Geometric deep learning on the sphere

Efficient generalised spherical CNNs

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Outline

- 1. Symmetry in deep learning
- 2. Spherical CNNs
- 3. Efficient generalised spherical CNNs
- 4. Numerical experiments

Symmetry in 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.

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Hard!

Deep Learning

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Hard!

 $\textbf{Physics} \quad \longleftrightarrow \quad \textbf{Deep Learning}$

Physics \longleftrightarrow Deep Learning

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

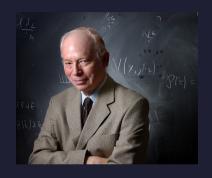
4

Physics \longleftrightarrow Deep Learning

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

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

4



"Symmetry: key to nature's secrets."

— Steven Weinberg

Mirror symmetry



Mirror symmetry



Mirror symmetry





Mirror symmetry



Rotational symmetry



Mirror symmetry





Mirror symmetry





Mirror symmetry





In physics we typically consider **continuous symmetries**, where system is symmetric (invariant) to continuous transformation.

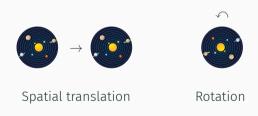


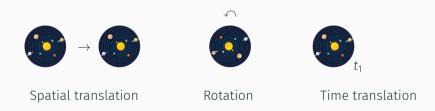
Spatial translation



Spatial translation









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Noether's theorem

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



Emmy Noether

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

Symmetries at the heart of physics:

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

(Energy not conserved in general relativity since time translation broken.)



Emmy Noether

Symmetry is the foundation underlying the fundamental laws of physics.



Symmetry in deep learning

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).

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Equivariance

Equivariance

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

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

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

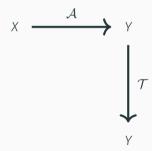
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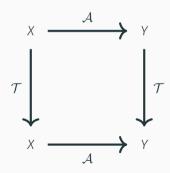
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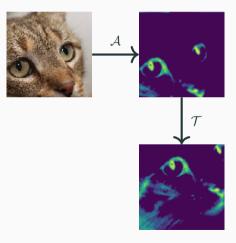
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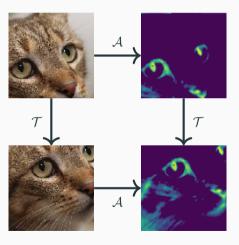
Planar (Euclidean) CNNs exhibit translational equivariance

Planar (Euclidean) convolution is translationally equivariant.



Planar (Euclidean) CNNs exhibit translational equivariance

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Importance of equivariance

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.

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In some sense, equivariance to a transformation means a pattern need only be learnt once, and may then be recognised in all transformed scenarios.

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Cat



Still a cat

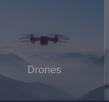
Spherical CNNs

Data on the sphere is prevalent

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Encode symmetries of the sphere and rotations













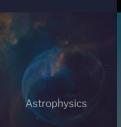
Data on the sphere arises in many applications







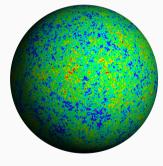






Cosmology and virtual reality

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



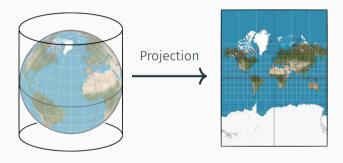
Cosmic microwave background



360° virtual reality

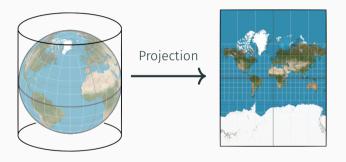
Why not standard (Euclidean) deep learning approaches?

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

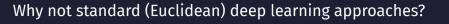


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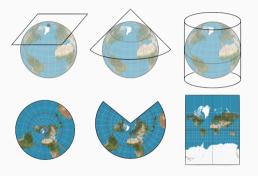
Greenland appears to be a similar size to Africa in the projected planar map, whereas it is over 10 times smaller.



Projection breaks symmetries and geometric properties of sphere.

