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Spherical convolutional neural network for diffusion MRI analysis





Overview

- Motivation to use spherical CNN
- Brain micro-structure modeling
- Theory behind
- Illustration of the architectures
- Experiments
- Conclusions & discussions

Signals on sphere



Figure 1. 3D object from ModelNet database and its projections on sphere [1]



Figure 2. Segmentation of atmospheric rivers [2]



Figure 4. 360° image ° [4]



Figure 3. Segmentation of molecular surfaces [3]

[1] Esteves, Carlos, et al. "3D object classification and retrieval with Spherical CNNs." arXiv preprint arXiv:1711.06721 (2017).

[2] Jiang, Chiyu, et al. "Spherical cnns on unstructured grids." arXiv preprint arXiv:1901.02039 (2019).

[3] Poulenard, Adrien, et al. "Effective Rotation-invariant Point CNN with Spherical Harmonics kernels." 2019 International Conference on 3D Vision (3DV). IEEE, 2019.
[4] Coors, Benjamin, Alexandru Paul Condurache, and Andreas Geiger. "Spherenet: Learning spherical representations for detection and classification in omnidirectional images." Proceedings of the European Conference on Computer Vision (ECCV). 2018.

Diffusion





Figure 5. Illustration of diffusion in free and restricted volumes

diffusion MRI (dMRI)

- Based on water molecule diffusion properties of underlying tissue
- Molecule motion in white matter (axons) is restricted
- Molecule motion in gray matter and cerebrospinal fluid is close to free
- Each voxel is a signal in 3D, often sampled on sphere
- Contains Rician noise
- Crucial for white matter analysis!



Brain micro-structure modeling

Fiber orientation distribution function (FOD)

- Function on a sphere that reveals how the axon bundles are oriented in a voxel
- Important for tracking of white matter pathways



Brain micro-structure modeling

Neurite orientation dispersion and density imaging (NODDI) [5]

- A biophysical model that explains dMRI signal as a linear combination of three compartments
 - Intra-cellular axons and dendrites
 - Extra-cellular neuron cell bodies and glial cells
 - Cerebrospinal fluid (CSF)
- Showed potential in evaluation of several neurodegenerative diseases



Convolution on a sphere

Planar correlation (convolution) of two R² signals is a signal in R² Spherical correlation (convolution) of two S² signals is a signal in SO(3)

Space of **translational** moves in plane (R²) is in R² (isomorphic to plane)



Figure 6. Translational movements of patterns in plane

Space of **3D rotational** moves on sphere (S²) is SO(3) manifold.



Figure 7. Rotational movements of patterns on sphere

3D rotational group or SO(3) manifold: group of all rotations around origin in 3D Euclidean space







Figure 8. 3D rotation (images generated by Google Earth)

Convolution on a sphere







Figure 9. Kernel movement in plane

Figure 10. Illustration of deformation introduced by projection of spherical signal on plane (**image source:** Spherical CNNs, Taco S. Cohen et al.) Figure 11. Kernel movement in SO(3) (image generated using Q-ball sampling tool)

Fourier transform





0

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Spherical signals can be represented as a linear combination of spherical harmonics:



$$f(\theta_k, \phi_k) = \sum_{l=0}^{L} \sum_{m=-l}^{m=l} \hat{f}_l^m Y_l^m(\theta_k, \phi_k)^{-1}$$

Image sources:

https://en.wikipedia.org/wiki/Multidimensional_transform#/media/File:Dctjpeg.png, 4 https://www.ti.uni-bielefeld.de/html/people/ddiffert/libShc/manual/fouriertransform.html



m 0

2

Spherical CNNs [6]





$$\begin{split} [\psi \star f](R) &= \langle L_R \psi, f \rangle = \int_{\mathrm{SO}(3)} \sum_{k=1}^K \psi_k(R^{-1}Q) f_k(Q) dQ. \\ \widehat{\psi \star f}^l &= \hat{f}^l \cdot \hat{\psi}^{l\dagger} \end{split}$$

SO(3) signals



Spherical CNNs [6]

Transformation from Fourier domain to SO(3) is given by:

$$f(R) = \sum_{l=0}^{b} (2l+1) \sum_{m=-l}^{l} \sum_{n=-l}^{l} \hat{f}_{mn}^{l} D_{mn}^{l}(R),$$

where $D_{mn}^{l}(R)$ are Wigner D matrices







 $f(R) = f(\varphi, \theta, \psi)$



[6] Spherical CNNs, Taco S. Cohen, Mario Geiger, Jonas Koehler, Max Welling

Adjustments to dMRI data properties



Antipodally symmetric \rightarrow basis of even order are

Figure 12. Illustration of spherical harmonics

Real signal \rightarrow real basis are sufficient for their representation

Real spherical harmonics

$$Y_{lm} = \begin{cases} \sqrt{2}(-1)^{m} \Im(Y_{l}^{|m|}), & \text{if } m < 0 \\ Y_{l}^{m}, & \text{if } m = 0 \\ \sqrt{2}(-1)^{m} \Re(Y_{l}^{m}), & \text{if } m > 0 \end{cases}$$

