DEEPSPHERE: AN ALMOST EQUIVARIANT GRAPH-BASED SPHERICAL CNN

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Applied Machine Learning Days 2020

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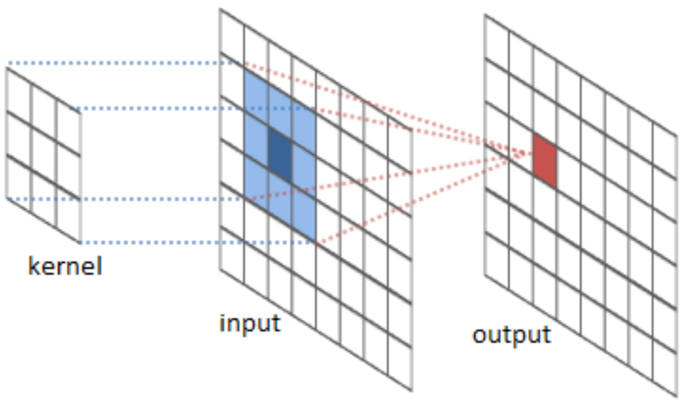
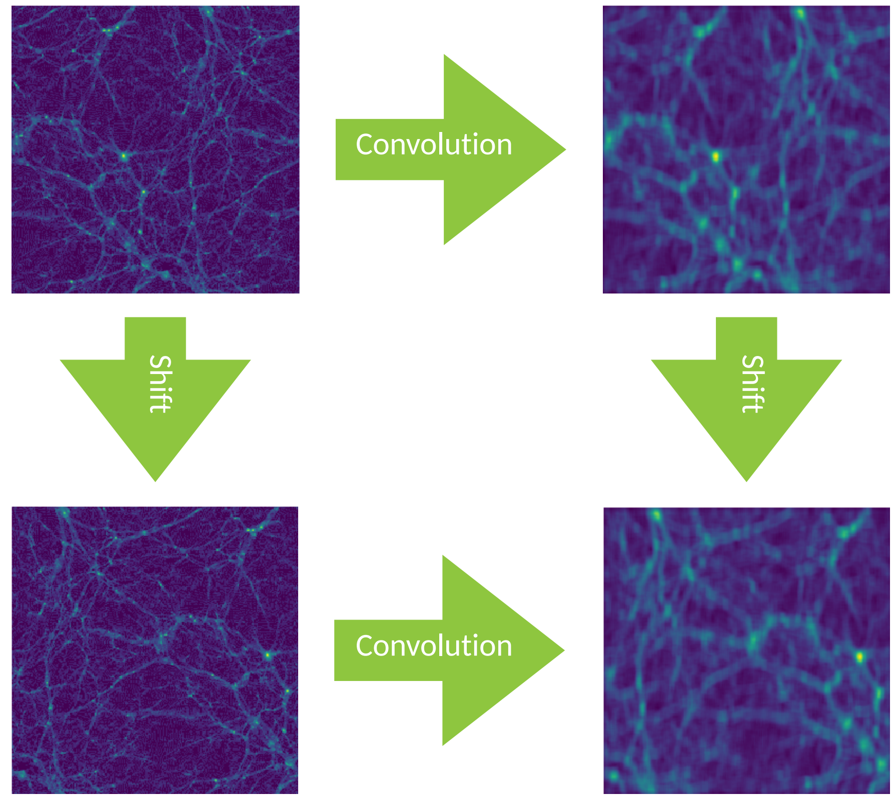
Why are CNNs so successful?

Efficiency



From the [River Trail documentation]

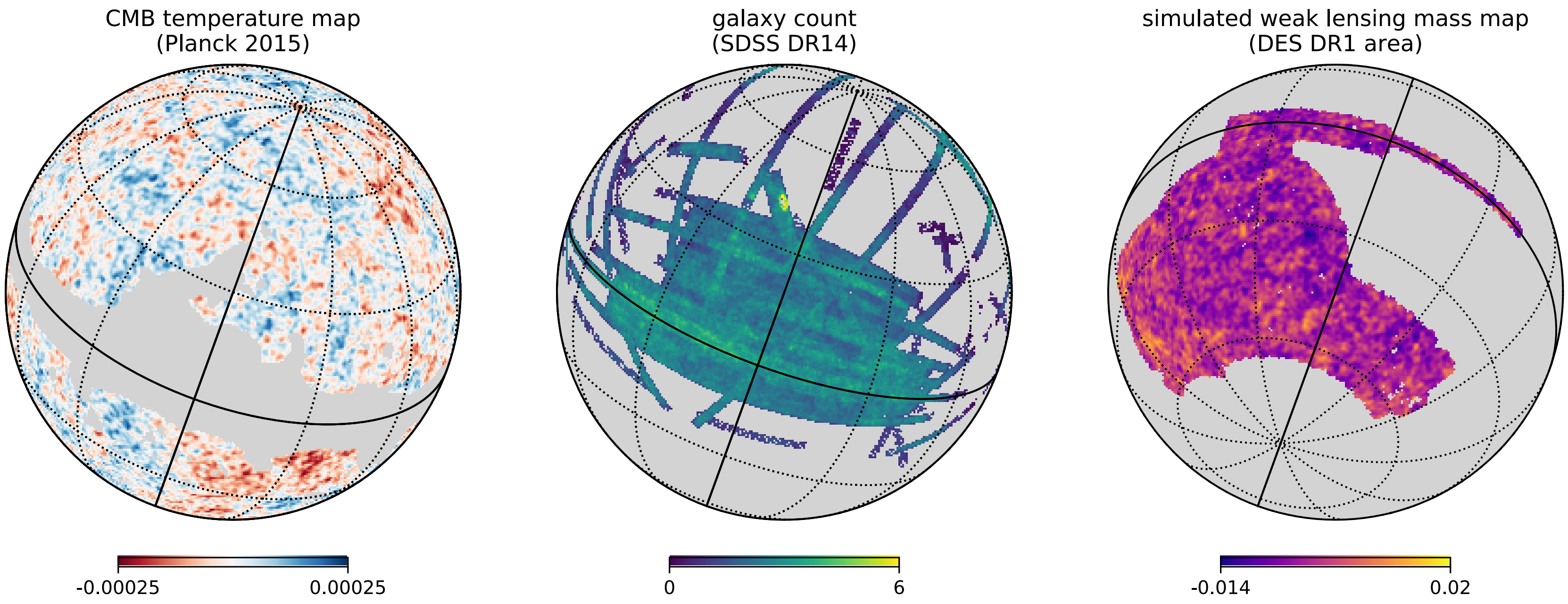
Translation equivariance



Allows for deep architecture

Data driven constraint

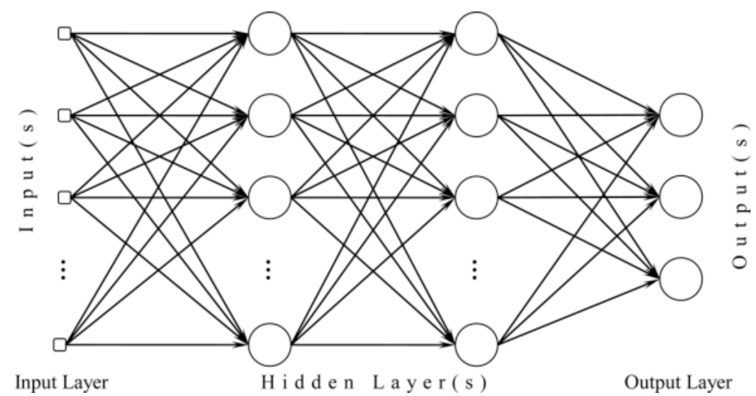
Irregular domain



Assume a manifold

How to build a convolution for an irregular domain?

