Geometric deep learning on the sphere

Scalable and equivariant spherical CNNs

Jason McEwen

www.jasonmcewen.org

Kagenova Limited Mullard Space Science Laboratory (MSSL), UCL

In collaboration with:

Jeremy Ocampo 🔸 Matthew Price 🔸 Oliver Cobb 🔸 Chris Wallis 🔸 Augustine Mavor-Parker 🔸 Augustin Marignier 🔸 Mayeul d'Avezac

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- 1. Symmetry in deep learning
- 2. Geometric deep learning on the sphere
- 3. Continuous spherical CNNs
- 4. Discrete-continuous spherical CNNs

Mentimeter

Give your input at https://www.menti.com/puiqjn97i9.

Or go to https://www.menti.com and enter voting code: 7439 9891.



Symmetry in deep learning

Physics and deep learning

Physics

Understanding the world by modelling from first principles for generative models and inference.

Deep Learning

Understanding the world by **learning informative representations** for generative models and inference.

Physics and deep learning

Physics

Understanding the world by modelling from first principles for generative models and inference.

Hard!

Deep Learning

Understanding the world by **learning informative representations** for generative models and inference.

Hard!

Physics \iff Deep Learning

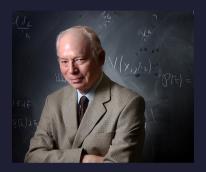
Physics \longleftrightarrow Deep Learning

Here we focus on integrating physics \rightarrow deep learning (in other works focus on reverse: physics \leftarrow deep learning).

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As we will see, this key factor driving the deep learning revolution.



"Symmetry: key to nature's secrets."

- Steven Weinberg

Mirror symmetry



Mirror symmetry



Mirror symmetry





Mirror symmetry





Mirror symmetry





Mirror symmetry



Rotational symmetry



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Mirror symmetry







Spatial translation



Spatial translation





Spatial translation

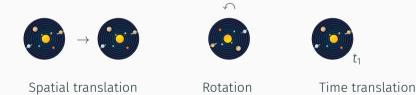
Rotation





Spatial translation

Rotation





Spatial translation



Rotation



Time translation

Noether's theorem

For every continuous symmetry of the universe, there exists a conserved quantity.



Emmy Noether

Noether's theorem

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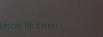
Symmetries at the heart of physics:

- + Translational symmetry \Leftrightarrow conservation of momentum
- + Rotational symmetry \Leftrightarrow conservation of angular momentum
- + Time translational symmetry \Leftrightarrow conservation of energy



Emmy Noether

Symmetry is the foundation underlying the fundamental laws of physics.



Encoding symmetry in deep learning models captures fundamental properties about the underlying nature of our world.

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Key factor driving the deep learning revolution, with the advent of CNNs.

- CNNs resulted in a step-change in performance.
- Convolutional structure of CNNs capture translational symmetry (i.e. translational equivariance).

Equivariance

Equivariance

An operator ${\mathcal A}$ is equivariant to a transformation ${\mathcal T}$ if

$$\mathcal{T}(\mathcal{A}(f)) = \mathcal{A}(\mathcal{T}(f))$$

for all possible signals f.

Transforming the signal after application of the operator, is equivalent to transformation of the signal first, followed by application of the operator.

Equivariance

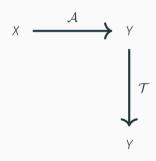
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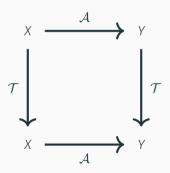
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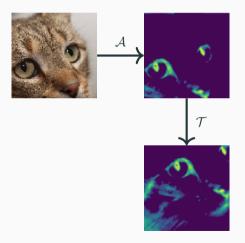
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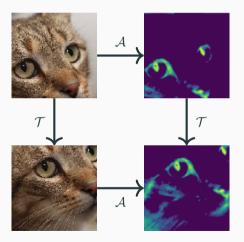
Planar (Euclidean) CNNs exhibit translational equivariance

Planar (Euclidean) convolution is translationally equivariant.



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Imposing inductive biases in deep learning models, such as equivariance to symmetry transformations, allows models to be learned in a more principled and effective manner.

Capture fundamental physical understanding of generative process.