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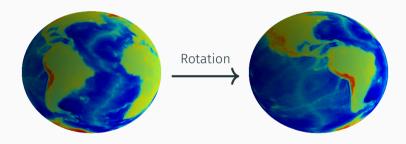


No projection of the sphere to the plane can preserve both shapes and areas ⇒ distortions are unavoidable.

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

Rotational equivariance

On the sphere, the analog of translations are rotations.

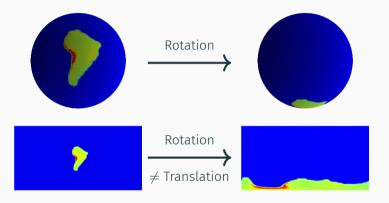


Would like spherical CNNs to exhibit rotational equivariance.

(Just as planar CNNs exhibit translational equivariance.)

Rotational equivariance

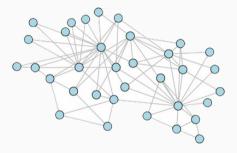
Rotational equivariance not captured by translational equivariance of planar CNNs.



(Harmonic networks constructed to capture rotational equivariance for planar images by Worral et al. 2017.)

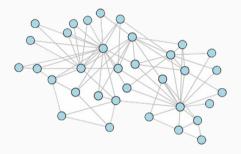
Why not graph-based geometric deep learning?

Could construct graph representation of sphere and apply graph CNNs.



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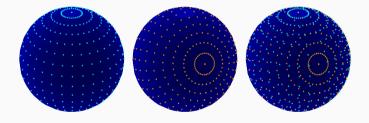
Again, breaks symmetries and geometric properties of sphere.

Cannot capture rotational equivariance.

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.

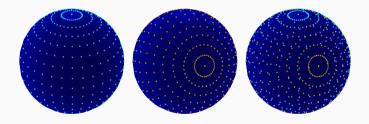


Capturing strict equivariance with operations defined directly in discretised (pixel) space **not possible** due to structure of sphere.

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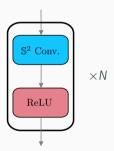


Capturing strict equivariance with operations defined directly in discretised (pixel) space **not possible** due to structure of sphere.

Instead, consider Fourier approach \rightarrow access to underlying continuous representations.

Spherical CNN

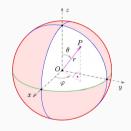
Spherical CNNs constructed by analog of Euclidean CNNs but using convolution on the sphere and with pointwise non-linear activations functions, e.g. ReLU (Cohen et al. 2018; Esteves et al. 2018).



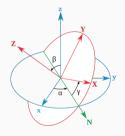
(Alternative, real space constructions have also been developed but do not exhibit rotational equivariance so not considered further; e.g. Boomsma & Frellsen 2017, Jiang et al. 2019, Perraudin et al. 2019.)

Signals on the sphere and rotation group

Consider signals $f \in L^2(\Omega)$ on the sphere $(\Omega = \mathbb{S}^2)$ or rotation group $(\Omega = SO(3))$.



 $\mbox{Sphere } \Omega = \mathbb{S}^2 \mbox{ with coordinates } (\theta,\phi) \in \mathbb{S}^2 \mbox{}$



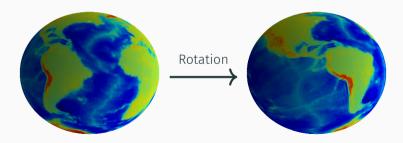
Rotation group $\Omega={\rm SO(3)}$ with coordinates $\rho=(\alpha,\beta,\gamma)\in{\rm SO(3)}$

Rotation of signals

Rotation of signals in spatial domain

A signal $f \in L^2(\Omega)$ on the sphere $(\Omega = \mathbb{S}^2)$ or rotation group $(\Omega = SO(3))$ can be rotated by $\rho \in SO(3)$ by

$$\mathcal{R}_{\rho}f(\omega) = f(\rho^{-1}\omega), \quad \text{for } \omega \in \Omega.$$



Convolution of signals

Convolution of signals in spatial domain

Convolution of two signals $f,\psi\in L^2(\Omega)$ is given by

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

where $d\mu(\omega)$ denotes the Haar measure on Ω and \cdot^* complex conjugation.

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Since no regular discretization of the sphere, compute in Fourier space to ensure equivariant.

