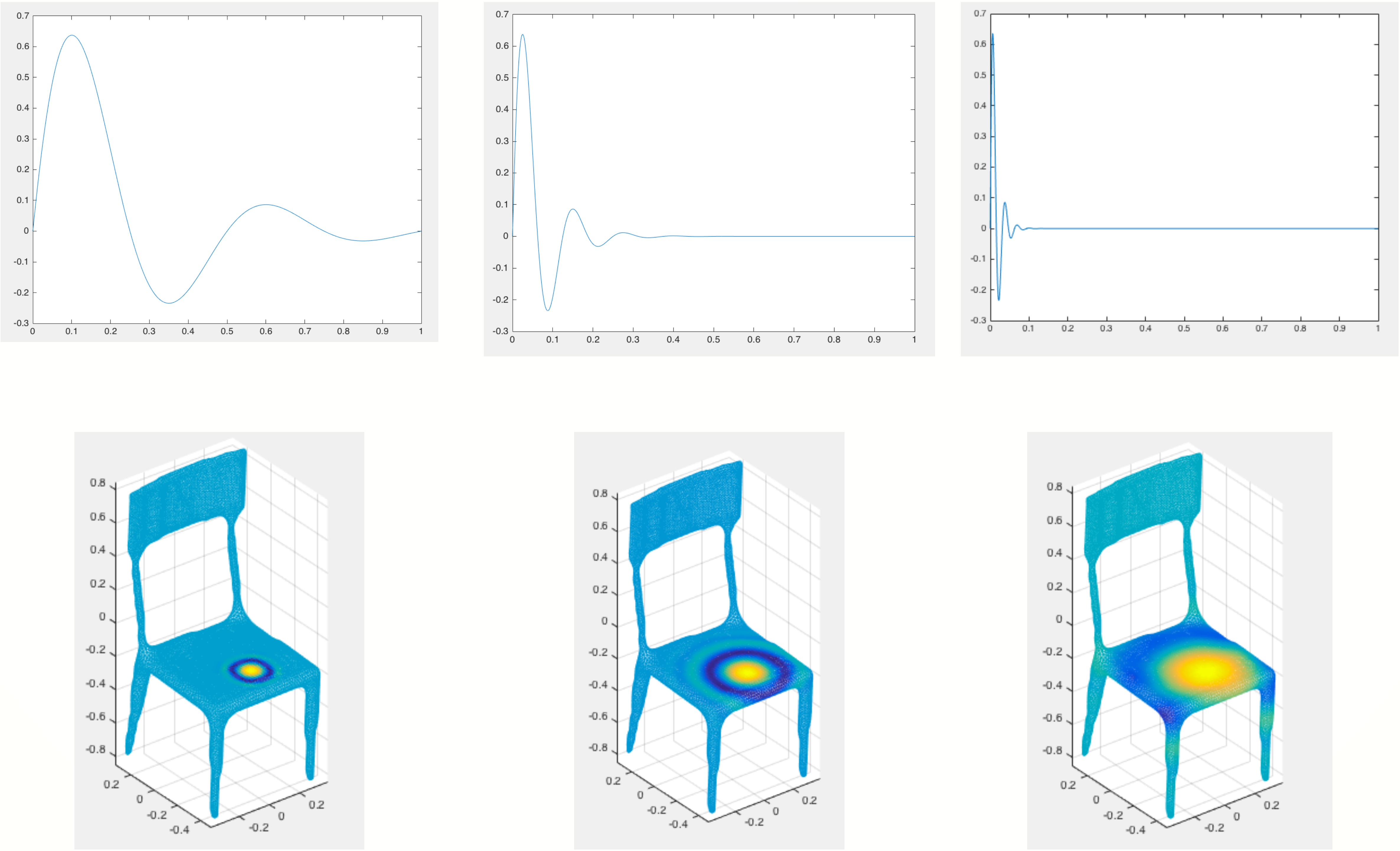

spectral pooling

Li Yi et al. 2017

Spectral CNN

- Issues:
  - Convolution kernels are not shift-invariant.
  - No effective pooling → Introduce spectral counterpart for spatial pooling
