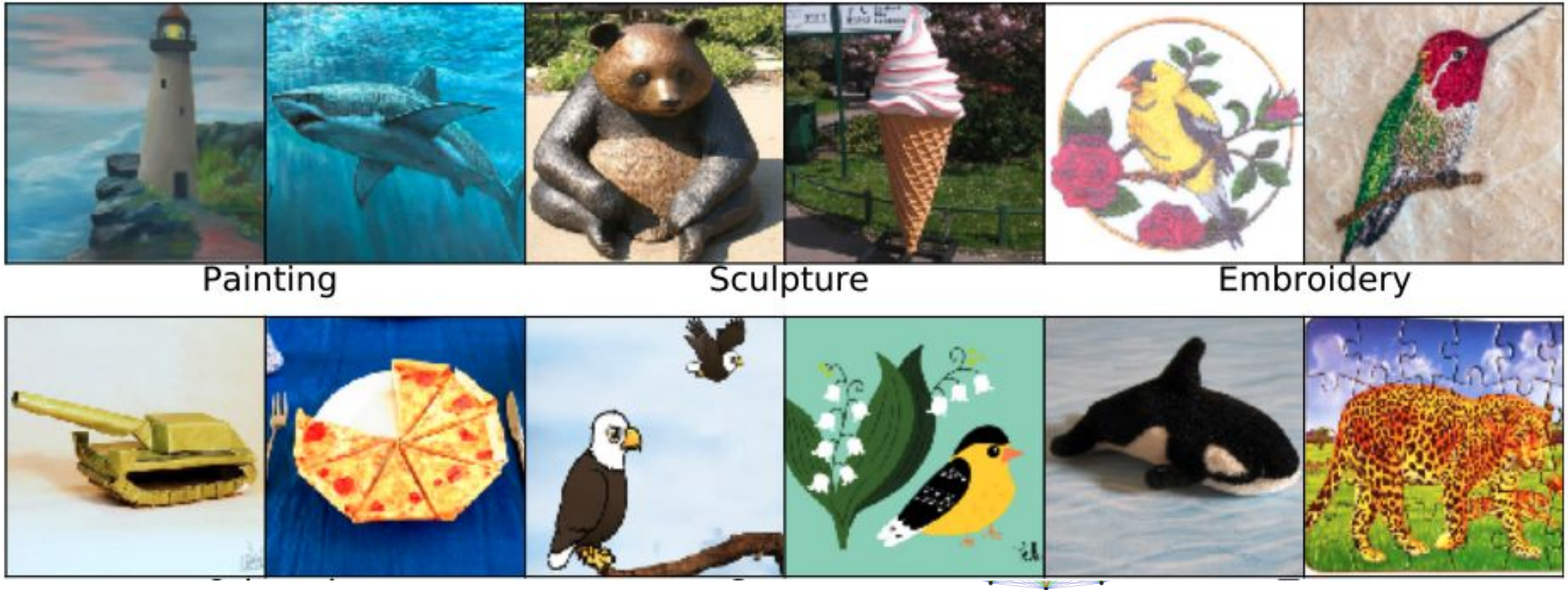
Geometric structures in machine learning

