Deep learning on the celestial sphere

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17 December 2020

Research interests

Physics and 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
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Hard!

Deep Learning

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Hard!

Physics and deep learning

Physics $\longleftrightarrow$ Deep Learning

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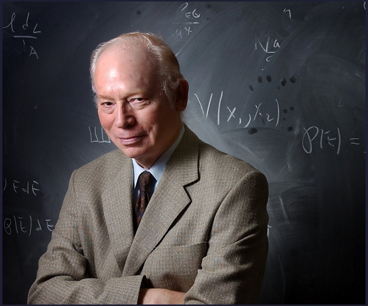
As we will see, this key factor driving the deep learning revolution.

Symmetry in deep learning



"Symmetry: key to nature's secrets."

— Steven Weinberg

Noether's theorem

Noether's theorem

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

Symmetries at the heart of physics:

- **Translational** symmetry ⇔ conservation of **momentum**
- **Rotational** symmetry ⇔ 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.

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).

Geometric deep learning on the celestial sphere

Data on the sphere is prevalent in astronomy and beyond

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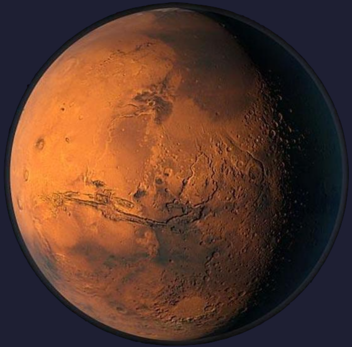

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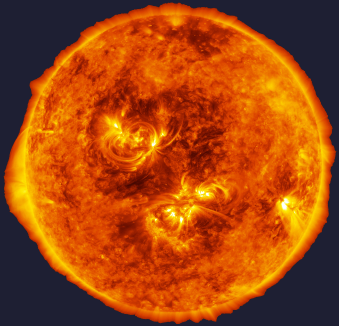

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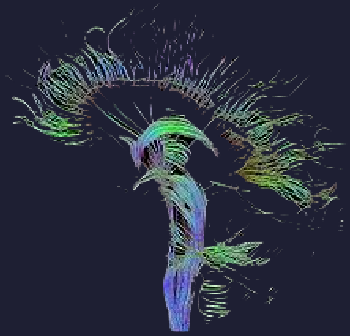

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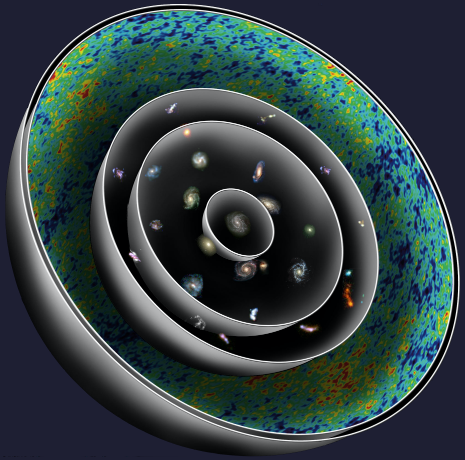

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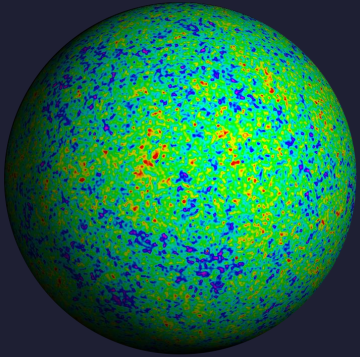


Generalised spherical CNNs

Efficient generalised spherical CNNs developed by McEwen and colleagues (Cobb et al. 2020; arXiv:2010.11661).

Consider the s-th layer of a generalised spherical CNN to take the form of a triple

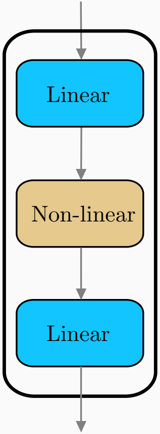
$$\mathcal{A}^{(s)} = (\mathcal{L}_1, \mathcal{N}, \mathcal{L}_2),$$

such that

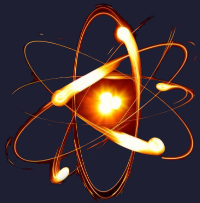
$$\mathcal{A}^{(s)}(f^{(s-1)}) = \mathcal{L}_2(\mathcal{N}(\mathcal{L}_1(f^{(s-1)}))),$$

where

- $\mathcal{L}_1, \mathcal{L}_2 : \mathcal{F}_L \rightarrow \mathcal{F}_L$ are linear operators (e.g. convolutions on $\mathbb{S}^2$, SO(3); generalised convolutions)
- $\mathcal{N} : \mathcal{F}_L \rightarrow \mathcal{F}_L$ is a non-linear activation operator (e.g. ReLUs, harmonic tensor product activations).



Group theoretic approach to construction
since group theory is the mathematical study of symmetry.

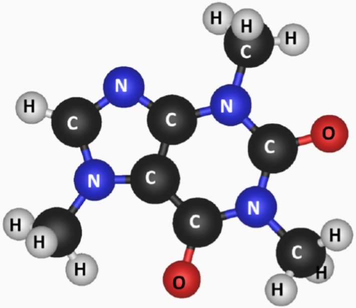


Since we’re concerned with rotational symmetry, leverage the machinery from the study of angular momentum in quantum mechanics.

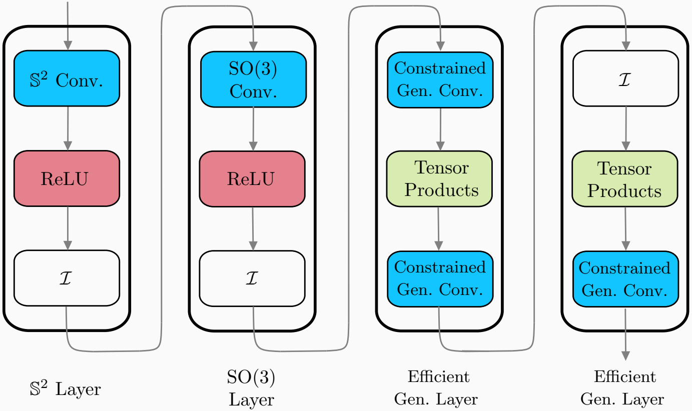
Illustration

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
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**