Importance of equivariance

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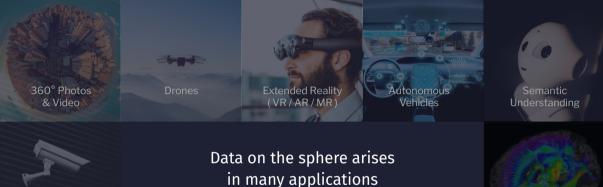






Still a cat

Geometric deep learning on the sphere



Surveillance & Monitoring

Molecular Chemistry Earth & Climate Science



Astrophysics

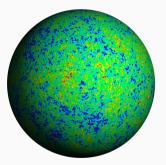
Medical Imaging



Communications

Cosmology and virtual reality

Whenever observe over angles, recover data on 2D sphere (or 3D rotation group).

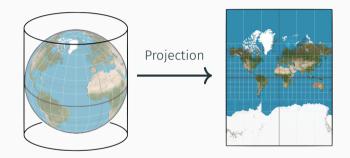


Cosmic microwave background

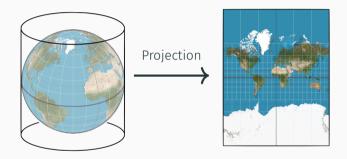


360° virtual reality

Could project sphere to plane and then apply standard planar CNNs.



Could project sphere to plane and then apply standard planar CNNs.

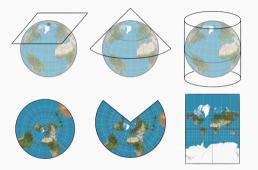


Greenland appears to be a similar size to Africa in the projected planar map, whereas it is over 10 times smaller.

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Projection breaks symmetries and geometric properties of sphere.

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No projection of the sphere to the plane can preserve both shapes and areas \Rightarrow distortions are unavoidable.

(Formally: a conformal, area-preserving projection does not exist.)

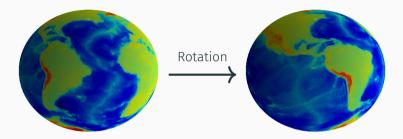
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Goals of geometric deep learning on the sphere

- 1. Capture geometry and symmetry of the sphere (rotational equivariance)
- 2. Computationally scalable to support high-resolution data

Rotational equivariance

On the sphere, the analog of translations are rotations.



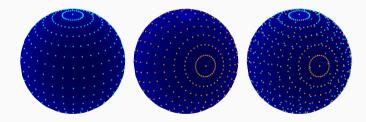
Would like spherical CNNs to exhibit rotational equivariance.

(Just as planar CNNs exhibit translational equivariance.)

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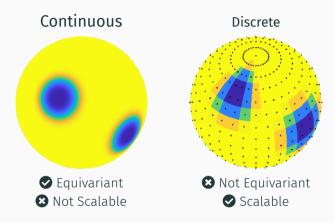
Capturing rotational equivariance in spherical CNNs

Well-known that regular discretisation of the sphere does not exist (e.g. Tegmark 1996). \Rightarrow Not possible to discretise sphere in a manner that is invariant to rotations.



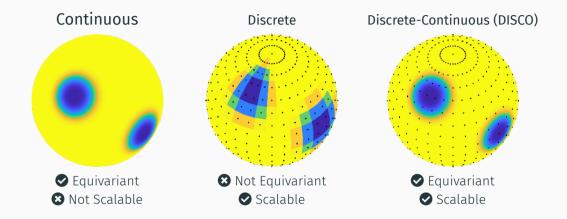
Capturing strict equivariance with operations defined directly in discretised (pixel) space **not possible** due to structure of sphere.

Categorisation of spherical CNNs frameworks



(Cohen et al. 2018; Esteves et al. 2018; Kondor et al. 2018; Cobb et al. 2021; McEwen et al. 2022) Jason McEwen (Jiang et al. 2019, Zhang et al. 2019, Perraudin et al. 2019, Cohen et al. 2019)

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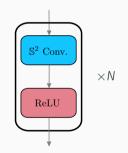


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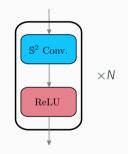
(Ocampo, Price & McEwen, 2022)

Continuous spherical CNNs

Spherical CNNs constructed by analog of Euclidean CNNs but using convolution on the sphere and with pointwise non-linear activations functions, e.g. ReLU (Cohen et al. 2018; Esteves et al. 2018).



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Consider Fourier representation \rightarrow access to underlying continuous representations.