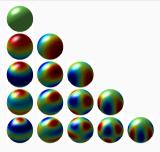
Fourier transforms on the sphere and rotation group

Fourier transform on sphere: spherical harmonic transform

A signal $f \in L^2(\mathbb{S}^2)$ can be decomposed into its harmonic representation by

$$f(\omega) = \sum_{\ell m} \hat{f}_m^{\ell}, Y_m^{\ell}(\omega), \quad \text{ for } \omega \in \mathbb{S}^2.$$

where $\hat{f}_m^\ell = \langle f, Y_m^\ell \rangle$ (also denoted \hat{f}^ℓ).



Spherical harmonics

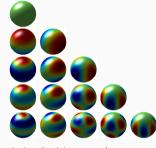
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Spherical harmonics

Fourier transform on rotation group: Wigner transform

A signal $f \in L^2(SO(3))$ can be decomposed into its harmonic representation by

$$f(\rho) = \sum_{\ell m} \frac{2\ell+1}{8\pi} \hat{f}_{mn}^{\ell} D_{mn}^{\ell*}(\rho), \quad \text{for } \rho \in SO(3).$$

where $\hat{f}_{mn}^{\ell} = \langle f, D_{mn}^{\ell*} \rangle$ (also denoted \hat{f}^{ℓ}).

Harmonic computations

Rotation of signals in harmonic domain

The rotation $f\mapsto \mathcal{R}_{\rho}f$ of a signal $f\in L^2(\Omega)$ can be described in harmonic space by

$$\hat{f}^\ell \mapsto D^\ell(\rho)\hat{f}^\ell.$$

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

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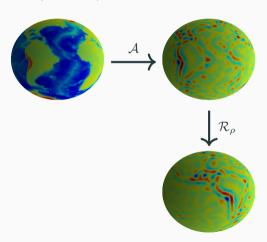
By computing convolutions in harmonic space, discretisation effects are eliminated.

Furthermore, fast harmonic transform algorithms can be leveraged (as we will see later).

Convolution is rotationally equivariant

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

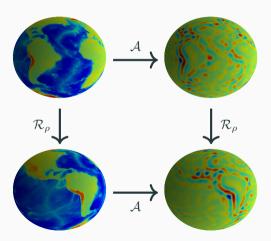
$$((\mathcal{R}_{\rho}f)\star\psi)(\rho')=(\mathcal{R}_{\rho}(f\star\psi))(\rho').$$



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Pointwise activation

While pointwise activations are rotationally equivariant in the continuous limit, they are not equivariant in practice when applied to discretised signals (since regular discretisation of sphere does not exist).

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Equivariance errors

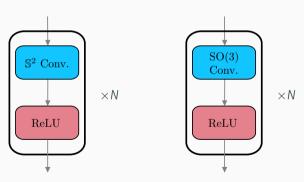
Layer	Mean Relative Error*
\mathbb{S}^2 to \mathbb{S}^2 conv. \mathbb{S}^2 to SO(3) conv. SO(3) to SO(3) conv.	4.4×10^{-7} 5.3×10^{-7} 9.3×10^{-7}
\$2 ReLU SO(3) ReLU	3.4×10^{-1} 3.7×10^{-1}

^{*} Floating point precision.

Spherical CNNs

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

Despite imperfect equivariance, find empirically that such models maintain a reasonable degree of equivariance and generally perform well.



3

Efficient generalised spherical CNNs

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Group theory is the mathematical study of symmetry.



Since we're concerned with rotational symmetry, leverage the machinery from the study of angular momentum in quantum mechanics.

Generalised signals

Consider generalised signal representations and convolutions of Kondor et al. (2018).

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Generalised signals

Consider set of variable length vectors of the form

$$f = {\hat{f}_t^{\ell} \in \mathbb{C}^{2\ell+1} : \ell = 0, .., L-1; \ t = 1, ..., \tau_f^{\ell}},$$

for t-th fragment of degree ℓ . Let \mathcal{F}_L be the space of all such sets of variable length vectors, with type $\tau_f = (\tau_f^0, ..., \tau_f^{L-1})$ unconstrained.

