Geometric Deep Learning Self-Study Group

Session 1

August 11, 2025

Aaron Margolis
https://armargolis.github.io/

Why Geometric Deep Learning?

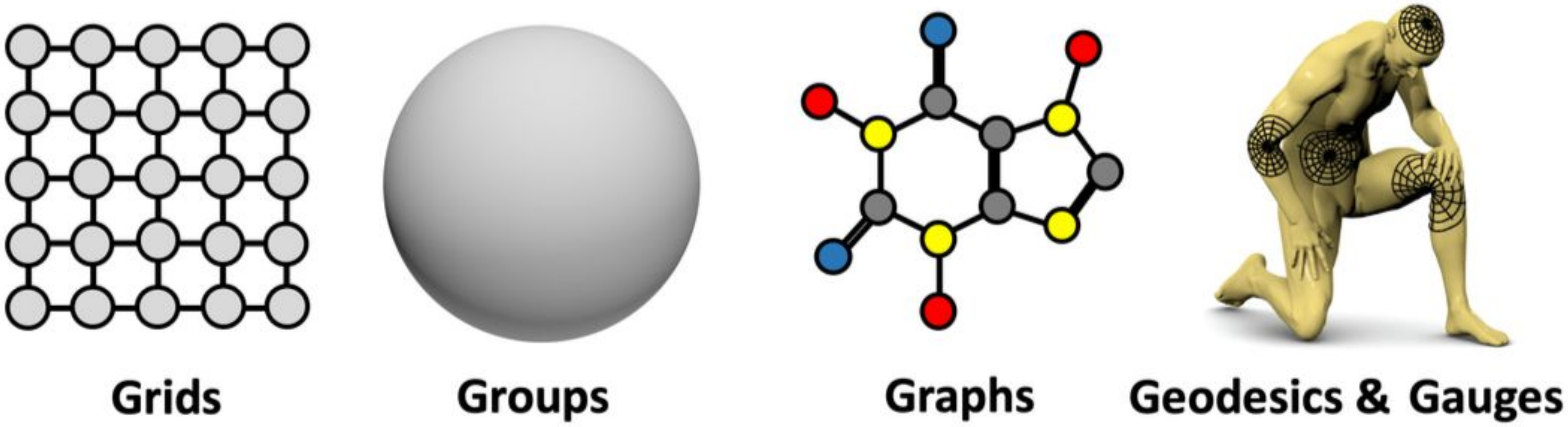
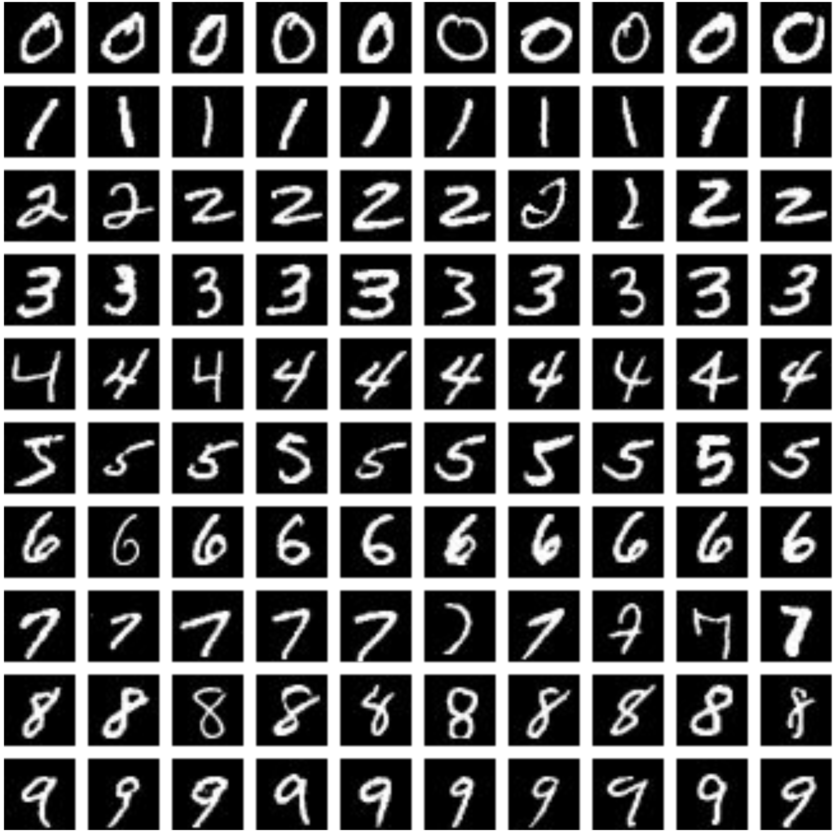
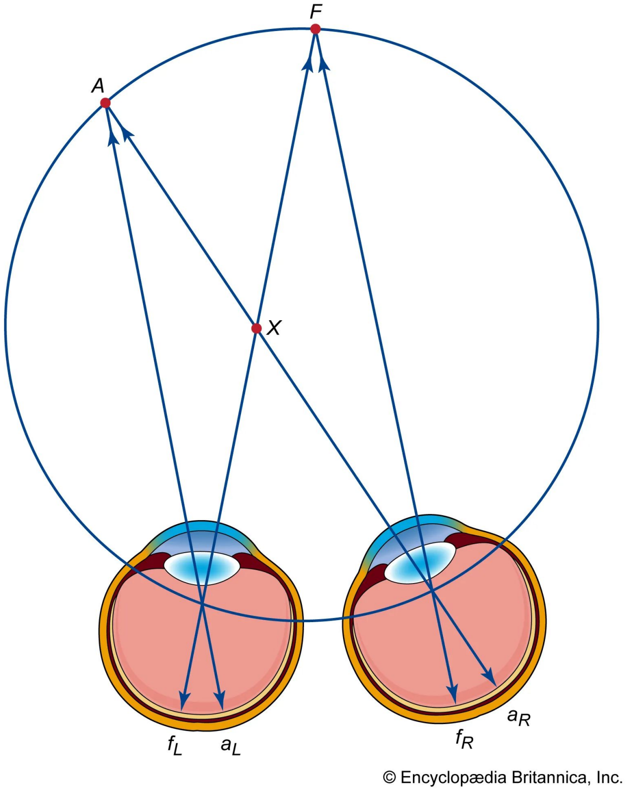