Convolution of signals on the sphere

Convolution of signals in spatial domain

Convolution of two signals $f, \psi \in L^2(\mathbb{S}^2)$ is given by

$$(f \star \psi)(\rho) = \langle f, R\psi \rangle = \int_{\mathbb{S}^2} \mathrm{d}\mu(\omega) f(\omega) \psi^*(\rho^{-1}\omega), \quad \text{for } \omega \in \mathbb{S}^2, \rho \in \mathrm{SO}(3),$$

where $d\mu(\omega)$ denotes the Haar measure on \mathbb{S}^2 and \cdot^* complex conjugation.

Since sphere is compact manifold, Fourier space is discrete and **sampling theorems** can be leveraged to compute Fourier representations exactly for bandlimited signals (e.g. McEwen & Wiaux 2011).

 \Rightarrow Provides access to underlying continuous signals and symmetries of sphere.

Convolution of signals in harmonic domain

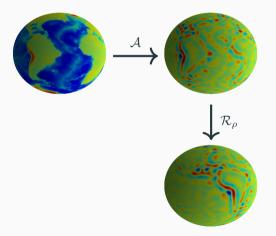
Convolution of two signals $f, \psi \in L^2(\mathbb{S}^2)$ can be computed as a product in harmonic space:

$$\widehat{(f\star\psi)}^\ell = \hat{f}^\ell \,\hat{\psi}^{\ell*}.$$

Convolution is rotationally equivariant

Convolution is rotationally equivariant (when computed in harmonic domain):

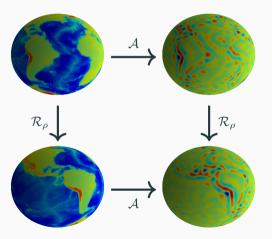
 $((\mathcal{R}_{\rho}f)\star\psi)(\rho')=(\mathcal{R}_{\rho}(f\star\psi))(\rho').$



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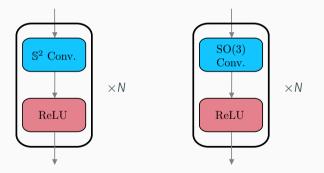
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Approach taken by Cohen et al. (2018) and Esteves et al. (2018).

Compute non-linear activation pixel-wise in spatial domain.



Given two harmonic fragments \hat{f}^{ℓ_1} and \hat{f}^{ℓ_2} , then

 $(C^{\ell_1,\ell_2,\ell})^{\top}(\hat{f}^{\ell_1}\otimes\hat{f}^{\ell_2}),$

where $C^{\ell_1,\ell_2,\ell}$ are Clebsch-Gordan coefficients, which is non-linear in f and rotationally equivariant (Kondor et al. 2018).

Consider the s-th layer of a generalized spherical CNN to take the form of a triple (Cobb et al. 2021; arXiv:2010.11661)

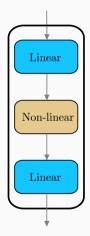
$$\mathcal{A}^{(s)} = (\mathcal{L}_1, \mathcal{N}, \mathcal{L}_2)_{s}$$

such that

$$\mathcal{A}^{(s)}(f^{(s-1)}) = \mathcal{L}_2(\mathcal{N}(\mathcal{L}_1(f^{(s-1)}))),$$

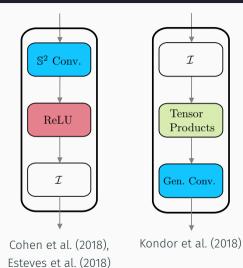
where

- $\mathcal{L}_1, \mathcal{L}_2 : \mathcal{F}_L \to \mathcal{F}_L$ are spherical convolution operators,
- $\mathcal{N} : \mathcal{F}_L \to \mathcal{F}_L$ is a non-linear, spherical activation operator.



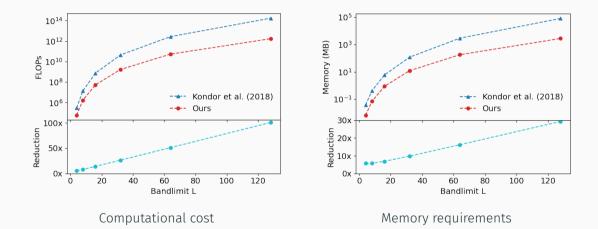
Efficient generalised spherical CNNs

- Build on other **influential equivariant spherical CNN** constructions:
 - Cohen et al. (2018)
 - Esteves et al. (2018)
 - Kondor et al. (2018)
- Encompass other frameworks as special cases.
- General framework supports hybrids models.
- Significant efficiency improvements.