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for t-th fragment of degree ℓ . Let \mathcal{F}_{ℓ} be the space of all such sets of variable length vectors, with type $\tau_f = (\tau_f^0, ..., \tau_f^{\ell-1})$ unconstrained.

Includes signals on the sphere and rotation group as special cases:

- \cdot $au_f^\ell=$ 1 for signals on the sphere
- \cdot $au_f^\ell = 2\ell + 1$ for signals on the rotation group

Rotation of generalised signals

Rotation of generalised signals

The rotation $f\mapsto \mathcal{R}_{\rho}f$ of a signal $f\in \mathcal{F}_{L}$ can be described by

$$\hat{f}_t^\ell \mapsto D^\ell(\rho) \hat{f}_t^\ell.$$

We may therefore extend the usual notion of rotational equivariance to \mathcal{F}_{L} .

Convolution of generalised signals

Convolution of generalised signals

Generalised convolution of a signal $f \in \mathcal{F}_L$ with a filter ψ is given by

$$(f * \psi)_t^{\ell} = \sum_{t'=1}^{\tau_f^{\ell}} \hat{f}_{t'}^{\ell} \, \hat{\psi}_{t,t'}^{\ell},$$

for a filter $\psi = \{\hat{\psi}^{\ell} \in \mathbb{C}^{\tau_f^{\ell} \times \tau_{(f*\psi)}^{\ell}} : \ell = 0, ..., L-1\}.$

Do not force the filter ψ to occupy the same domain as the signal f, allowing control over the type $\tau_{(f*\psi)}$ of transformed signal.

Provides generalised rotationally equivariant linear operator.

Non-linear transforms of generalised signals

How introduce non-linearity in an equivariant manner?

Non-linear transforms of generalised signals

How introduce non-linearity in an equivariant manner?

Consider irreducible representations of the rotation group SO(3) and leverage the decomposability of the tensor product between these representations (Thomas et al. 2018, Kondor et al. 2018).

Representation theory is concerned with the representation of abstract algebraic structures, e.g. groups, by linear transformations.

Consider tensor product of representation spaces (generalisation of outer product).

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Consider tensor product of representation spaces (generalisation of outer product).

 $D^{\ell}: SO(3) \to GL(\mathbb{C}^{2\ell+1})$ is an irreducible group representation of SO(3) on $\mathbb{C}^{2\ell+1}$ (since it is a group homomorphism from SO(3) to the general linear group $GL(\mathbb{C}^{2\ell_1+1})$).

Tensor-product group representation $D^{\ell_1} \otimes D^{\ell_2}$ is defined such that

$$(D^{\ell_1}\otimes D^{\ell_2})(\rho)=D^{\ell_1}(\rho)\otimes D^{\ell_2}(\rho),$$

which is not irreducible.

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Recover irreducible representation through change of basis such that $(D^{\ell_1} \otimes D^{\ell_2})(\rho)$ is block diagonal, where for each ℓ there is a block equal to $D^{\ell}(\rho)$.

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Decomposition of tensor product representations

Change of basis for $\hat{u}^{\ell_1} \otimes \hat{v}^{\ell_2} \in \mathbb{C}^{2\ell_1+1} \otimes \mathbb{C}^{2\ell_2+1}$ to recover an irreducible representation is

$$(\hat{u}^{\ell_1} \otimes \hat{v}^{\ell_2})_m^{\ell} = \sum_{m_1 = -\ell_1}^{\ell_1} \sum_{m_2 = -\ell_2}^{\ell_2} C_{m_1, m_2, m}^{\ell_1, \ell_2, \ell} \, \hat{u}_{m_1}^{\ell_1} \, \hat{v}_{m_2}^{\ell_2},$$

where $C_{m_1,m_2,m}^{\ell_1,\ell_2,\ell} \in \mathbb{C}$ denote Clebsch-Gordan coefficients.

Why is the tensor product decomposition useful?

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

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

is non-linear in f and rotationally equivariant (used shorthand notation for Glebsch-Gordan decomposition).

Non-linearly transforming generalised signals

Simply compute $(C^{\ell_1,\ell_2,\ell})^{\top}(\hat{f}^{\ell_1}\otimes\hat{f}^{\ell_2})$ for all pairs of input fragments and collect them into a generalised signal (Kondor et al. 2018).