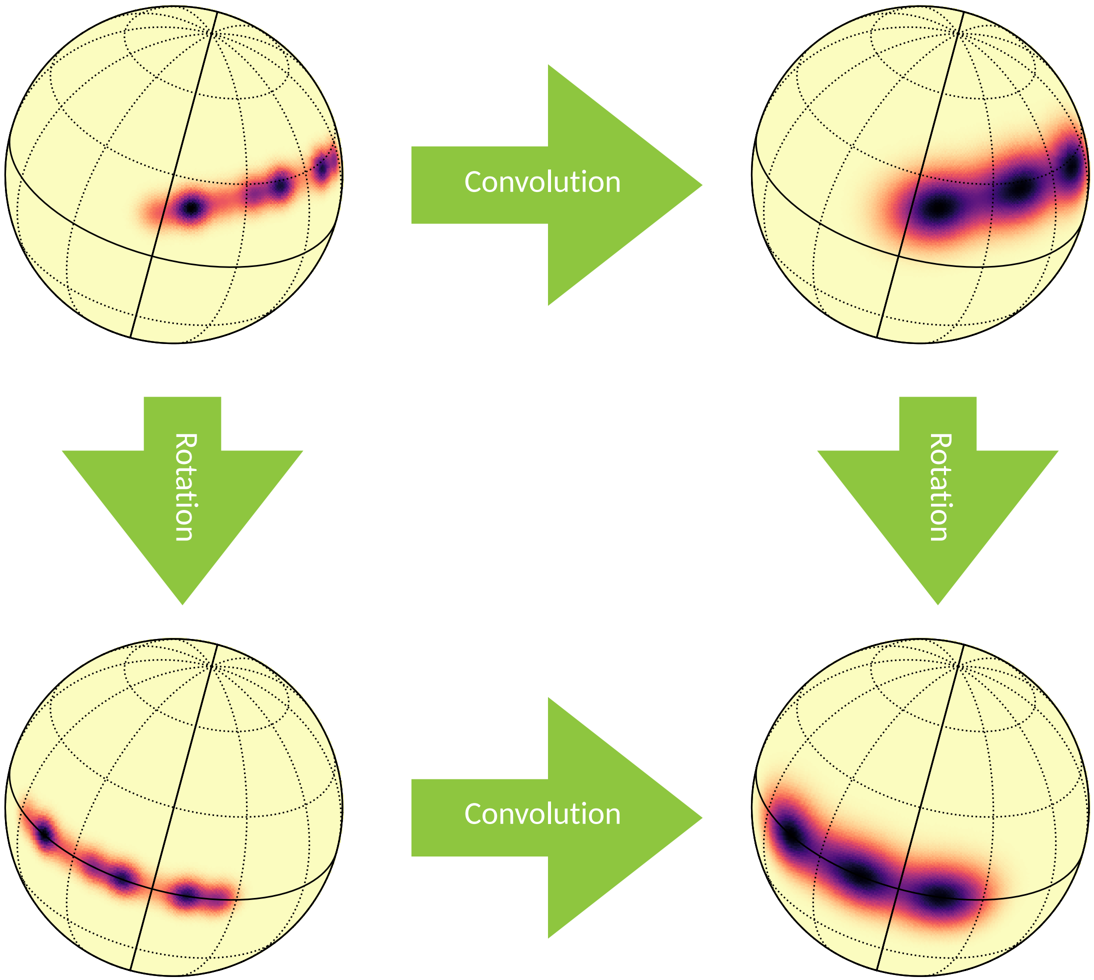
- Fully connected architectures are not the solution
  - No structure



- Goal
  1. Parameter sharing
  2. Efficient
  3. Backpropagable
  4. Some equivariance/invariance properties?

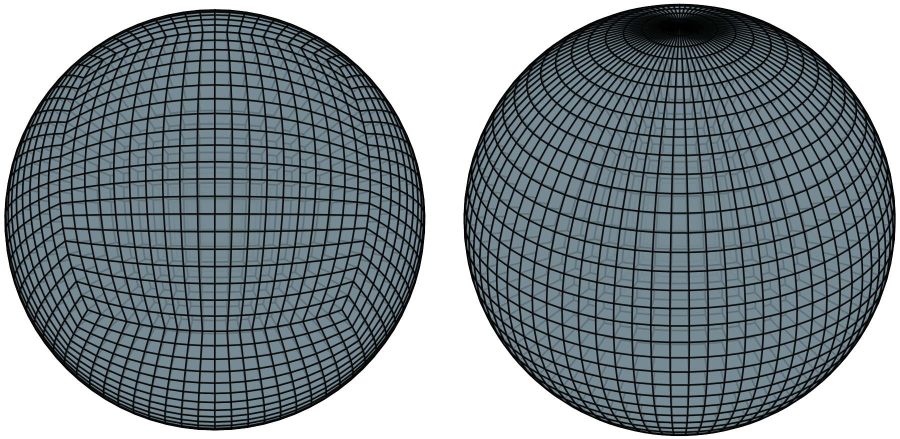
Example: sphere -> visual, lot of symmetries

Rotation equivariance on the SO(3) group



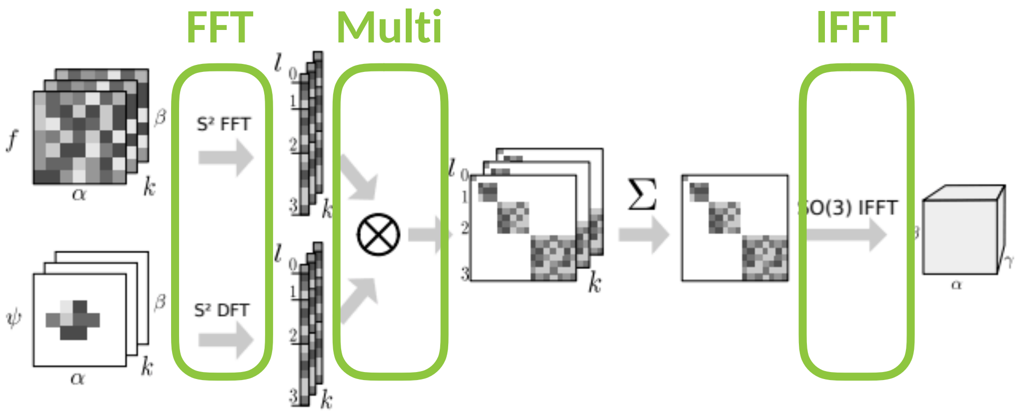
Convolution on the sphere (Brut force)

- Special sampling [Boomsma & Frellsen (2017)]
  - Fast
  - Simple
  - Not spherical
  - Not equivariant
  - Works only for specific samplings / not generalisable



Convolution on the SO(3) group

- Use spherical harmonics - [Cohen et al. (2018), Kondor et al. (2018)]
  - Spherical
  - Rotation equivariant
  - Slow
  - Complex
  - Generalizable? works only for known manifolds



GRAPHS BASICS

Graph signal processing basics

- Connected, undirected, weighted graph

$$\mathcal{G} = \{\mathcal{V}, \mathcal{E}, W\}$$

- Degree matrix: D
  - zeros except diagonals, which are sums of weights of edges incident to corresponding node
- Non-normalized Laplacian:

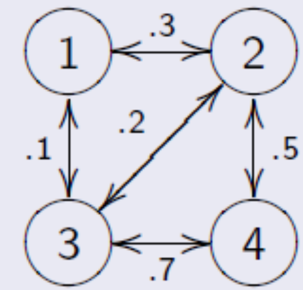
$$L = D - W$$

- Complete set of orthonormal eigenvectors - **Fourier basis**

$$L = U \Lambda U^*$$

- and associated real, non-negative eigenvalues - **frequency index**

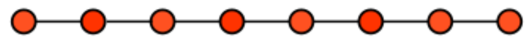
$$0 = \lambda_0 < \lambda_1 \leqslant \lambda_2 \leqslant \ldots \leqslant \lambda_{N-1} := \lambda_{max}$$



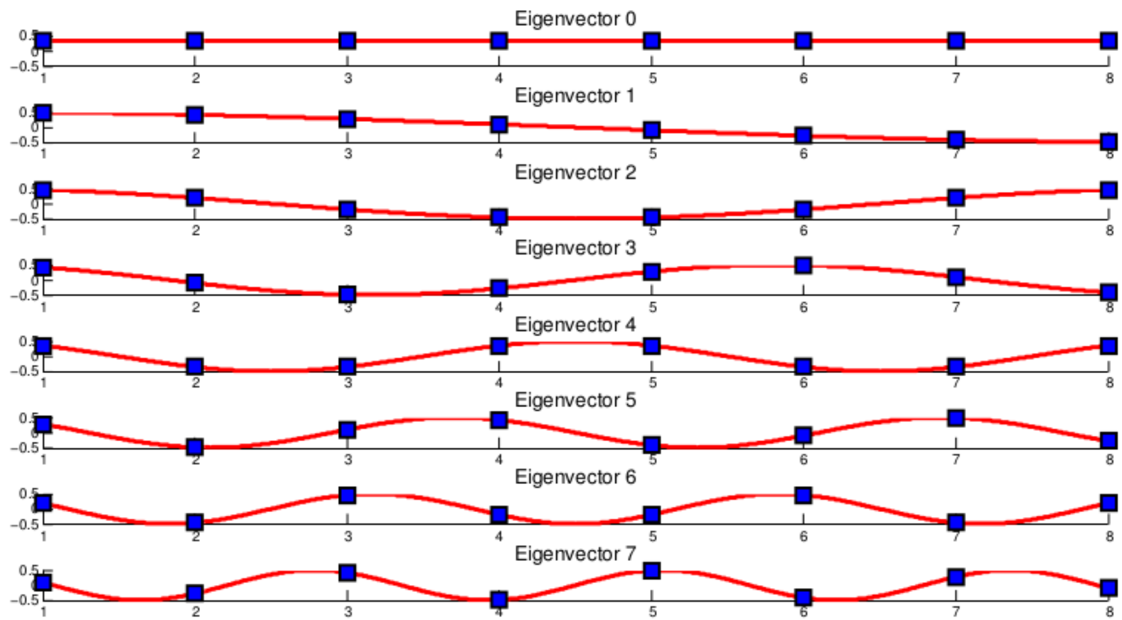
$$W = \begin{bmatrix} 0 & .3 & .1 & 0 \\ .3 & 0 & .2 & .5 \\ .1 & .2 & 0 & .7 \\ 0 & .5 & .7 & 0 \end{bmatrix}$$

$$D = \begin{bmatrix} .4 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1.2 \end{bmatrix}$$

Example: path

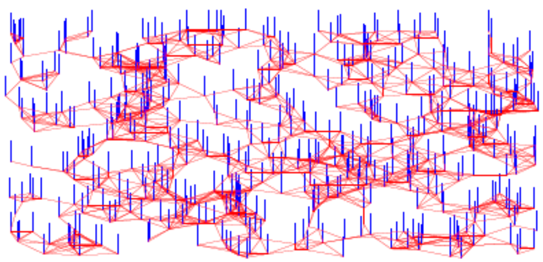


- $\lambda_\ell = 2 - 2\cos\left(\frac{\pi \ell}{N}\right)$
- $\chi_0(i) = \frac{1}{\sqrt{N}},\ \chi_\ell(i) = \sqrt{\frac{2}{N}} \cos\left(\frac{\pi \ell (i - 0.5)}{N}\right),\ \ \ell = 1, 2, \ldots, N-1$

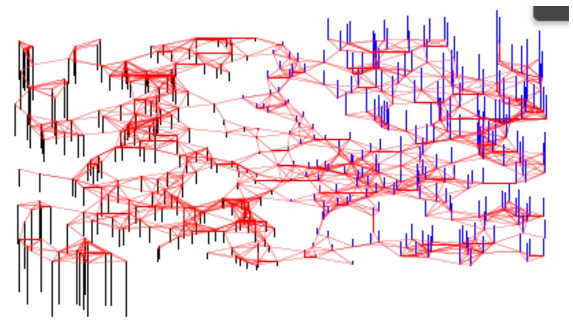


$\begin{bmatrix} | & & | \\ \chi_0 & \cdots & \chi_{N-1} \\ | & & | \end{bmatrix}$ is the Discrete Cosine Transform matrix (DCT-II, Strang, 1999), which is used in JPEG image compression

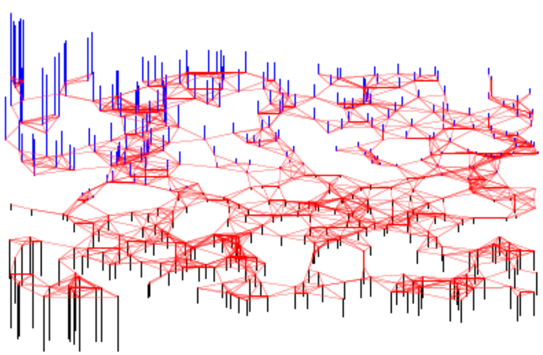
Example: Irregular sampling: sensor networks