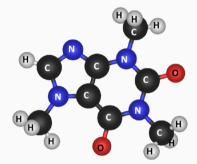
- 1. Channel-wise structure
- 2. Constrained generalized convolutions
- 3. Optimized degree mixing sets
- 4. Efficient sampling theory on the sphere and rotation group (McEwen & Wiaux 2011; McEwen et al. 2015)

Computational cost and memory requirements



Atomization energy prediction: problem

Predict atomization energy of molecule give the atom charges and positions.



Test root mean squared (RMS) error for QM7 regression problem

	RMS	Params
Montavon et al. 2012	5.96	-
Cohen et al. 2018	8.47	1.4M
Kondor et al. 2018	7.97	>1.1M
Ours (MST)	3.16	337k
Ours (RMST)	3.46	335k

Despite the efficient generalized approach

such equivariant spherical CNNs are limited to low-resolution data.

Introduce new initial layer, with following properties:

- 1. Scalable
- 2. Allow subsequent layers to operate at low-resolution (i.e. mixes information to low frequencies)
- 3. Rotationally equivariant
- 4. Stable and locally invariant representation (i.e. effective representation space)

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 \Rightarrow Scattering networks on the sphere (McEwen et al. 2022; arXiv:2102.02828)

Scattering on the sphere follows by direct analogue of Euclidian construction (Mallat 2012). Adopt scale-discretized wavelets on the sphere (e.g. McEwen et al. 2018, McEwen et al. 2015).

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 $U[j]f = |f \star \psi_j|.$

Modulus function is adopted for the activation function since non-expansive. Acts to mix signal content to low frequencies.

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Spherical cascade of propagators:

$$U[p]f = |||f \star \psi_{j_1}| \star \psi_{j_2}| \ldots \star \psi_{j_d}|,$$

for the path $p = (j_1, j_2, \dots, j_d)$ with depth d.

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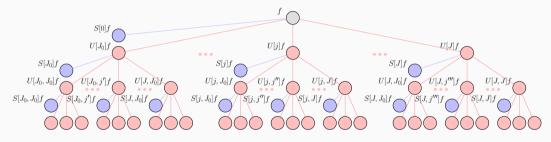
Scattering coefficients:

$$S[p]f = |||f \star \psi_{j_1}| \star \psi_{j_2}| \ldots \star \psi_{j_d}| \star \phi.$$

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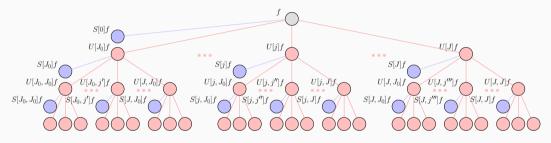
Scattering networks on the sphere

Spherical scattering network is collection of scattering transforms for a number of paths: $S_{\mathbb{P}}f = \{S[p]f : p \in \mathbb{P}\}, \text{ where the general path set } \mathbb{P} \text{ denotes the infinite set of all possible paths } \mathbb{P} = \{p = (j_1, j_2, \dots, j_d) : J_0 \le j_i \le J, 1 \le i \le d, d \in \mathbb{N}_0\}.$



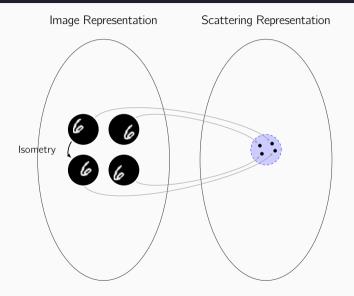
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Scattering networks are rotationally equivariant (since the spherical wavelet transform and modulus operator are rotationally equivariant).

Isometric invariance



Theorem (Isometric Invariance)

Let $\zeta \in \text{Isom}(\mathbb{S}^2)$, then there exists a constant C such that for all $f \in L^2(\mathbb{S}^2)$,

$$\|\mathcal{S}_{\mathbb{P}_{D}}f - \mathcal{S}_{\mathbb{P}_{D}}V_{\zeta}f\|_{2} \leq CL^{5/2}(D+1)^{1/2} |\chi|_{\infty} \|\zeta\|_{\infty} \|f\|_{2}.$$

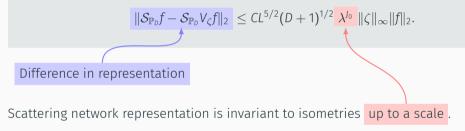
Difference in representation

Scattering network representation is invariant to isometries up to a scale .