Real Wigner D matrices

$$D_{lmn} = \begin{vmatrix} (-1)^{m+n} \Re (D_l^{mn}) + (-1)^m \Re (D_l^{m-n}) & \text{, for } m > 0, n > 0 \\ -(-1)^{m+n} \Im (D_l^{m|n|}) + (-1)^m \Im (D_l^{mn}), & \text{for } m > 0, n < 0 \\ (-1)^{m+n} \Im (D_l^{|m|n}) + (-1)^m \Im (D_l^{|m|-n}), & \text{for } m < 0, n > 0 \\ (-1)^{m+n} \Re (D_l^{|m||n|}) - (-1)^m \Re (D_l^{|m|n}), & \text{for } m < 0, n < 0 \end{vmatrix}$$

$$D_{l0n} = \begin{cases} \sqrt{2}(-1)^{n} \Im(D_{l}^{0|n|}), & \text{if } n < 0 \\ D_{l}^{0n}, & \text{if } n = 0 \\ \sqrt{2}(-1)^{n} \Re(D_{l}^{0n}), & \text{if } n > 0 \end{cases} \int_{lm0}^{m0} \int_{lm0}^{m0} D_{lm0} = \begin{cases} \sqrt{2}(-1)^{m} \Im(D_{l}^{|m|0}), & \text{if } m < 0 \\ D_{l}^{m0}, & \text{if } m = 0 \\ \sqrt{2}(-1)^{m} \Re(D_{l}^{m0}), & \text{if } m > 0 \end{cases}$$

Orthogonality loss

Continuous signals

Fourier Transform (FT)	$\hat{f}(\xi) = \int_{-\infty}^{\infty} f(t) e^{-i2\pi\xi t} dt$	$\hat{f}_l^m = \int_{\Omega} f(\theta, \phi) Y_l^{m*}(\theta, \phi) d\Omega$
inverse Fourier Transform (IFT)	$f(t) = \int_{-\infty}^{\infty} f(\xi) e^{i2\pi t\xi} d\xi$	$f(\theta,\phi) = \sum_{l=0}^{\infty} \sum_{m=-l}^{m=l} \hat{f}_l^m Y_l^m(\theta,\phi)$

Discrete signals



Figure 13. Illustration of gradient direction sampling scheme [7] (image source: http://www.emmanuelcaruyer.com/q-space-sampling.php)

 $Y_l^m(\theta_k,\phi_k)Y_l^m(\theta_k,\phi_k)^* \qquad Y_l^m(\theta_k,\phi_k)Y_l^m(\theta_k,\phi_k)^\dagger$





Figure 14. Loss of orthogonality of transposed and pseudo inverted basis

[7] Caruyer, Emmanuel, et al. "Design of multishell sampling schemes with uniform coverage in diffusion MRI." Magnetic resonance in medicine 69.6 (2013): 1534-1540.



NODDI parameter estimation – experiment

Golden standard generated by AMICO [8] with full sampling scheme



Experiments run on downsampled scheme



Full sampling scheme

Downsampled sampling scheme

Model trained to estimate three NODDI parameters: ${m v}_{ic} \,\, {m v}_{csf} \,\,\, {m OD}$

Spherical CNN model parameters:

- 4 convolutional + 4 fully connected layers
- Total number of trainable parameters: 103 891

Model trained on HCP [9] dataset:

- 30 subjects for training
- 10 subjects for validation
- 10 subjects for test

[8] Daducci, Alessandro, et al. "Accelerated microstructure imaging via convex optimization (AMICO) from diffusion MRI data." Neuroimage 105 (2015): 32-44.

[9] Van Essen, David C., et al. "The WU-Minn human connectome project: an overview." Neuroimage 80 (2013): 62-79.

image source: http://www.emmanuelcaruyer.com/q-space-sampling.php

NODDI parameter estimation – results





[10] Ye, Chuyang. "Tissue microstructure estimation using a deep network inspired by a dictionary-based framework." Medical image analysis 42 (2017): 288-299.

FOD estimation – experiment



[11] Ronneberger, Olaf, Philipp Fischer, and Thomas Brox. "U-net: Convolutional networks for biomedical image segmentation." International Conference on Medical image computing and computer-assisted intervention. Springer, Cham, 2015.





Conclusions & discussions

- We have investigated and shown how to use and adjust S2CNNs to dMRI data
- Promising results were obtained for two challenging tasks
- How to use synthetic data with known ground truth
- How to use another properties, such as axial symmetry of the signals generated by individual axon bundles
- How to avoid computationally expensive conversions to and from Fourier domain
- ...

Thank you for your attention! Questions?

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