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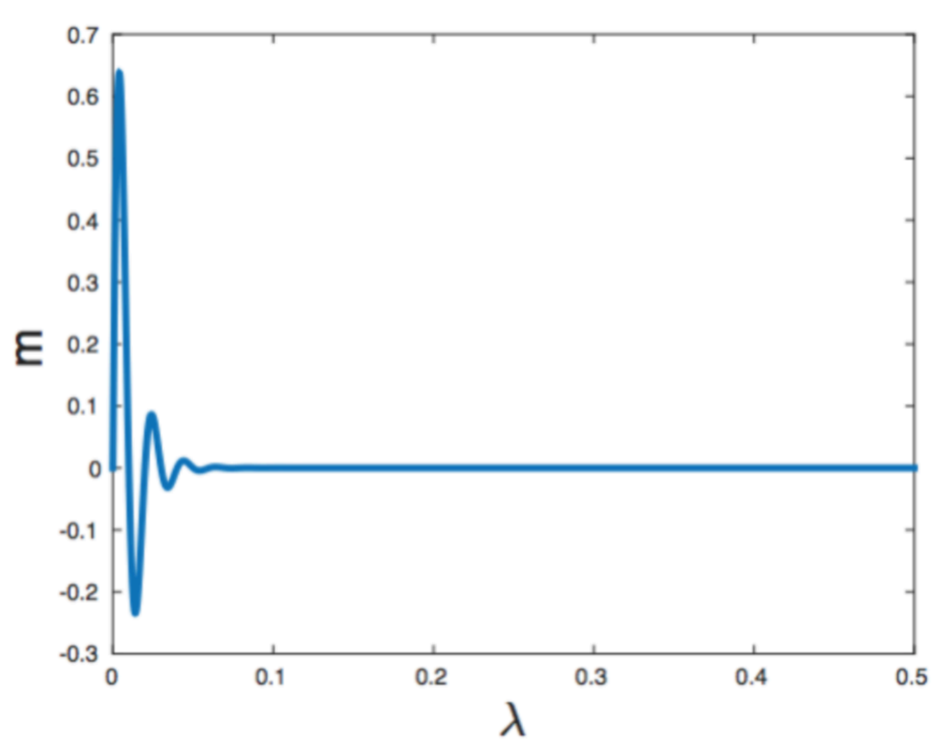
SyncSpecCNN

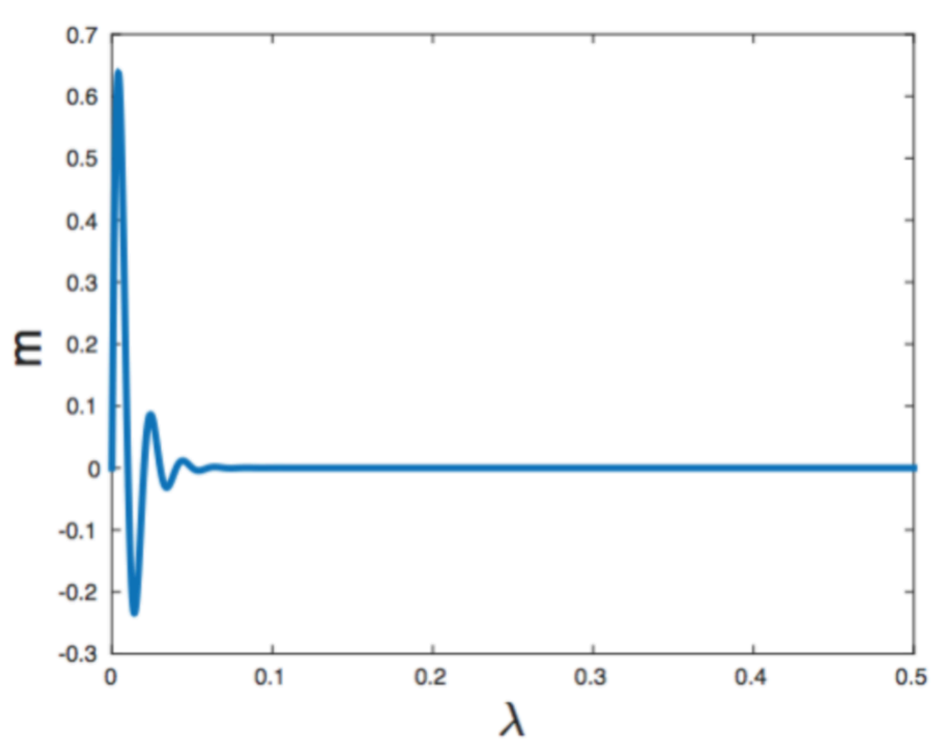
- Introduce spectral counterpart for spatial pooling
- Synchronize Fourier basis for better generalizability