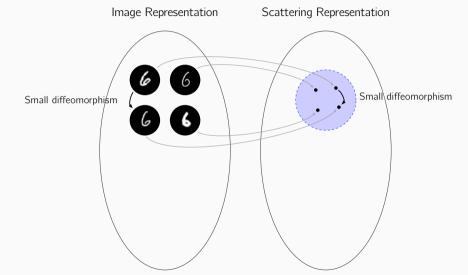
(Proof: Follows by straightforward extension of proof of Perlmutter et al. 2020.)

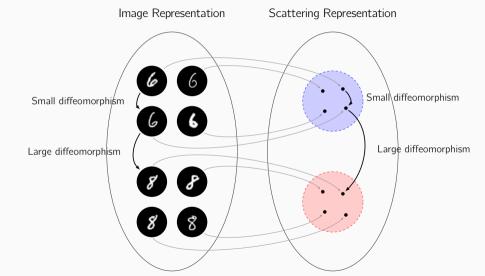
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Theorem (Stability to Diffeomorphisms)

Let $\zeta \in \text{Diff}(\mathbb{S}^2)$. If $\zeta = \zeta_1 \circ \zeta_2$ for some isometry $\zeta_1 \in \text{Isom}(\mathbb{S}^2)$ and diffeomorphism $\zeta_2 \in \text{Diff}(\mathbb{S}^2)$, then there exists a constant C such that for all $f \in L^2(\mathbb{S}^2)$,

$$\|\mathcal{S}_{\mathbb{P}_{D}}f - \mathcal{S}_{\mathbb{P}_{D}}V_{\zeta}f\|_{2} \leq CL^{2} \|\zeta^{2}\|_{\infty} + L^{1/2}(D+1)^{1/2}\lambda^{J_{0}} \|\zeta_{1}\|_{\infty} \|f\|_{2}.$$

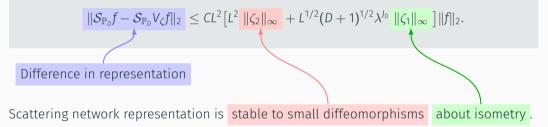
Difference in representation

Scattering network representation is stable to small diffeomorphisms about isometry .

(Proof: Follows by straightforward extension of proof of Perlmutter et al. 2020.)

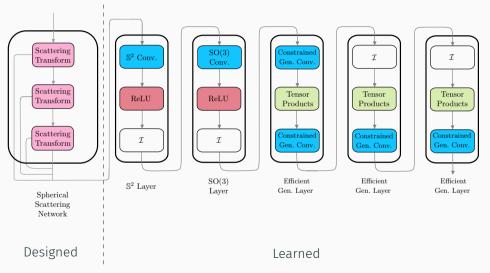
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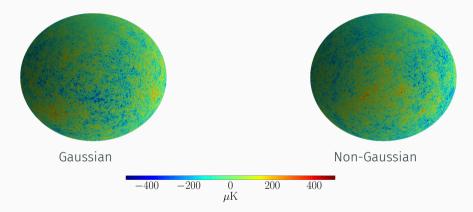
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Scalable and rotationally equivariant spherical CNNs



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Gaussianity of the cosmic microwave background



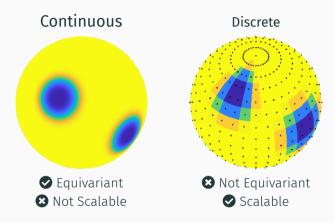
At L = 1024 (~2 million pixels), we achieve classification accuracy of: 53% without scattering network versus 95% with scattering network.

While spherical scattering networks help to scale to high-resolution input data,

high-resolution outputs for dense predictions are not supported.

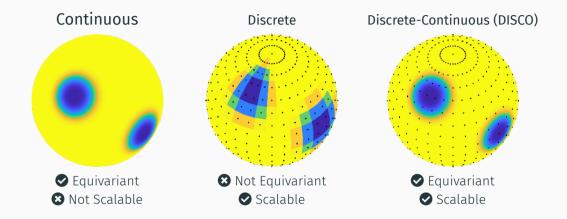
Discrete-continuous spherical CNNs

Categorisation of spherical CNNs frameworks



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(Ocampo, Price & McEwen, 2022)

Discrete-continuous (DISCO) spherical convolution

Scalable and Equivariant Spherical CNNs by Discrete-Continuous (DISCO) Convolutions (Ocampo, Price & McEwen 2022; arXiv:2209.13603)

Follows by a careful hybrid representation of the spherical convolution:

- · some components left continuous, to facilitate accurate rotational equivariance;
- while other components are discretized, to yield scalable computation.