MLRG summer, 2021

Geometric structures exist everywhere

Non-Euclidean Observations

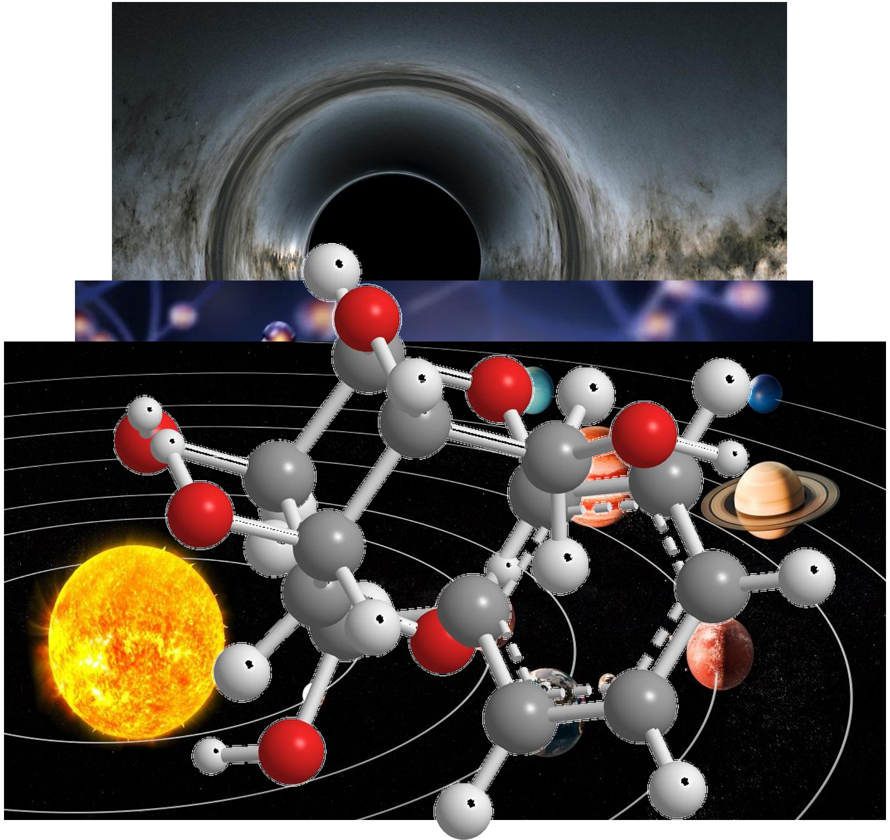
- Images



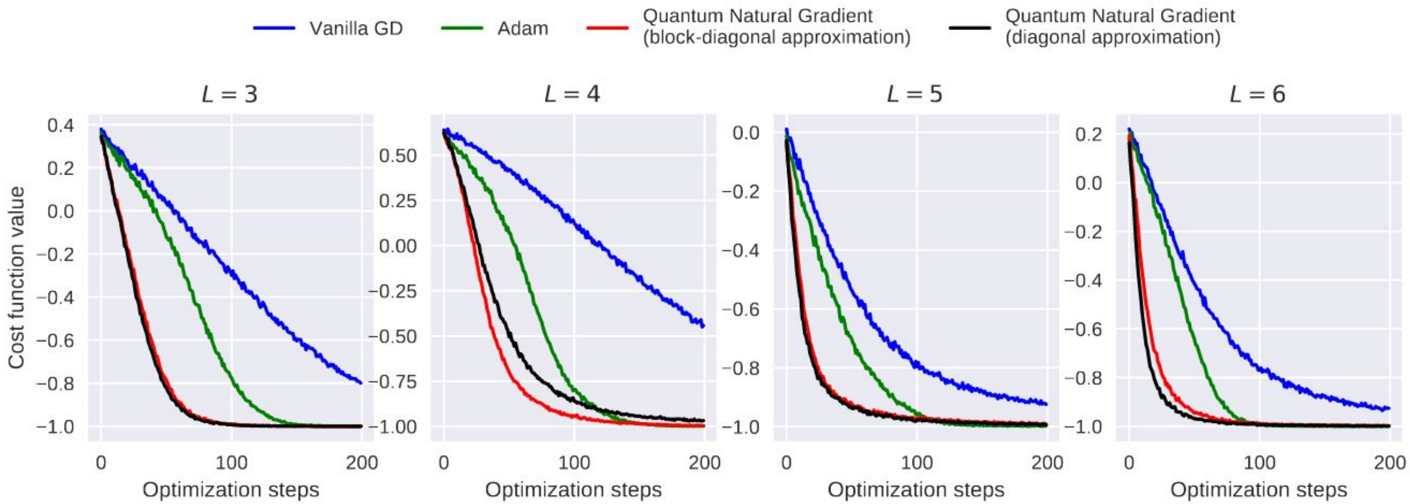
Geometric structures exist everywhere

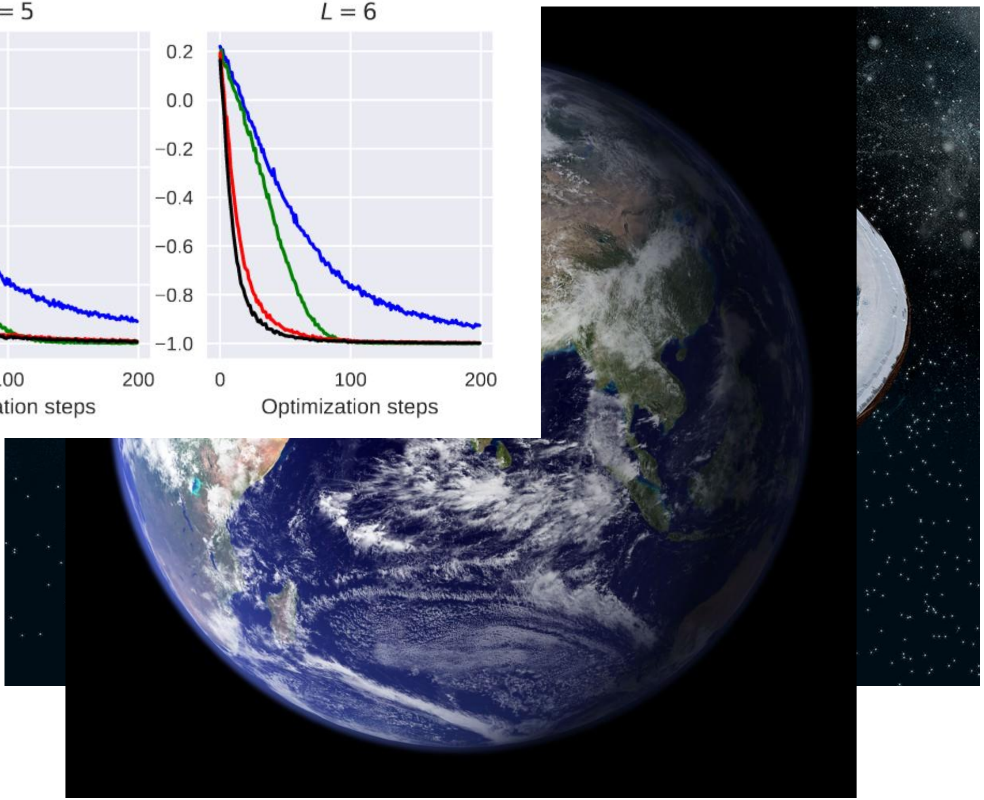
Natural Science

- Black holes (general relativity)
- Elementary particles (particle physics)
- Planetary motion (classical mechanics)
- Organic compounds (chemistry)



Why use Geometric structures?

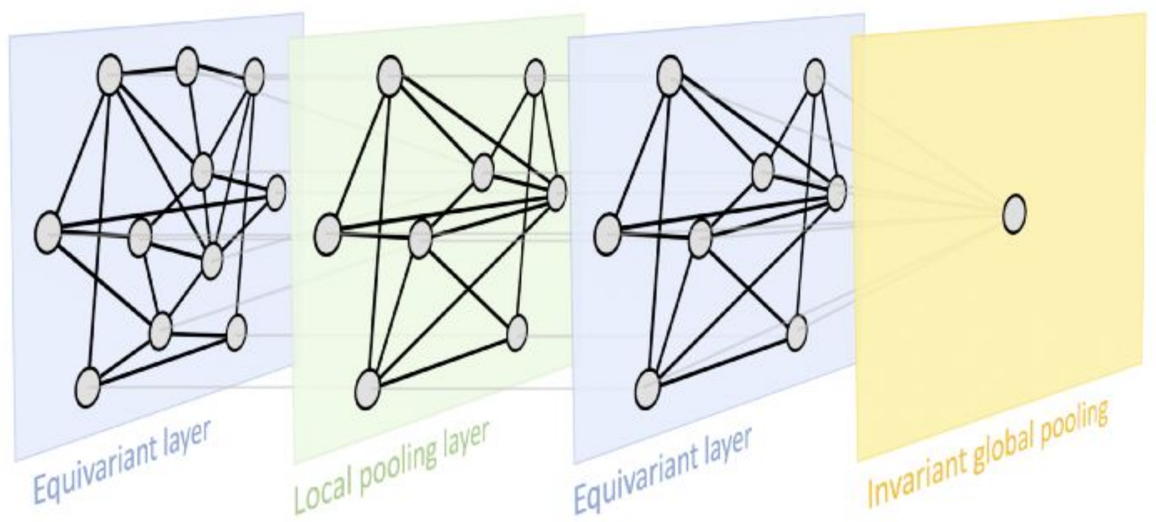




Geometric methods are more efficient

Why Geometric structures?

Geometric priors are encoded in many useful NNs (e.g., CNN, RNN, GNN)



Challenges

Difficulties of exploiting geometric structures

- Unawareness (less fashionable)

- non-standard math for ML (time investment)