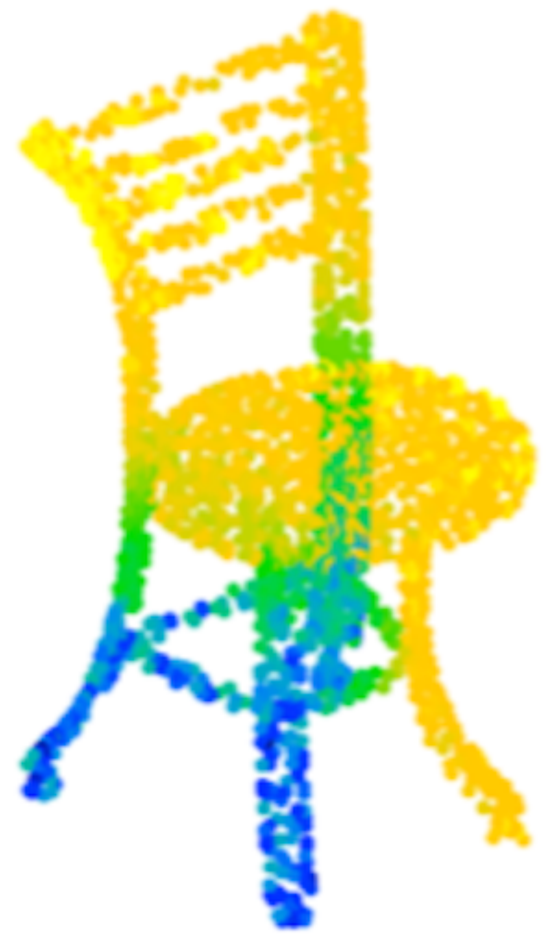
Cross domain discrepancy

Spectral Domain 1



Spectral Domain 2





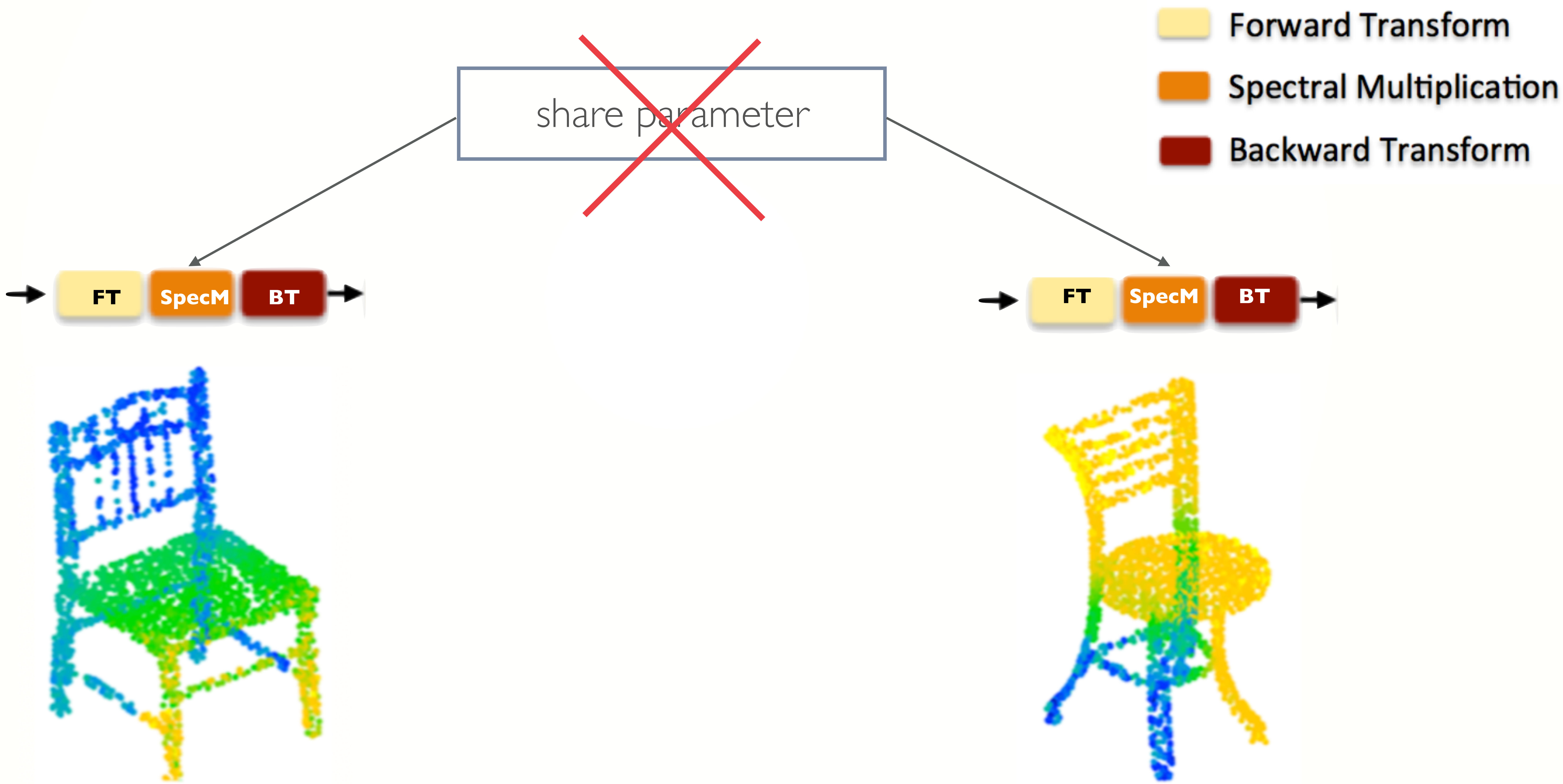
Spectral domain is independently defined for each shape graph

The same spectral function would induce very different spatial functions on different graphs