Figure 9: The 5G of Geometric Deep Learning: grids, groups & homogeneous spaces with global symmetry, graphs, geodesics & metrics on manifolds, and gauges (frames for tangent or feature spaces).

Computer Vision uses grids



Natural Vision uses Spheres



GDL: Mathematicians vs Practitioners

[Submitted on 7 Jul 2016 (v1), last revised 11 Jul 2016 (this version, v2)]

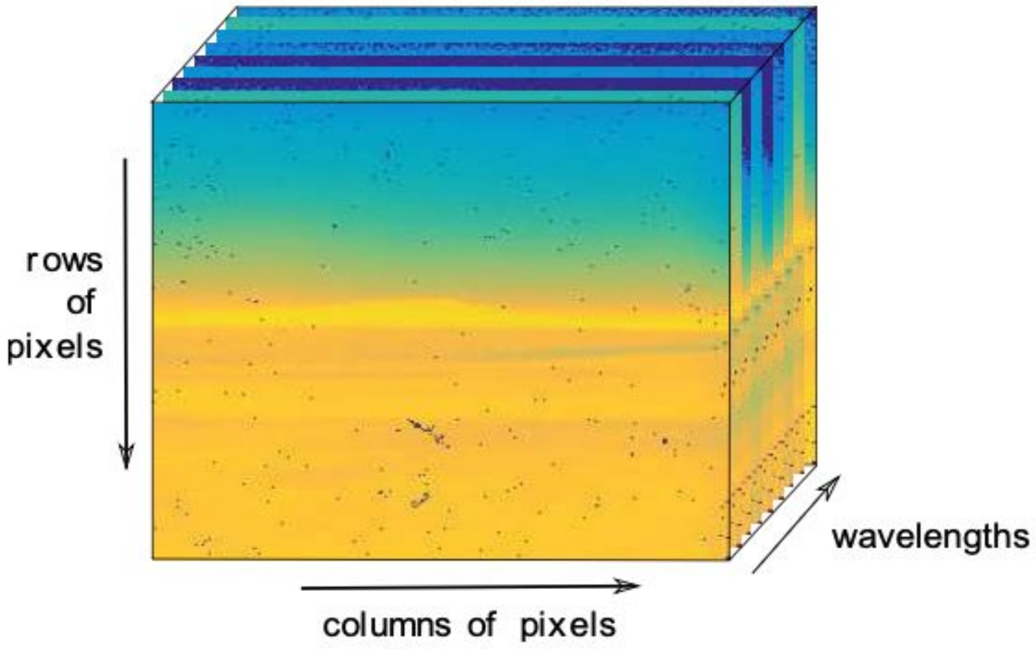
Persistent Homology on Grassmann Manifolds for Analysis of Hyperspectral Movies

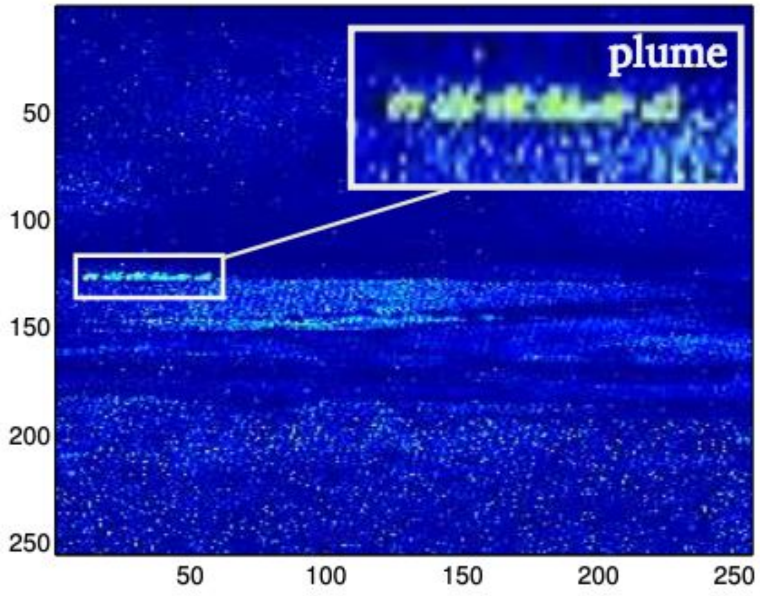
Sofya Chepushtanova, Michael Kirby, Chris Peterson, Lori Ziegelmeier