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DISCO spherical convolution

Spherical convolution can be carefully approximated by the DISCO representation

$$(f \star \psi)(R) = \int_{\mathbb{S}^2} f(\omega) \psi(R^{-1}\omega) \mathrm{d}\omega \approx \sum_i f[\omega_i] \psi(R^{-1}\omega_i) \delta\omega_i,$$

where, for now, we consider 3D rotations $R \in SO(3)$.

Rotations restricted to the quotient space may be written $R = Z(\alpha)Y(\beta) \in SO(3)/SO(2)$.

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Analogous to Euclidean planar CNNs, where filters are translated across the image but are *not* rotated in the plane.

However, as the space SO(3)/SO(2) is **not a group**, when restricting rotations in this manner important differences to the usual setting arise since we no longer have a group convolution.

SO(3) rotational equivariance

DISCO spherical convolution $f \star \psi$ for rotations $Q, R \in SO(3)$ satisfies SO(3) rotational equivariance:

$$\begin{aligned} ((\mathcal{Q}f) \star \psi)(R) &\approx \sum_{i} (\mathcal{Q}f)[\omega_{i}]\psi(R^{-1}\omega_{i})\delta\omega_{i} \\ &= \sum_{i} f[\omega_{i}]\psi((Q^{-1}R)^{-1}\omega_{i})\delta\omega_{i} \\ &\stackrel{(**)}{\approx} (f \star \psi)(Q^{-1}R) \\ &= (\mathcal{Q}(f \star \psi))(R). \end{aligned}$$

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$$= \sum_{i} f[\omega_{i}]\psi((Q^{-1}R)^{-1}\omega_{i})\delta\omega_{i}$$
$$\stackrel{(**)}{\approx} (f \star \psi)(Q^{-1}R)$$
$$= (\mathcal{Q}(f \star \psi))(R).$$

Note that step (**) only holds since SO(3) exhibits a group structure and so $Q^{-1}R \in SO(3)$.

DISCO spherical convolution $f \circledast \psi$ for rotations $Q, R \in SO(3)/SO(2)$ does not satisfy SO(3) or SO(3)/SO(2) rotational equivariance (since SO(3)/SO(2) is not a group).

DISCO spherical convolution $f \otimes \psi$ for rotations $Q, R \in SO(3)/SO(2)$ does not satisfy SO(3) or SO(3)/SO(2) rotational equivariance (since SO(3)/SO(2) is not a group).

But DISCO spherical convolution $f \oplus \psi$ does satisfy asymptotic SO(3)/SO(2) equivariance. Recover asymptotic SO(3)/SO(2) rotational equivariance as $\beta \to 0$, for $Q = Z(\alpha)Y(\beta)$. DISCO spherical convolution $f \otimes \psi$ for rotations $Q, R \in SO(3)/SO(2)$ does not satisfy SO(3) or SO(3)/SO(2) rotational equivariance (since SO(3)/SO(2) is not a group).

But DISCO spherical convolution $f \otimes \psi$ does satisfy asymptotic SO(3)/SO(2) equivariance. Recover asymptotic SO(3)/SO(2) rotational equivariance as $\beta \to 0$, for $Q = Z(\alpha)Y(\beta)$.

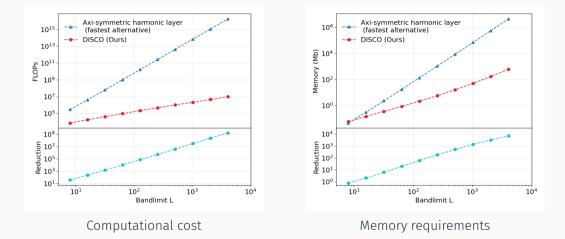
Asymptotic SO(3)/SO(2) equivariance of significant practical use since content in spherical signals often orientated and similar content appears at similar latitudes, particularly for 360° panoramic photos and video.

DISCO convolution affords a computationally scalable implementation.

- 1. Spare tensor representation.
- 2. Memory compression.
- 3. Custom sparse gradients.