Cross domain parameter sharing is not valid

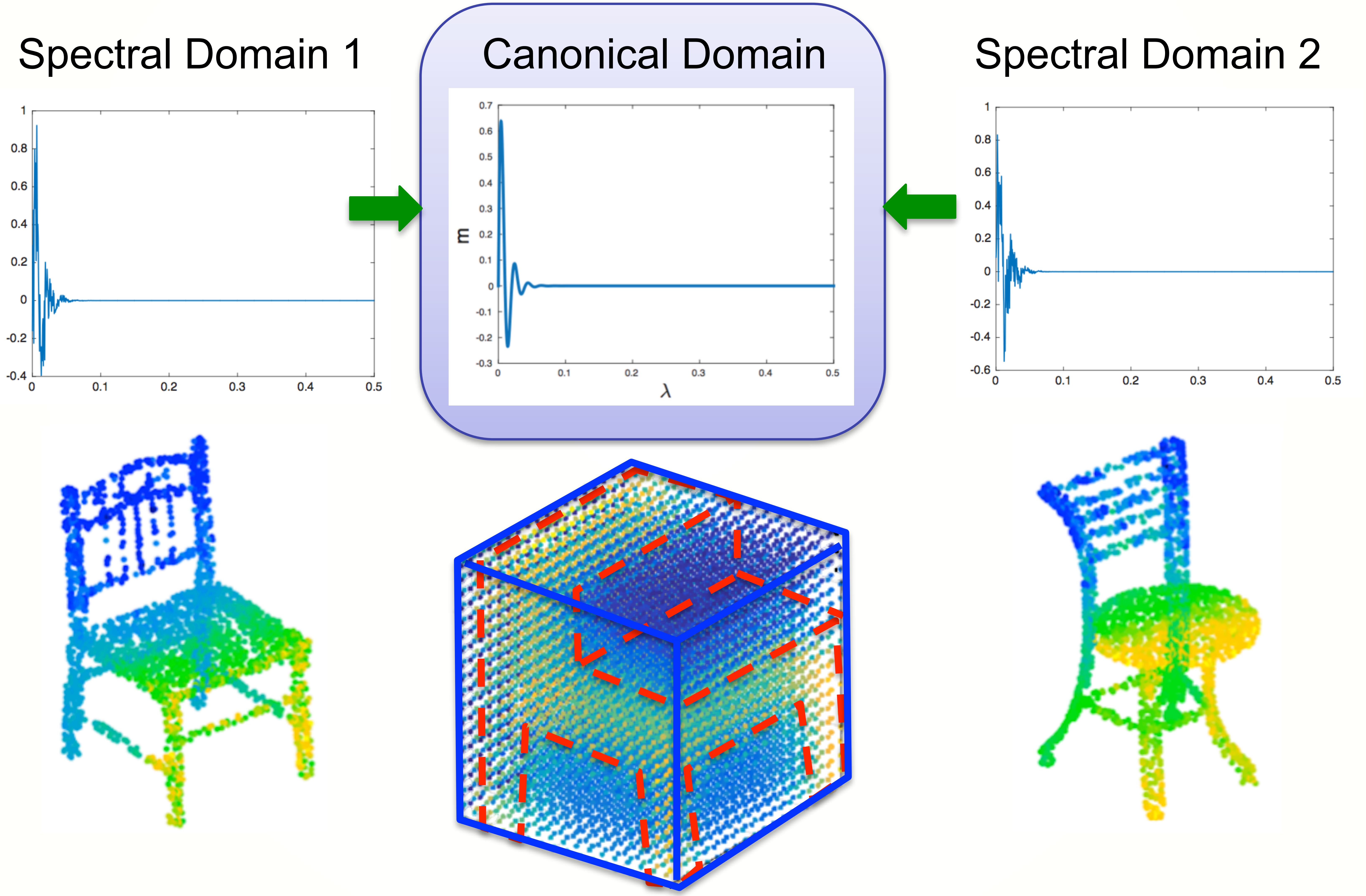
Li Yi et al. 2017

Cross domain discrepancy



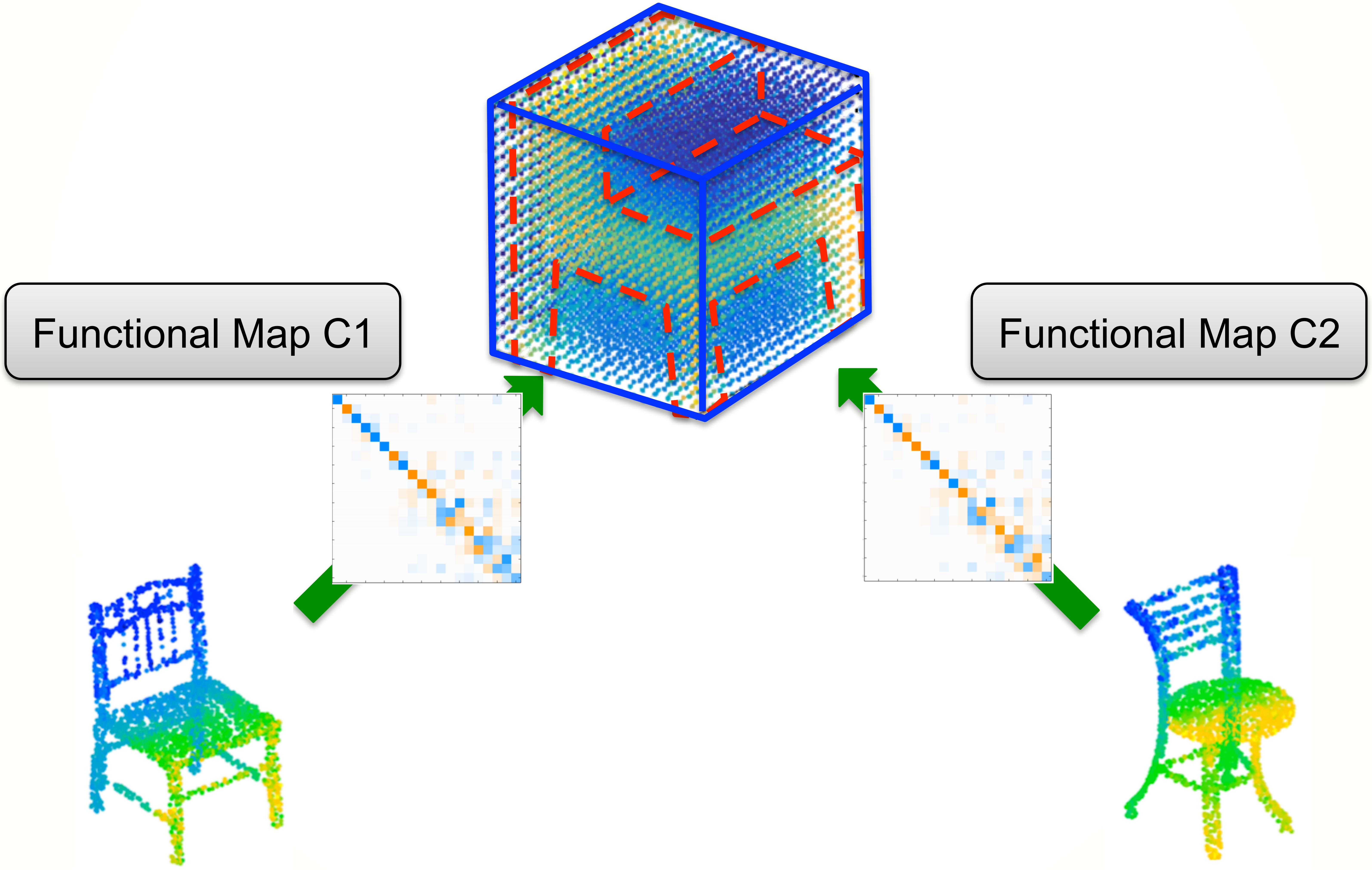
Li Yi et al. 2017