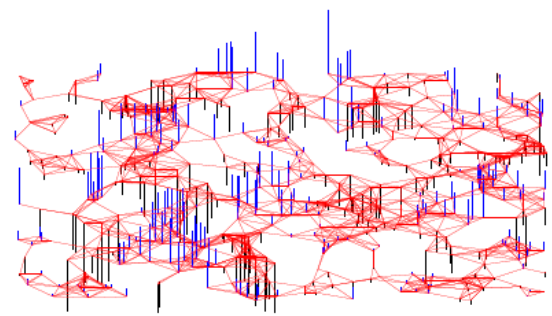
χ_0



χ_1

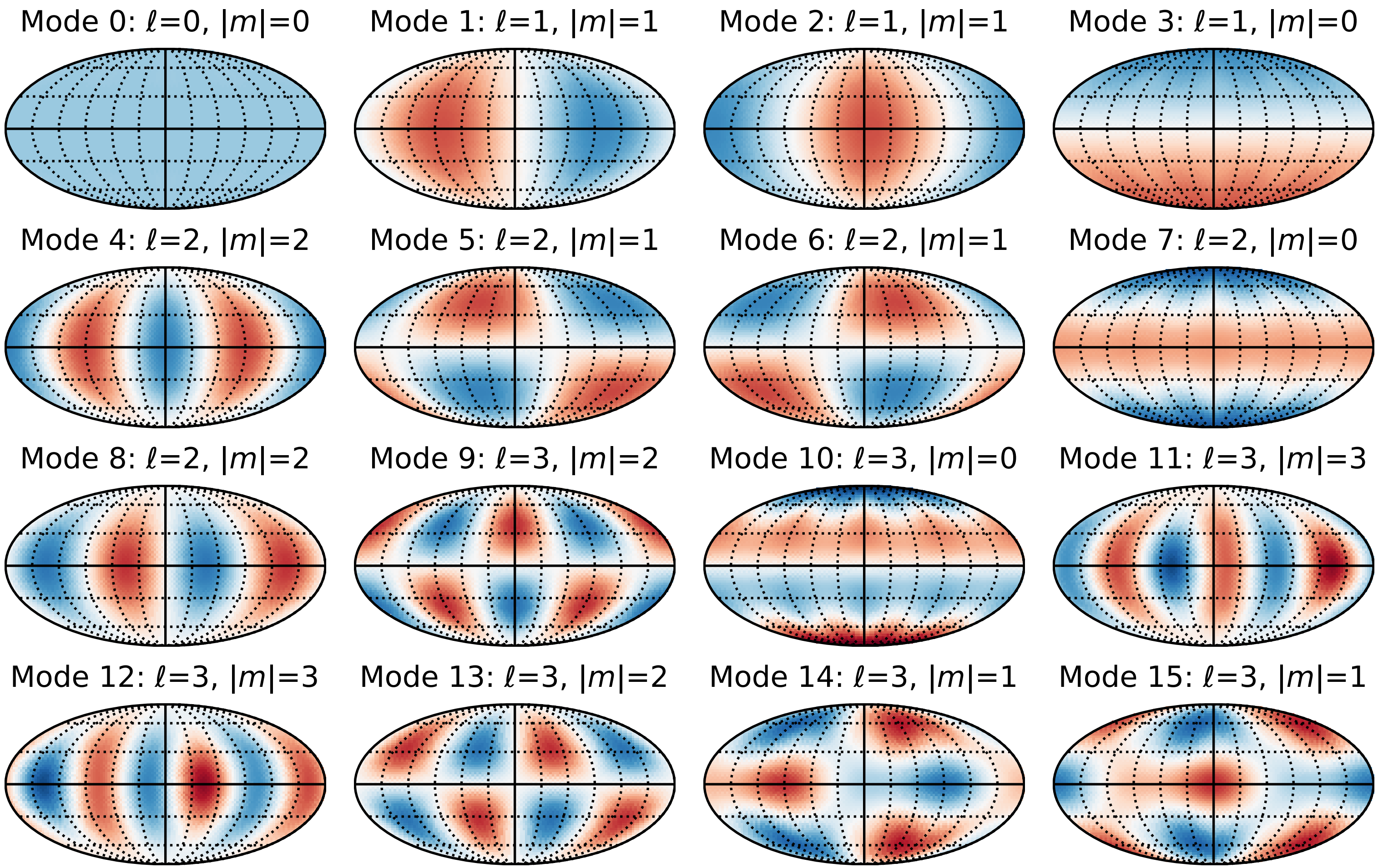


χ_2



χ_{50}

Graph Fourier basis on the sphere



Use HEALpix sampling

Defining convolution on graphs

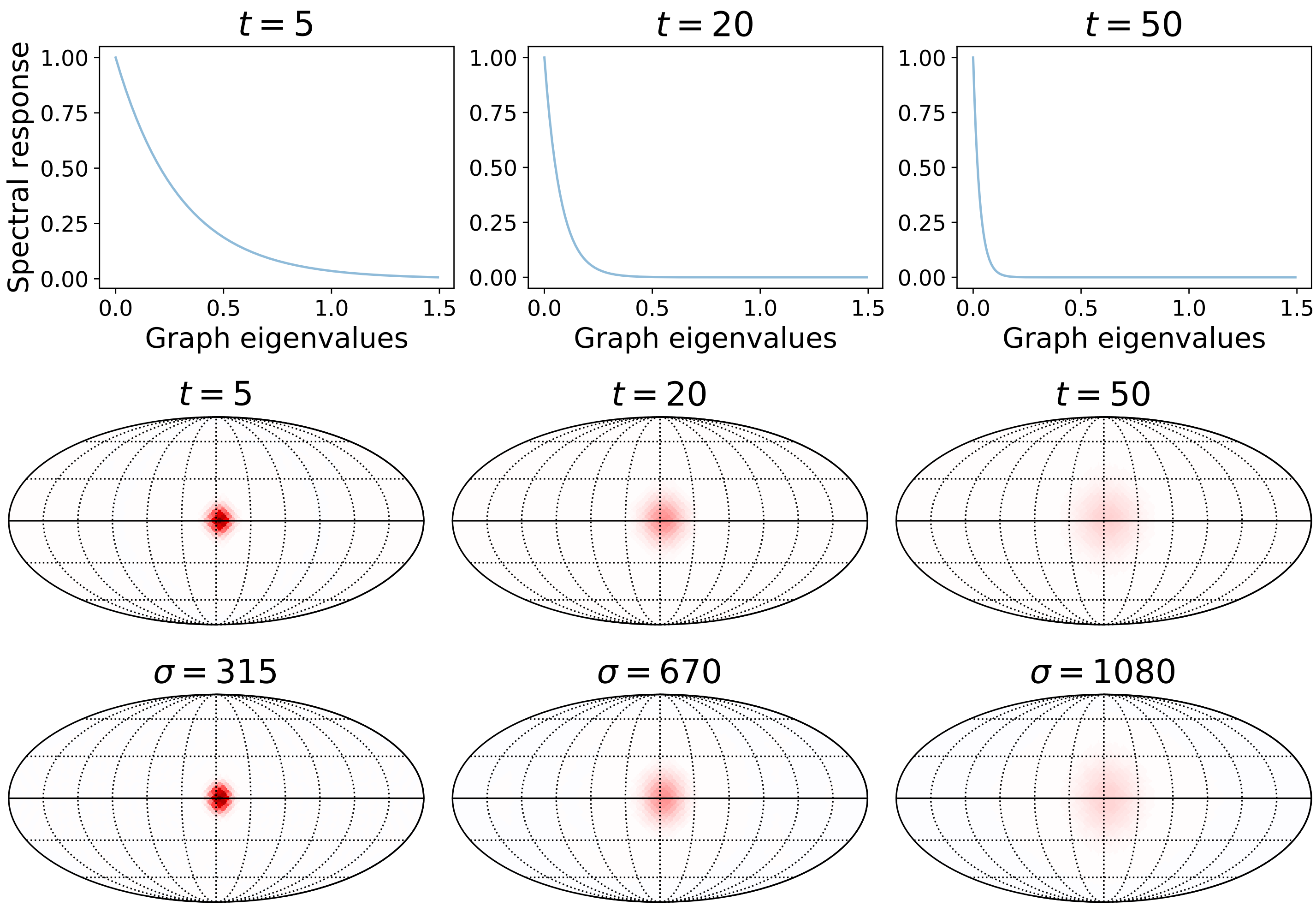
- Fourier transform: $\hat{s} = U^* s$
- Inverse Fourier transform: $s = U \hat{s}$
- Convolution
  (multiplication in the Fourier domain)

$$h(L)s := \underbrace{\boxed{U}}_{\text{Inverse Fourier transform}} \underbrace{\boxed{h(\Lambda)}}_{\text{Multiplication with a kernel/filter}} \underbrace{\boxed{U^*}}_{\text{Fourier transform}} s$$

Parameter sharing: all nodes share the same kernel!