Linear scaling in number of pixels on the sphere $O(N) = O(L^2)$ for both computational cost and memory usage.

Computational cost and memory requirements



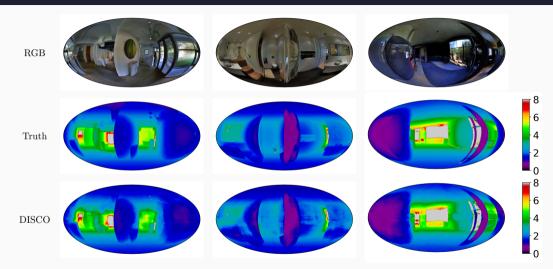
For 4k spherical image, 10⁹ saving in computational cost and 10⁴ saving in memory usage.

DISCO spherical CNNs exhibit excellent rotational equivariance properties and

are computationally scalable

supporting high-resolution input and output data for dense-prediction tasks.

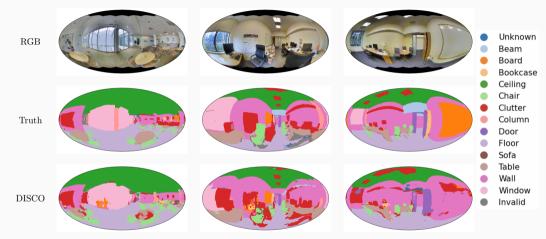
Depth estimation for Pano3D



Example predictions for depth estimation of Pano3D data (depth plotted in meters). Jason McEwen

Model	Parameters	Depth Error Metrics			Depth Accuracy Metrics				
		WRMSE	WRMSLE	wAbsRel	wSqRel	$\delta_{1.05}^{ m ico}$	$\delta_{1.1}^{\mathrm{ico}}$	$\delta^{ m ico}_{ m 1.25}$	$\delta^{ m ico}_{ m 1.25^2}$
Planar UNet	27M	0.4520	0.1300	0.1147	0.0811	36.68%	60.59%	88.31%	96.96%
DISCO-Directional (Ours)	658k	0.5063	0.1695	0.1109	0.0852	38.32%	62.12%	88.65%	97.29%

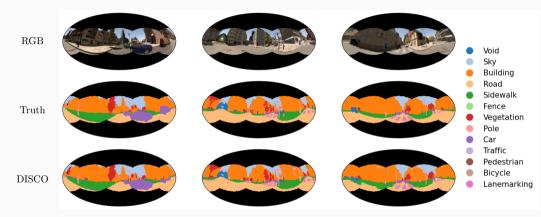
Semantic segmentation for 2D3Ds dataset



Example predictions for semantic segmentation of 2D3DS data.

Model	mloU	mAcc
Planar UNet	35.9	50.8
UGSCNN	38.3	54.7
GaugeNet	39.4	55.9
HexRUNet	43.3	58.6
SWSCNNs	43.4	58.7
CubeNet	45.0	62.5
MöbiusConv	43.3	60.9
DISCO-Axisymmetric (Ours)	39.7	54.1
DISCO-Directional-Separable (Ours)	43.9	60.9
DISCO-Directional (Ours)	45.2	61.5
DISCO-Directional-Aug (Ours)	45.7	62.7

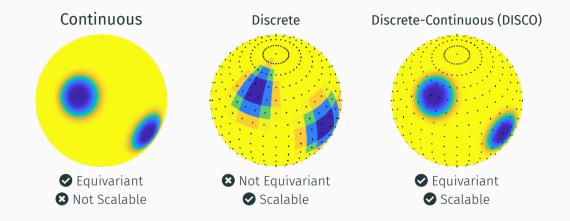
Semantic segmentation for Omni-SYNTHIA dataset



Example predictions for semantic segmentation of Omni-SYNTHIA data.

Model	mloU	mAcc
Planar UNet	44.6	52.6
UGSCNN	37.6	48.9
HexUNet	48.3	57.1
DISCO-Directional-Separable (Ours)	48.3	59.3
DISCO-Directional-Separable-Aug (Ours)	49.2	63.7

Summary



(Cohen et al. 2018; Esteves et al. 2018; Kondor et al. 2018; Cobb et al. 2021; McEwen et al. 2022) Jason McEwen (Jiang et al. 2019, Zhang et al. 2019, Perraudin et al. 2019, Cohen et al. 2019)

(Ocampo, Price & McEwen, 2022)