Different domain needs to be synchronized



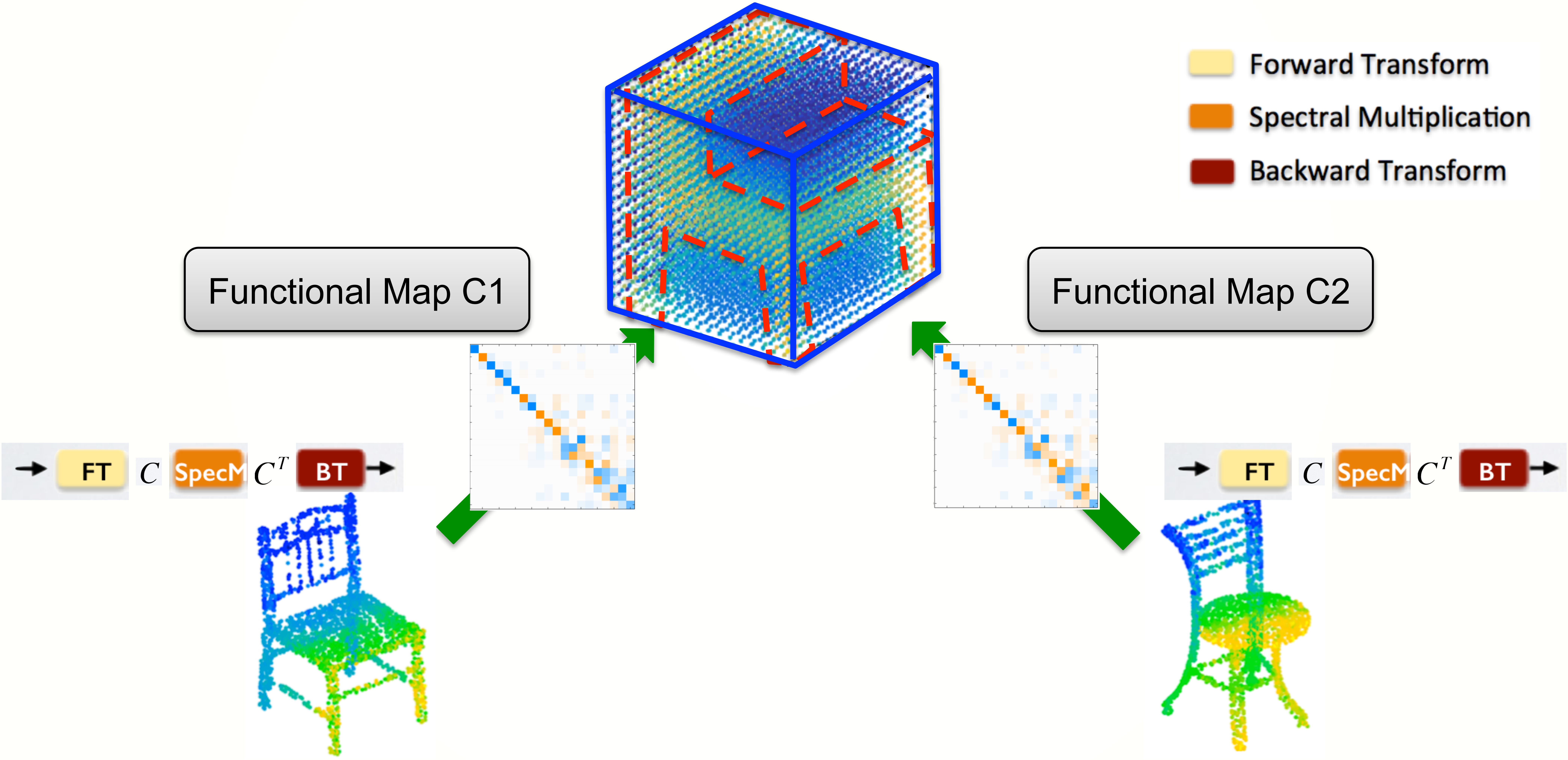
Li Yi et al. 2017

Functional map for domain synchronization



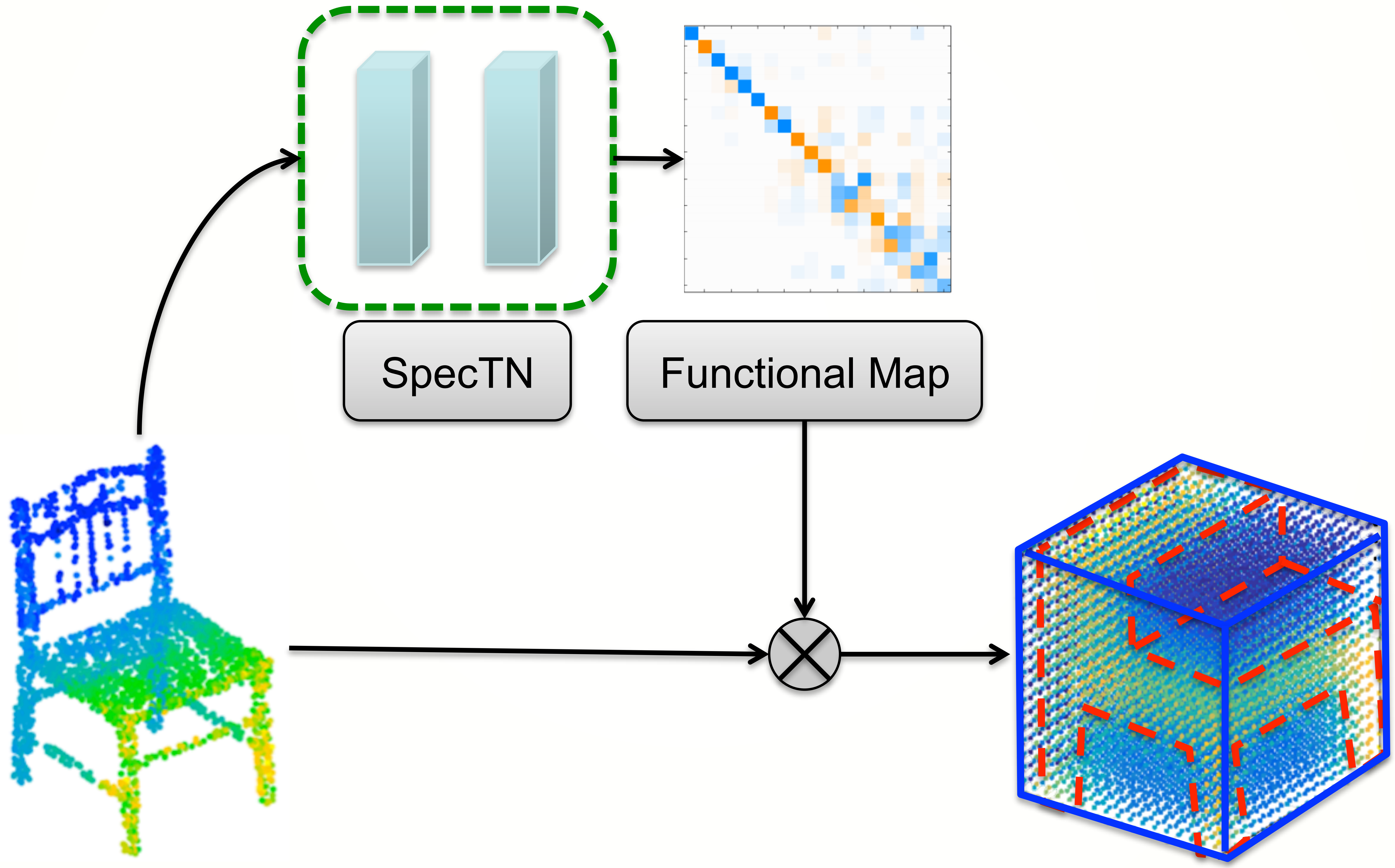