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Tensor-product based activation of generalised signals

A generalised signal $f \in \mathcal{F}_L$ may be equivariantly and non-linearly transformed by an operator $\mathcal{N}_{\otimes} : \mathcal{F}_L \to \mathcal{F}_L$ defined as

$$\mathcal{N}_{\otimes}(f) = \{ (C^{\ell_1,\ell_2,\ell})^{\top} (\hat{f}_{t_1}^{\ell_1} \otimes \hat{f}_{t_2}^{\ell_2}) : \ell = 0, ..., L-1; \ (\ell_1,\ell_2) \in \mathbb{P}_L^{\ell}; \ t_1 = 0, ..., \tau_f^{\ell_1}; \ t_2 = 0, ..., \tau_f^{\ell_2} \},$$

where for each degree the set

$$\mathbb{P}_L^{\ell} = \{(\ell_1, \ell_2) \in \{0, ..., L-1\}^2 : |\ell_1 - \ell_2| \le \ell \le \ell_1 + \ell_2\}$$

is defined in order to avoid the computation of trivially equivariant all-zero fragments.

Non-linearly transforming generalised signals

Equivariance errors

Layer	Mean Relative Error*
Tensor-product activation $ ightarrow$ Generalized conv.	5.0×10^{-7}
\mathbb{S}^2 ReLU	3.4×10^{-1}
SO(3) ReLU	3.7×10^{-1}

^{*} Floating point precision.

Consider the s-th layer of a generalised spherical CNN to take the form of a triple (Cobb et al. 2020)

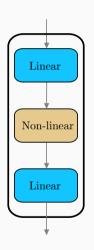
$$\mathcal{A}^{(s)} = (\mathcal{L}_1, \mathcal{N}, \mathcal{L}_2),$$

such that

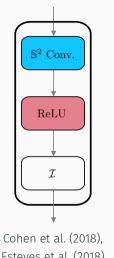
$$\mathcal{A}^{(s)}(f^{(s-1)}) = \mathcal{L}_2(\mathcal{N}(\mathcal{L}_1(f^{(s-1)}))),$$

where

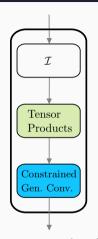
- $\mathcal{L}_1, \mathcal{L}_2 : \mathcal{F}_L o \mathcal{F}_L$ are linear operators,
- $\cdot \mathcal{N}: \mathcal{F}_L \to \mathcal{F}_L$ is a non-linear activation operator.



· Encompass other frameworks as special cases.

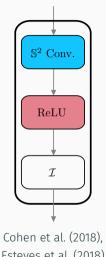


Esteves et al. (2018)

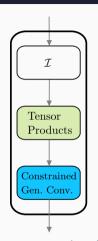


Kondor et al. (2018)

- · Encompass other frameworks as special cases.
- · General framework supports hybrids models.



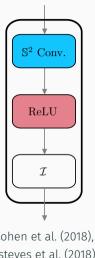
Esteves et al. (2018)



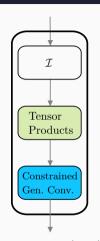
Kondor et al. (2018)

- · Encompass other frameworks as special cases.
- · General framework supports hybrids models.

Construct more efficient lavers...



Cohen et al. (2018), Esteves et al. (2018)



Kondor et al. (2018)

Computational cost of strictly equivariant layers

For strictly equivariant layers the non-linear transformation is **prohibitively costly**.

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Computing
$$g = \mathcal{N}_{\otimes}(f)$$
 is
$$\mathcal{O}(\mathit{C}^{2}\mathit{L}^{5}),$$

where C is representational capacity and L spatial resolution (bandlimit):

- $\mathcal{O}(C^2L^3)$ fragments,
- cost of computing each fragment is $\mathcal{O}(L^2)$.

Channel-wise structure

Let network activations take form $(f_1,...,f_K) \in \mathcal{F}_L^K$ where $f_i \in \mathcal{F}_L$ all same type τ_f .

