Deep Learning for the Sciences

Escaping the black box

This is deep learning

> Solve anything, with big data, big models, and big compute

“Normal” users dispose of none of these.

Could DL be conceptualized differently?

Yes!

- Let domain-/task-derived principles guide choice of architecture (*Geometric Deep Learning*)
- Make use of pre-existing, subject-specific *domain knowledge*

Geometric Deep Learning (GDL)

Neural network design is subject to *constraints* derived from the domain and the task:

- *Symmetries* correspond to conserved quantities
  - Invariances
  - Equivariances
- Scale separation (coarse-graining)

High-level intro: Beyond alchemy: A first look at geometric deep learning

GDL: Why it matters

- Standard DL algorithms/architectures do not satisfy constraints inherent in many tasks. E.g., convolution is not rotation-equivariant.
- Practical GDL research builds *tools* to handle these tasks.
- Such tasks are everywhere:
  - Medicine (MRI …)
  - Earth sciences (the Earth is not flat …)
  - Computer vision (need deformation, and other non-linear transformations)

Field-specific domain knowledge

- Ranges from foundational (Newton’s second law) to very concrete (pressure increases with depth).
- Commonly incorporated by
  - Custom loss functions / regularizations
  - Custom layers / architectures
  - Stochasticity
  - Custom operators acting in the spectral domain

Field-specific domain knowledge: Why it matters

[Answering the rhetorical question anyway.]

- Reliability
- Explainability
- Trust
- Why waste resources to learn what we know?

Example 1: Geometric Deep Learning

TBD

Example 1: Field-specific domain knowledge

TBD