SPHERICAL CONVOLUTION

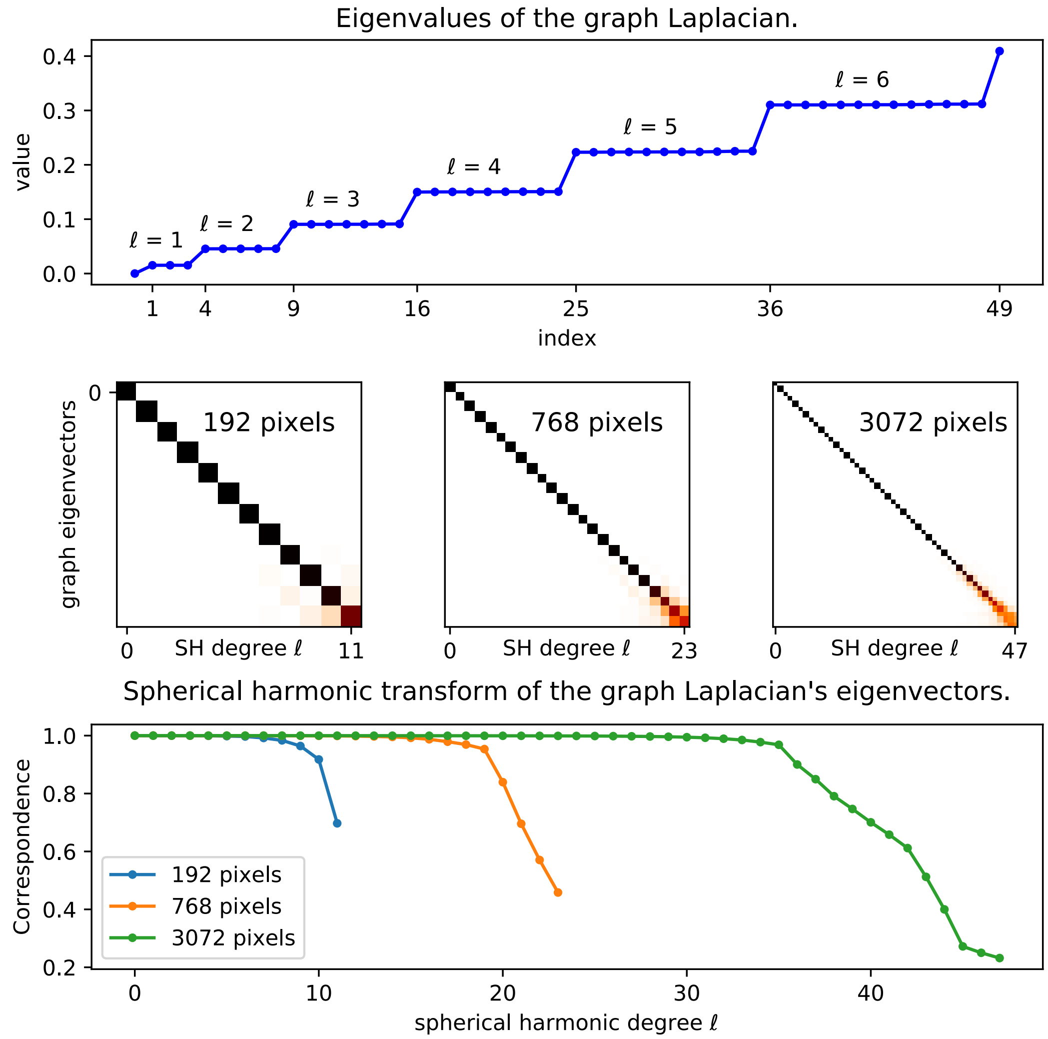
Example heat diffusion



Solution of the heat equation: $\tau \boldsymbol{L} \boldsymbol{f}(t) = -\partial_t \boldsymbol{f}(t)$

Is graph convolution on a sphere equivariant?

- We observe empirical alignment of Fourier bases.
- We proved point wise convergence toward the Laplace-Beltrami operator.



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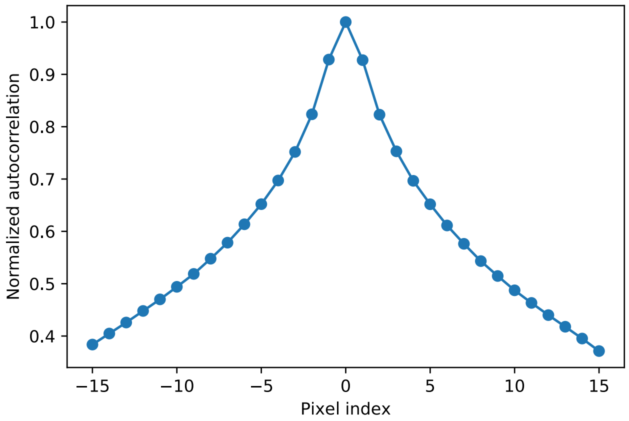
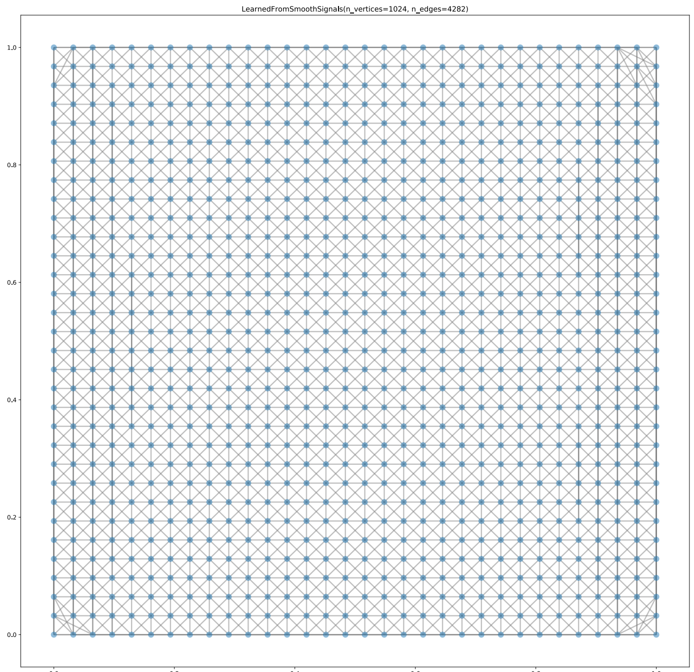
What if I do not know the structure?

- Graph learning techniques based on correlation.

  Kalofolias, V. and Perraudin, N., 2019. Large Scale Graph Learning From Smooth Signals. *International Conference on Learning Representations*



- Example:
  - CIFAR10 -> recover the expected grid of normal convolution.



More generally

- Graphs are good representations to capture the structural properties of a manifold.
- In some setting, the graph Laplacian converges toward the Laplace Beltrami operator.

Belkin, M., & Niyogi, P. (2007). Convergence of Laplacian eigenmaps. In *Advances in Neural Information Processing Systems* (pp. 129-136).

- You can do parameter sharing on a general manifold, but the notion of equivariance remains to be defined precisely.