Li Yi et al. 2017

Functional map for domain synchronization



Li Yi et al. 2017

Spectral transformer network



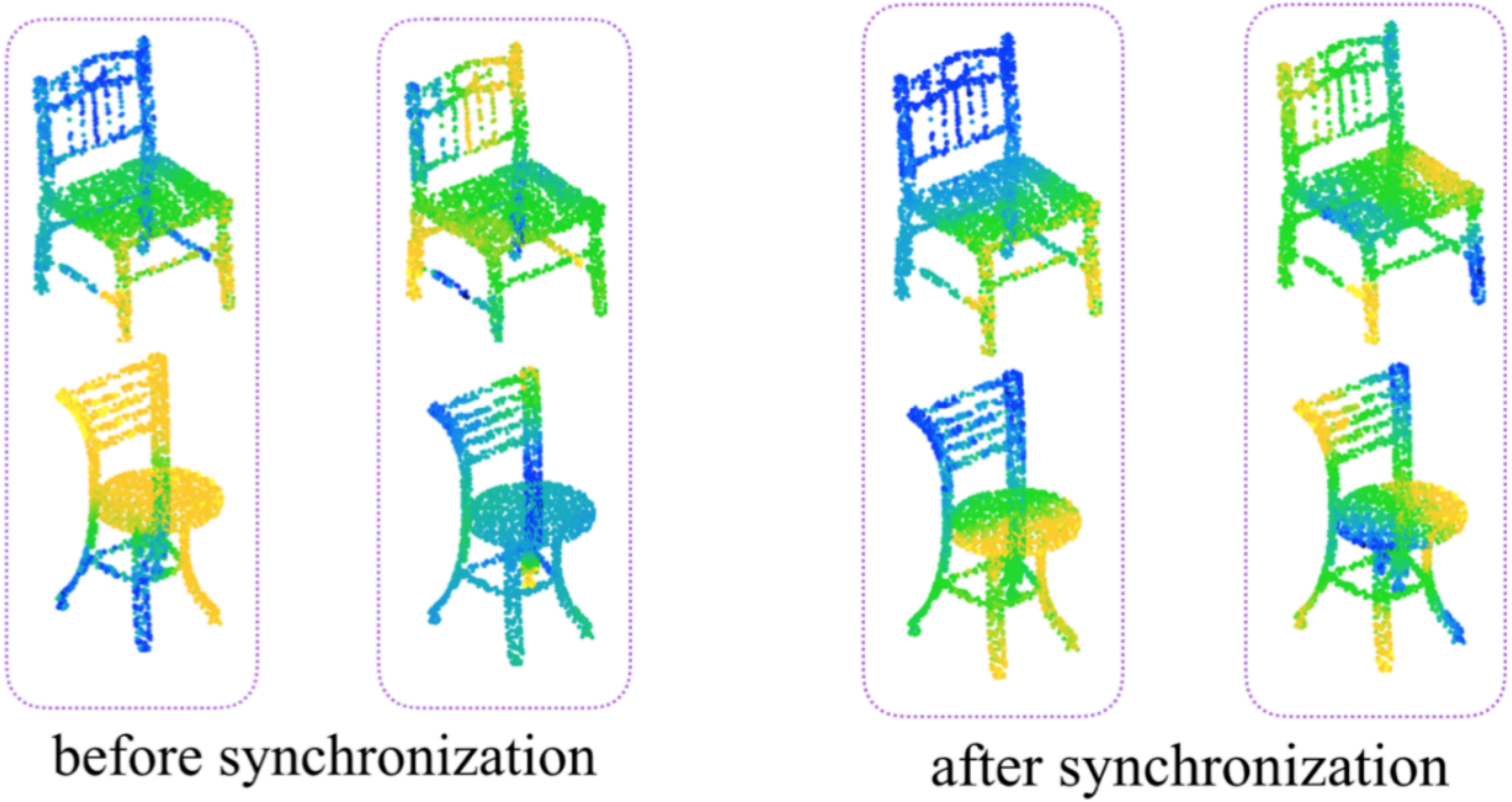
Li Yi et al. 2017

Spectral transformer network

- Generates high dimensional transformation, sensitive to initialization (15x45 matrix)
- Pre-trained to get a good starting point
- Fine tuned with the end task learning