Apply \mathcal{N}_{\otimes} to each of K channels separately \Rightarrow cost is reduced by K times relative to single channel with the same total number of fragments.



Prior approach to applying a tensor-product based non-linear operator



Ours (Cobb et al. 2020)

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Prior approach to applying a tensor-product based non-linear operator

Ours (Cobb et al. 2020)

Using C = K to control representational capacity, reduce $\mathcal{O}(C^2)$ to $\mathcal{O}(C)$.

Constrained generalised convolution

Under new multi-channel structure we decompose the generalized convolution into three separate linear operators:

- 1. **Uniform convolution**: linear projection uniformly across channels to project down onto the desired type (interpreted as learned extension of \mathcal{N}_{\otimes} to undo the drastic expansion of representation space).
- 2. **Channel-wise convolution**: linear combinations of the fragments within each channel.
- 3. Cross-channel convolution: linear combinations to learn new features.

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Computational and parameter efficiency dramatically improved.

Non-linear operators must perform **degree mixing** (equivariant linear operators cannot mix information corresponding to different degrees).

But, it is not necessary to compute all possible tensor-product based fragments.

Recall, degree mixing set \mathbb{P}_{L}^{ℓ} :

$$\mathbb{P}^{\ell}_{L} = \{(\ell_{1},\ell_{2}) \in \{0,...,L-1\}^{2} : |\ell_{1}-\ell_{2}| \leq \ell \leq \ell_{1}+\ell_{2}\}.$$

Consider subsets of \mathbb{P}^{ℓ}_{L} that scale better than $\mathcal{O}(L^{2})$.

Consider the graph $G_L^{\ell} = (\mathbb{N}_L, \mathbb{P}_L^{\ell})$ with nodes $\mathbb{N}_L = \{0, ..., L-1\}$ and edges \mathbb{P}_L^{ℓ} .

- Some notion of relationship between ℓ_1 and ℓ_2 is captured if there exists a path between the two nodes in G_L^{ℓ} .
- Select smallest subgraph such that all relationships are preserved ⇒ minimum spanning tree (MST). Weight edges by computational cost to minimise overall cost.

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Two optimised degree mixing sets:

1. **MST**: reduce resolution complexity from $\mathcal{O}(L^5)$ to $\mathcal{O}(L^4)$, whilst preserving performance.

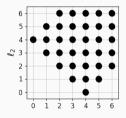
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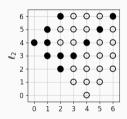
Two optimised degree mixing sets:

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- 2. Reduced MST (logarithmic subsampling): reduce to $\mathcal{O}(L^3 \log L)$, with small but insignificant performance degradation that is offset by computational saving.

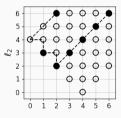
Visualization of the degree mixing set \mathbb{P}_{l}^{ℓ} for L=7 and $\ell=4$.



Full \mathbb{P}^{ℓ}_{L} set of size $\mathcal{O}(L^{2})$



MST subset of size $\mathcal{O}(L)$



RMST subset of size $\mathcal{O}(\log L)$

Efficient sampling theory and fast harmonic transforms

Adopt **efficient sampling theory** and **fast algorithms** to compute harmonic transforms on the sphere and rotation group.

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Novel sampling theorem on sphere (McEwen & Wiaux 2011)



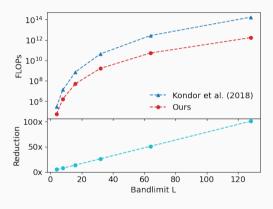
SSHT: Spin spherical harmonic transforms
www.spinsht.org

Novel sampling theorem on rotation group (McEwen et al. 2015)