- Few practical implementations (examples in low-dimensions)

The goal of this MLRG

Learn some basics of geometric structures and how to exploit them in ML

Basics:

Optimization on manifolds (sub-topic 1)

Information geometry (sub-topic 2)

Geometric deep learning (sub-topic 3)

8 meetings (2 meetings for the basics, 6 meetings for related papers)

Pick at least one paper from each subtopic

Basics: (I will cover the basics of manifolds and information geometry)

Geodesic Convex Optimization

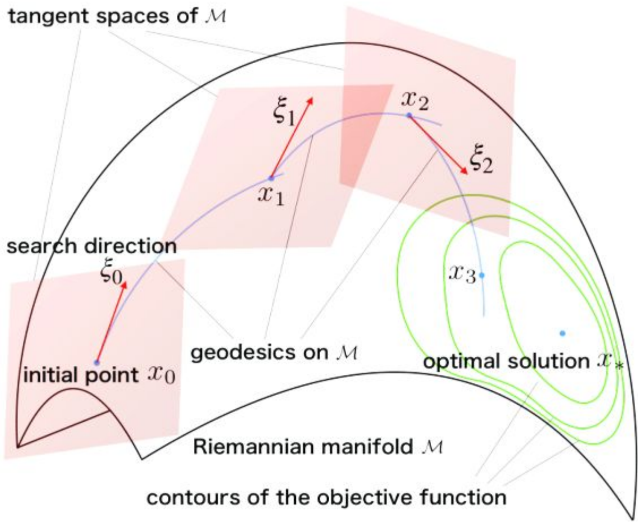
https://arxiv.org/abs/1806.06373

An elementary introduction to information geometry

https://arxiv.org/abs/1808.08271

Geometric Deep Learning: Grids, Groups, Graphs, Geodesics, and Gauges,
https://arxiv.org/abs/2104.13478,
https://www.youtube.com/watch?v=w6Pw4MOzMuo (**Presenter ?**)