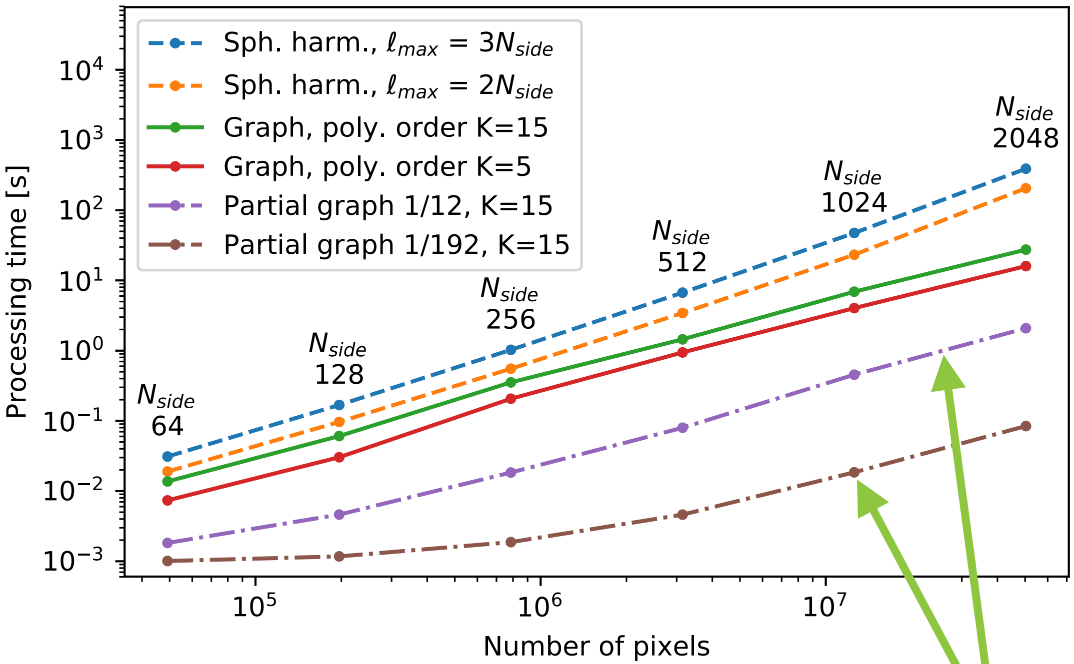
Efficient filtering

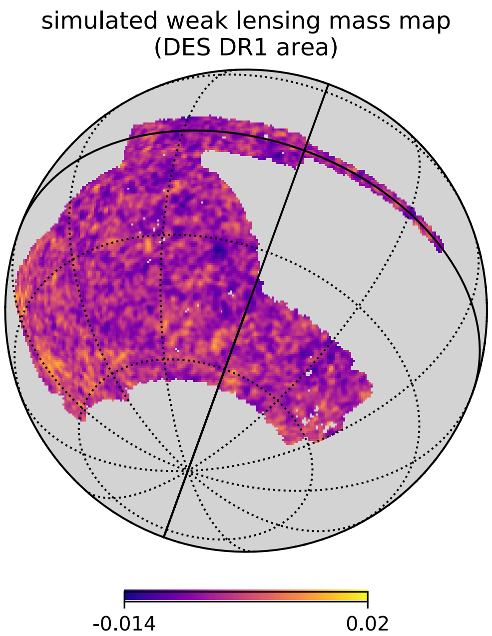
- Computing the Eigen-decomposition is not scalable!
- If the **kernel is a polynomial** and **L is sparse**

$$p(L)s = Up(\Lambda)U^*s = U\left(\sum_{i=0}^{K}\alpha_i\Lambda^i\right)U^*s = \sum_{i=0}^{K}\alpha_i L^i s$$

- Filtering is the result of a few sparse multiplications
- O(E), where E is the number of edges

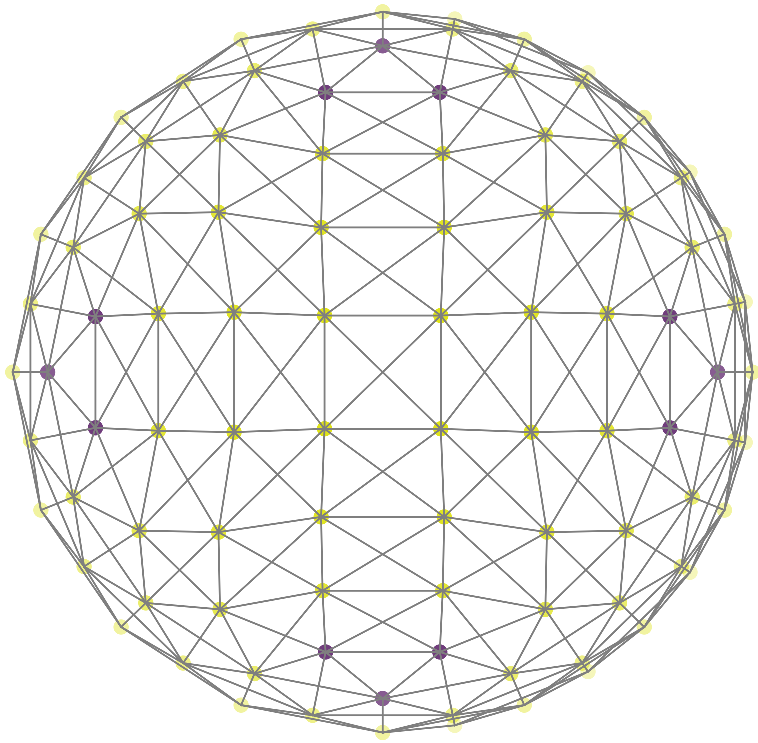
Filtering speed





The graph allows for flexibility

Summary



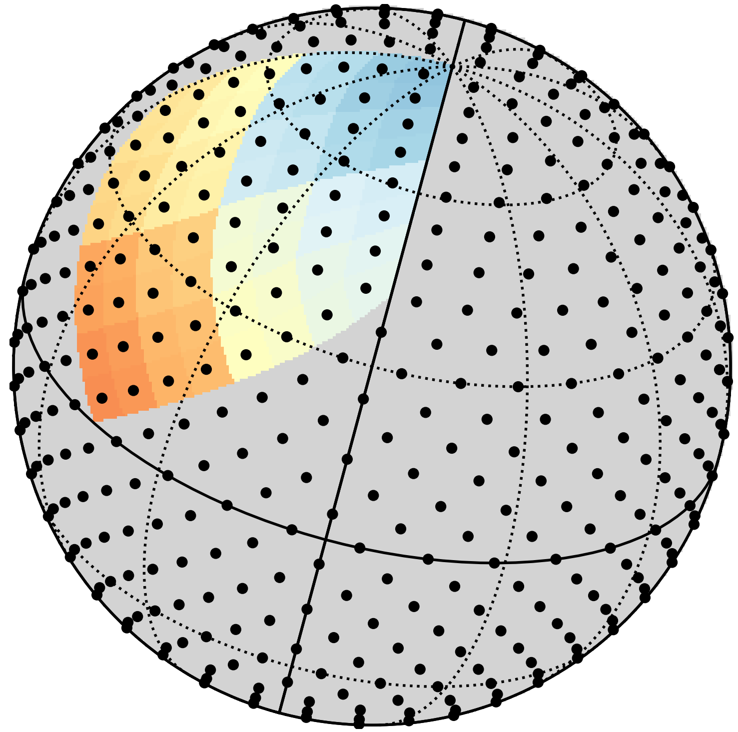
- Approximates the sphere
- Almost rotational equivariant
- Efficient (use only the neighbours information)
- Flexible (can be applied on a sphere subpart)
- Relatively simple
- Generalizable