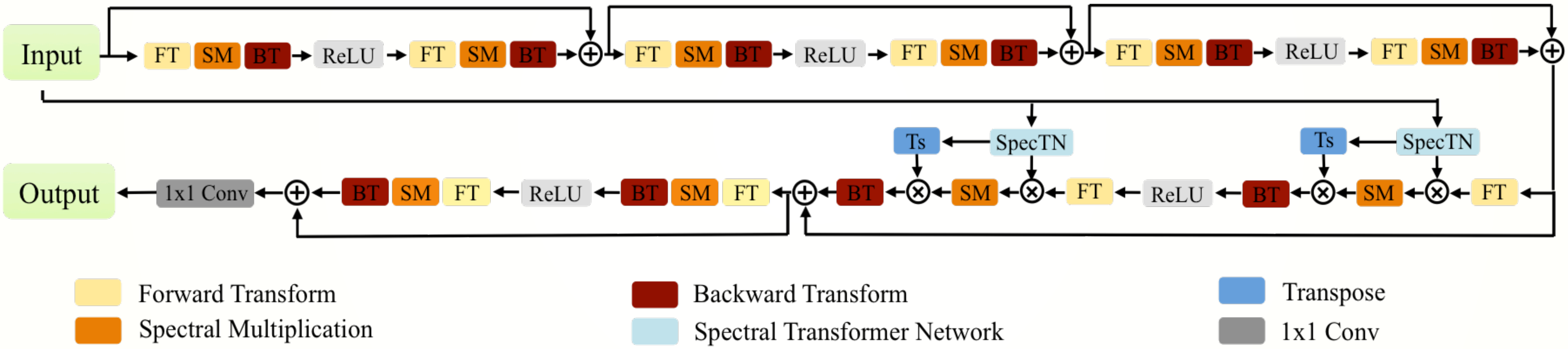
Li Yi et al. 2017

Synchronization visualization



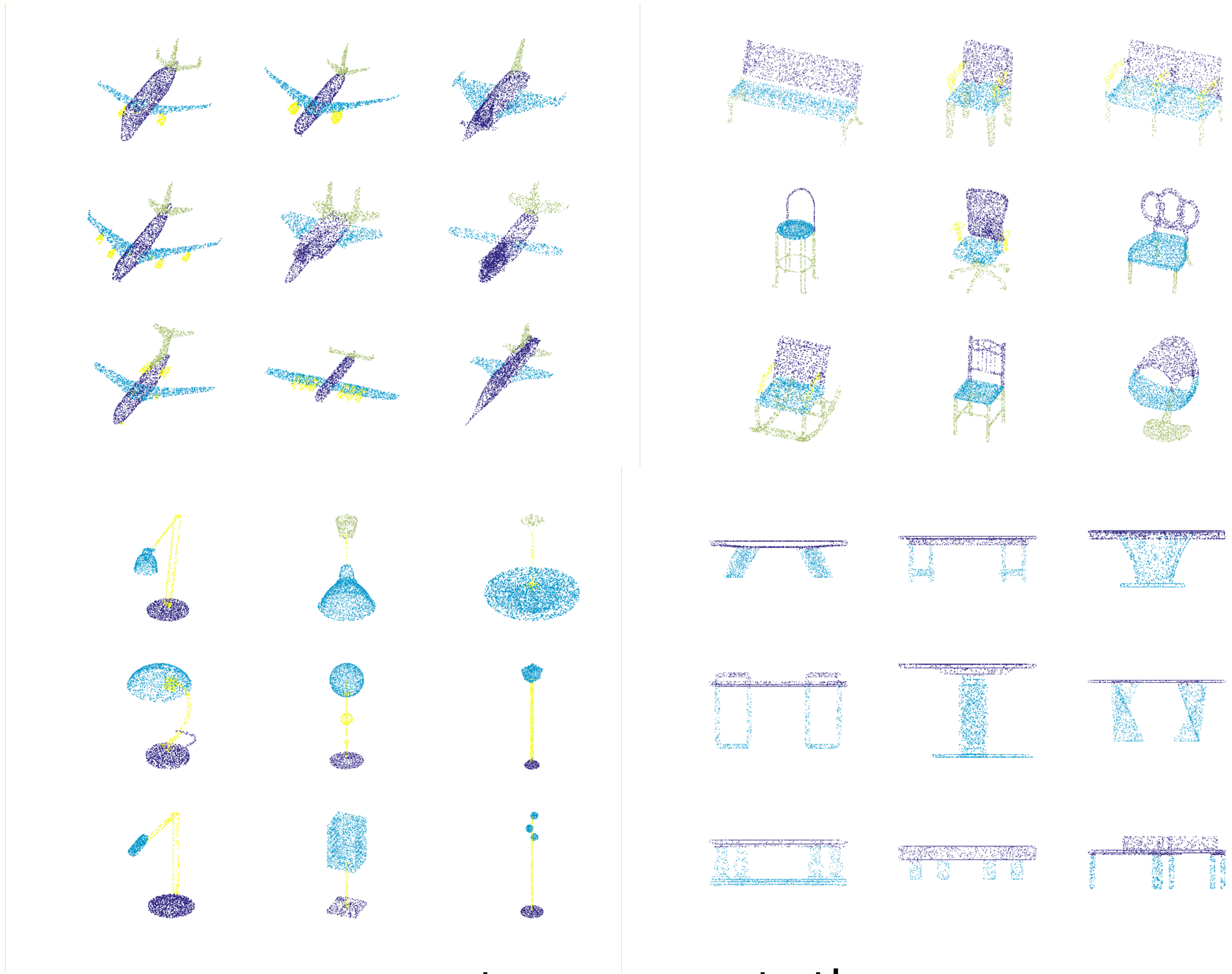
Li Yi et al. 2017

SyncSpecCNN



Li Yi et al. 2017

SyncSpecCNN



part segmentation

key point prediction

Li Yi et al. 2017

Discussion

- Spatial construction is usually more efficient but less principled
- Spectral construction is more principled but usually slow (computing Laplacian eigenvectors for large scale data could be painful)
- On going research tries to bridge the gap

Convolutional Neural Networks on Graphs with Fast Localized Spectral Filtering, Defferrard et al. 2016

no need to compute eigen decomposition;
reduce filtering complexity from $O(|\mathcal{V}| \cdot |\mathcal{V}_{\text{trunc}}|)$ to $O(|\mathcal{E}| \cdot K)$

Discussion

- Spatial construction is usually more efficient but less principled
- Spectral construction is more principled but usually slow (computing Laplacian eigenvectors for large scale data could be painful)
- On going research tries to bridge the gap
- Generalization issue on generic graphs is still a challenge