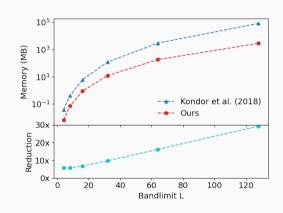


SO3: Fast Wigner transforms on rotation group www.sothree.org

Computational cost and memory requirements



Computational cost

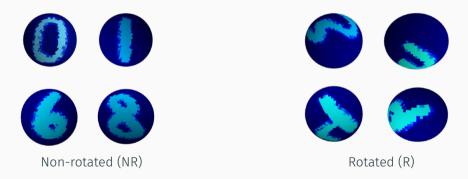


Memory requirements

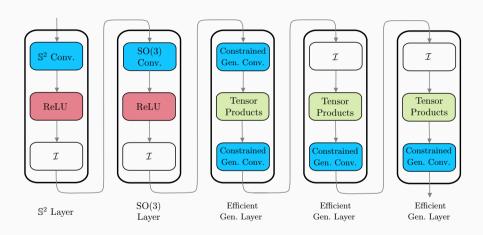


Spherical MNIST: problem

Canonical benchmark problem of classifying MNIST digits projects onto the sphere.



Spherical MNIST: architecture



Test accuracy for spherical MNIST digits classification problem

	NR/NR	R/R	NR/R	Params
Planar CNN Cohen et al. 2018 Kondor et al. 2018 Esteves et al. 2018	99.32 95.59 96.40 99.37			58k 58k 286k 58k
Ours (MST) Ours (RMST)	99.35 99.29			58k 57k

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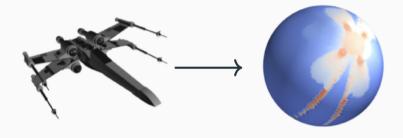
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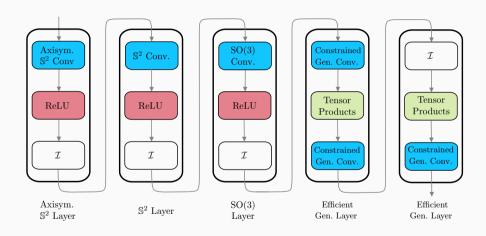
3D shape classification: problem

Classify 3D meshes and perform shape retrieval.



[Image credit: Esteves et al. 2018]

3D shape classification: architecture



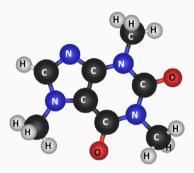
3D shape classification: results

SHREC'17 object retrieval competition metrics (perturbed micro-all)

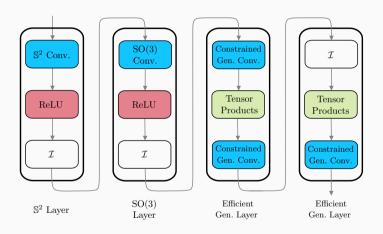
	P@N	R@N	F1@N	mAP	NDCG	Params
Kondor et al. 2018	0.707	0.722	0.701	0.683	0.756	>1M
Cohen et al. 2018	0.701	0.711	0.699	0.676	0.756	1.4M
Esteves et al. 2018	0.717	0.737	-	0.685	-	500k
Ours	0.719	0.710	0.708	0.679	0.758	250k

Atomization energy prediction: problem

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



Atomization energy prediction: architecture



Atomization energy prediction: results

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

RMS	Params
5.96	-
8.47	1.4M
7.97	>1.1M
3.16	337k
3.46	335k
	5.96 8.47 7.97 3.16

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- Reviewed **spherical CNNs constructions**, with a focus on rotational equivariance (Cohen et al. 2018, Esteves et al. 2018, Kondor et al. 2018).

Summary '

- Importance of encoding **equivariance to symmetry transforms** in order to capture fundamental physical understanding of generative process.
- Need for geometric deep learning techniques constructed natively on manifolds, such as the sphere.
- Reviewed **spherical CNNs constructions**, with a focus on rotational equivariance (Cohen et al. 2018, Esteves et al. 2018, Kondor et al. 2018).
- Efficient generalised spherical CNNs (Cobb et al. 2020; arXiv:2010.11661)
 - General framework that encompasses others as special cases.
 - $\boldsymbol{\cdot}$ Supports hybrid models to leverage strength of alternatives alongside each other.
 - · New efficient layers to be used as primary building blocks.
 - · State-of-the-art performance, both in terms of accuracy and parameter efficiency.



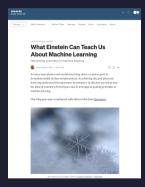
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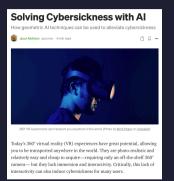
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