Picking Presenters



Related papers

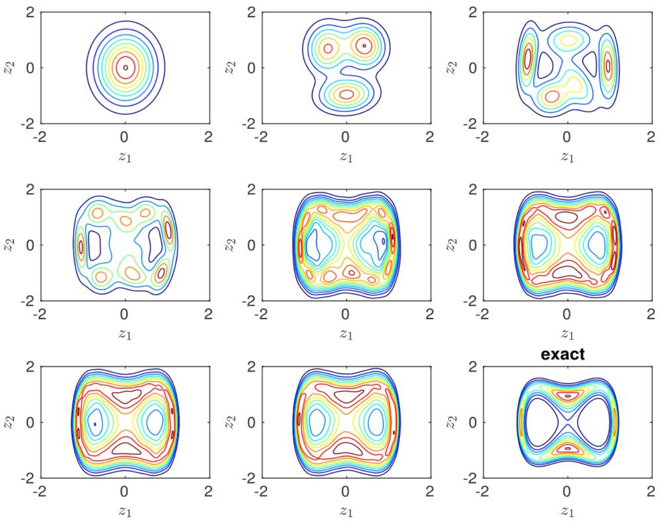
Sub-topic 1

Manifold optimization

[1] Momentum Improves Optimization on Riemannian Manifolds, https://arxiv.org/abs/2002.04144

[2] Projection-free nonconvex stochastic optimization on Riemannian manifolds, https://arxiv.org/abs/1910.04194

Picking Presenters



Sub-topic 2

Information geometry

[1] Natural Wake-Sleep Algorithm,

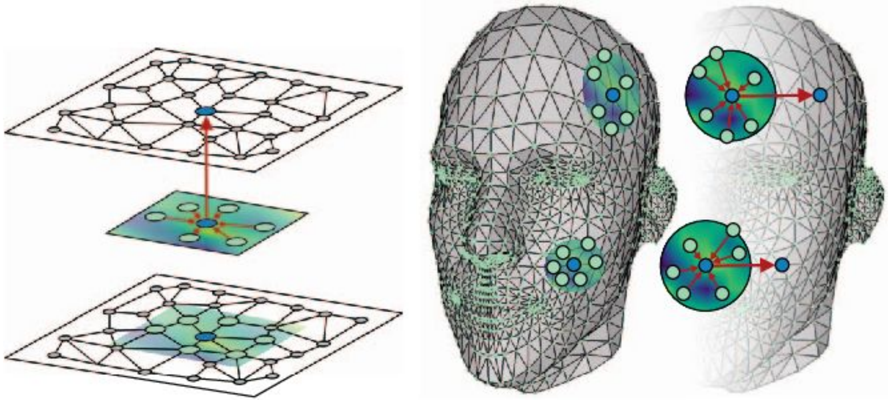
https://arxiv.org/abs/2008.06687

[2] Quantum Natural Gradient,

https://arxiv.org/abs/1909.02108

[3] NGBoost: Natural Gradient Boosting for Probabilistic Prediction,
https://arxiv.org/abs/1910.03225

Picking Presenters



Sub-topic 3

Geometric deep learning

[1] Group Equivariant Convolutional Networks,

https://arxiv.org/abs/1602.07576

[2] Modeling polypharmacy side effects with graph convolutional networks, https://arxiv.org/abs/1802.00543

[3] Predicting anticancer hyperfoods with graph convolutional networks, https://pubmed.ncbi.nlm.nih.gov/34099048/

[4] Generalizing Convolutional Neural Networks for Equivariance to Lie Groups on Arbitrary Continuous Data, https://arxiv.org/abs/2002.12880

[5] LieTransformer: Equivariant Self-Attention for Lie Groups, https://arxiv.org/abs/2012.10885

Schedule

July 7	Introduction
July 14	Basics of geometric DL (graph, group) [Nick]
July 21	Basics of manifolds [Wu]
July 28	Optimization [Fred]
August 4	Wake-Sleep [Christian]
August 11	Something (Momentum or Quantum) [Victor]
August 18	NGBoost (Wilder)
August 25	GCNNs (Emmanuel)

September 1 : AntiCancer [Betty]