Similar idea in a different context [Khasanova & Frossard, 2017]

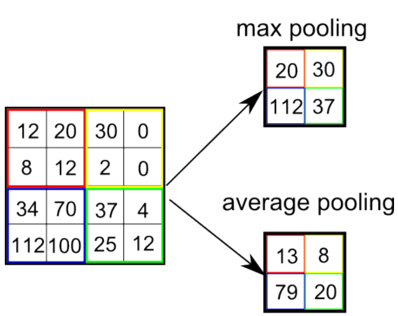
DEEPSPHERE

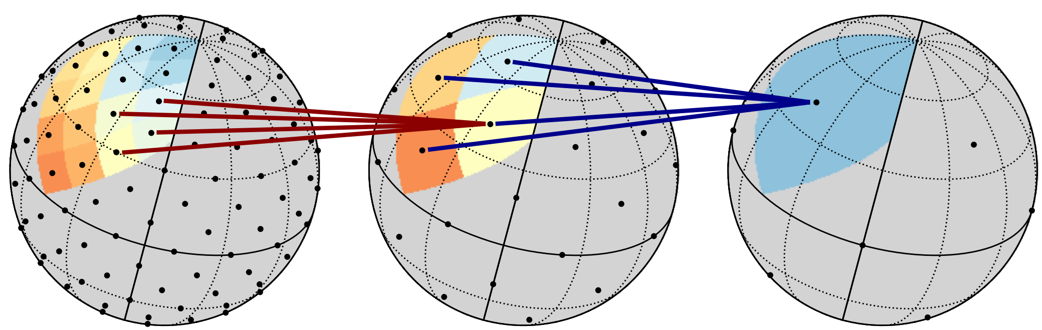
HEALpix

- Hierarchical
- Equal Area
- isoLatitude
- Pixelisation

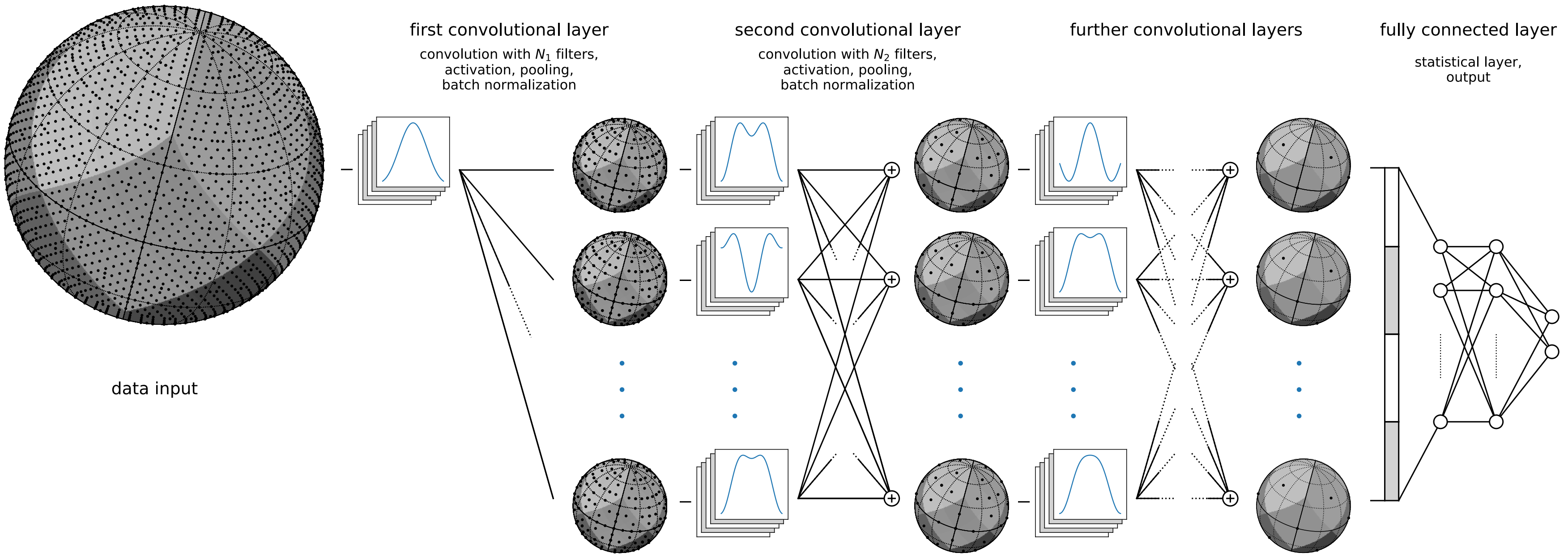


Natural pooling



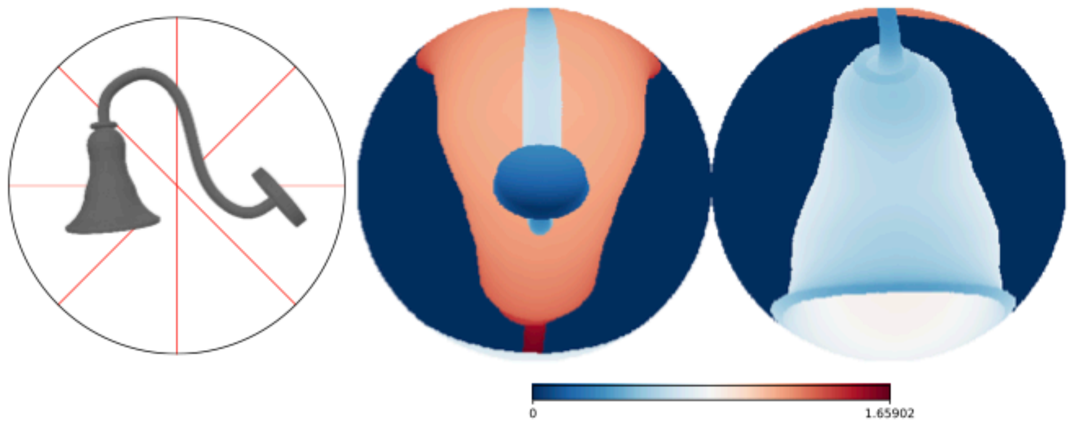


DeepSphere



data input
first convolutional layer
convolution with N_1 filters,
activation, pooling,
batch normalization
second convolutional layer
convolution with N_2 filters,
activation, pooling,
batch normalization
further convolutional layers
fully connected layer
statistical layer,
output

Shape classification



Projection of a 3D shape from SHREC-17.

	performance		size	speed	
Method	F1	mAP	params	inference [ms]	training
Cohen et al. (a)	78.85	67.6	1.4M	38	50h
Esteves et al.	79.36	68.5	500k	10	2h52
DeepSphere *Equiangular*	79.36	66.5	190k	1	50m
DeepSphere *HEALPix*	80.65	68.6	190k	1	50m

Table 2: Performance of different models for SHREC'17 task. F1-score computed with sklearn, mAP from the official script of the competition.

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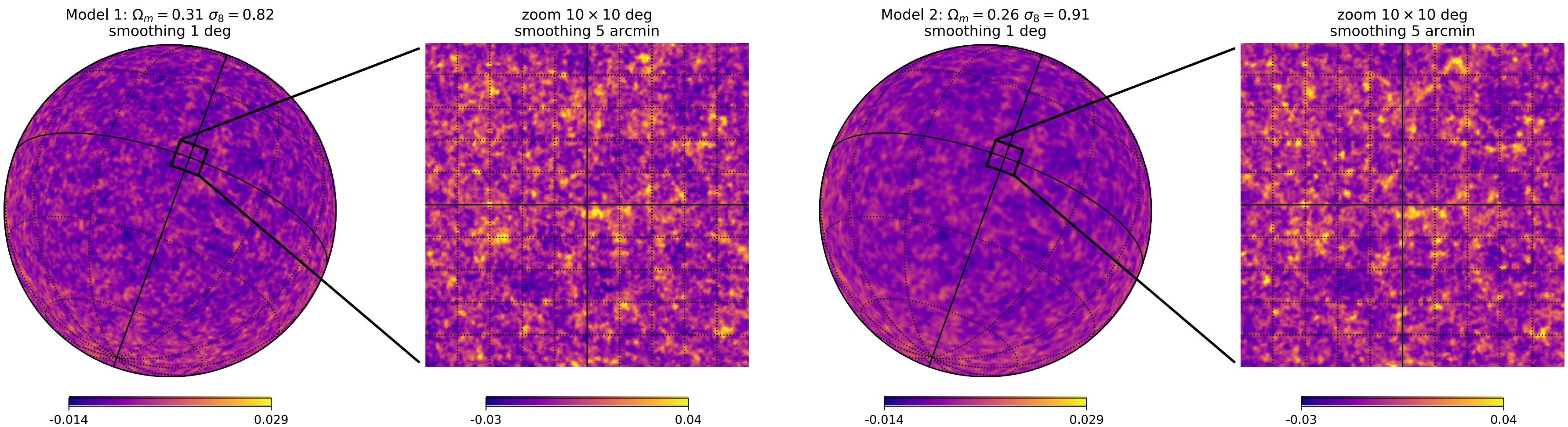
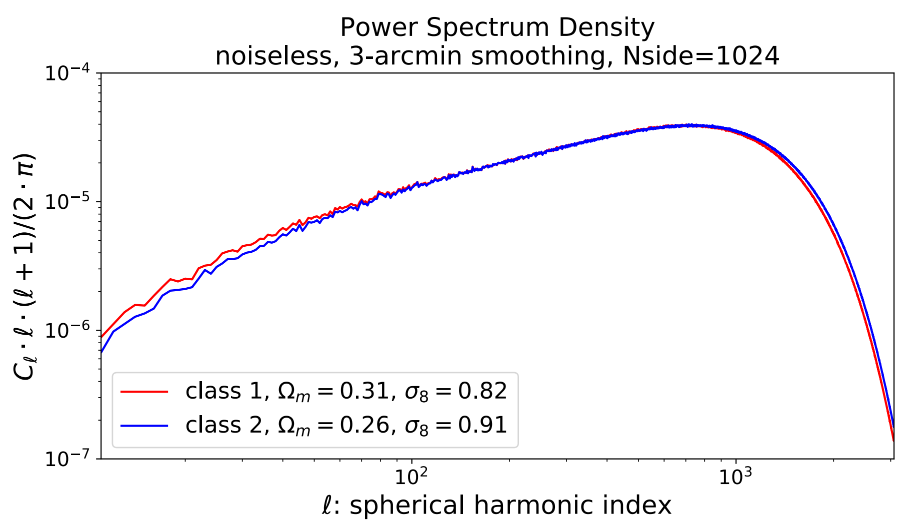
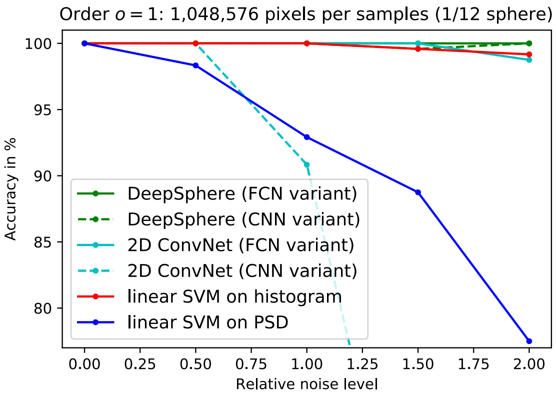
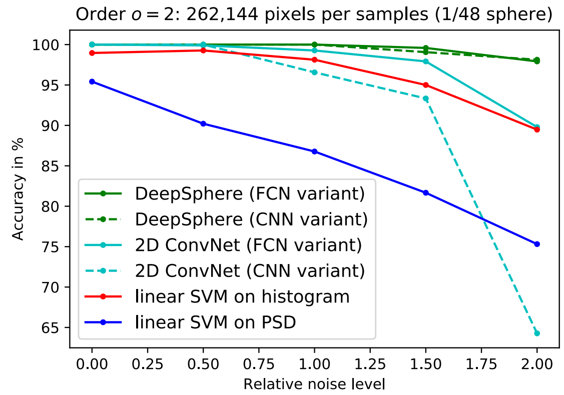
The convergence maps dataset

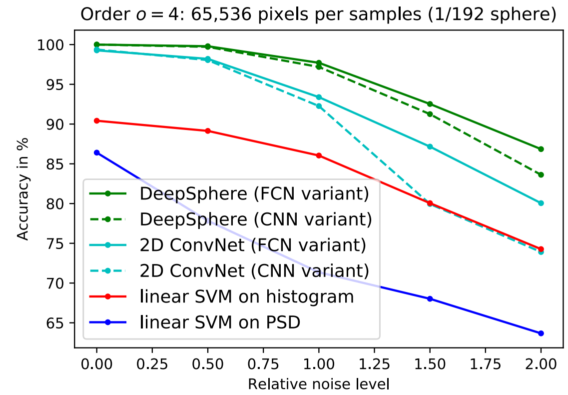


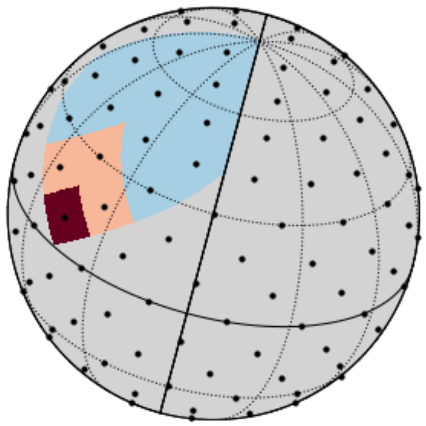


Results: better than 2D CNNs.









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Conclusive words

- Deepsphere is an excellent tradeoff between computational complexity and equivariance.
- If you work with data on irregular data domain, think about graphs!
- Disclaimer: they exists plenty of other graph methods and the one presented here is definitely not the most used.
- Code: https://github.com/SwissDataScienceCenter/DeepSphere
- Papers

  - **Perraudin, N.**, Defferrard, M., Kacprzak, T., & Sgier, R. (2019). DeepSphere: Efficient spherical convolutional neural network with HEALPix sampling for cosmological applications. *Astronomy and Computing*, *27*, 130-146.
  - Defferrard, M., Milano M., Gusset F. & **Perraudin N.** (2020). DeepSphere: a graph-based spherical CNN. *International Conference on Learning Representations*.

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Discussion

Thanks for your attention

- Questions?

- Suggestions?

- Discussion…