The existence of characteristic structure, or shape, in complex data sets has been recognized as increasingly important for mathematical data analysis. This realization has motivated the development of new tools such as persistent homology for exploring topological invariants, or features, in large data sets. In this paper we apply persistent homology to the characterization of gas plumes in time dependent sequences of hyperspectral cubes, i.e. the analysis of 4-way arrays. We investigate hyperspectral movies of Long-Wavelength Infrared data monitoring an experimental release of chemical simulant into the air. Our approach models regions of interest within the hyperspectral data cubes as points on the real Grassmann manifold $G(k,n)$ (whose points parameterize the k-dimensional subspaces of $\mathbb{R}^n$), contrasting our approach with the more standard framework in Euclidean space…

https://arxiv.org/abs/1607.02196

Finding the Data of Interest in a 4D Dataset





References and Resources

Main Reference:
Geometric Deep Learning: Grids, Groups, Graphs, Geodesics, and Gauges
Michael M. Bronstein, Joan Bruna, Taco Cohen, Petar Veličković
https://geometricdeeplearning.com/book/ We'll use the chapters rather than the big pdf
For September 1: Introduction https://geometricdeeplearning.com/book/introduction.html
Lecture: "ICLR 2021 Keynote: GDL: The Erlangen Programme of ML by M Bronstein"
https://www.youtube.com/watch?v=w6Pw4MOzMuo
For September 22: Graphs https://geometricdeeplearning.com/book/graphs.html
Lecture: "Deep learning on graphs: successes, challenges | GNN | M Bronstein"
https://www.youtube.com/watch?v=PLGcx65MhCc

Additional References:
Mathematical Foundations of Geometric Deep Learning by Borde and Bronstein
https://www.arxiv.org/abs/2508.02723
Introduction to Geometric Deep Learning by Patrick Nicolas
https://patricknicolas.substack.com/p/introduction-to-geometric-deep-learning

Further Reading:
Valence Labs
https://portal.valencelabs.com

Graph Learning on Wednesdays
https://sites.google.com/view/graph-learning-on-weds

Session Outline

Felix Klein vs. Dmitri Mendeleev
The 5Gs: Grids, Groups, Graphs, Geodesics and Gauges

Group Discussion

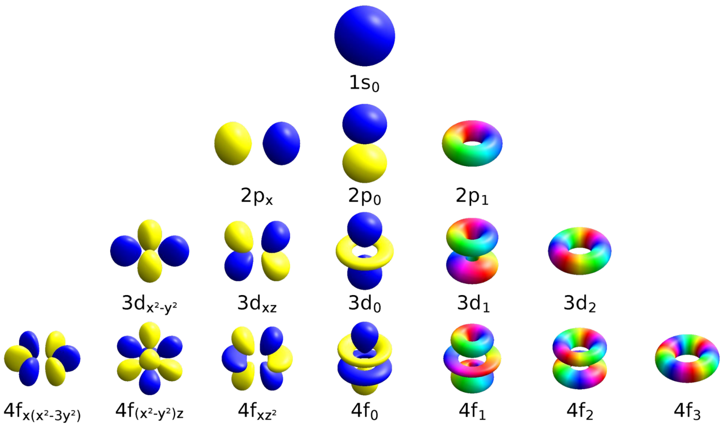
Geometric Deep Learning on Microscopy
Q&A

Periodic Table vs. Underlying Structure

Mendeleev's Periodic Table (1869)

I	II	III	IV	V	VI	VII	VIII		
H 1.01									
Li 6.94	Be 9.01	B 10.8	C 12.0	N 14.0	O 16.0	F 19.0			
Na 23.0	Mg 24.3	Al 27.0	Si 28.1	P 31.0	S 32.1	Cl 35.5			
K 39.1	Ca 40.1		Ti 47.9	V 50.9	Cr 52.0	Mn 54.9	Fe 55.9	Co 58.9	Ni 58.7
Cu 63.5	Zn 65.4			As 74.9	Se 79.0	Br 79.9			
Rb 85.5	Sr 87.6	Y 88.9	Zr 91.2	Nb 92.9	Mo 95.9		Ru 101	Rh 103	Pd 106
Ag 108	Cd 112	In 115	Sn 119	Sb 122	Te 128	I 127			
Ce 133	Ba 137	La 139		Ta 181	W 184		Os 194	Ir 192	Pt 195
Au 197	Hg 201	Ti 204	Pb 207	Bi 209					
			Th 232		U 238				

Atomic orbitals
m-eigenstates and
superpositions



Periodic Table of Machine Learning

Supervisory Signal

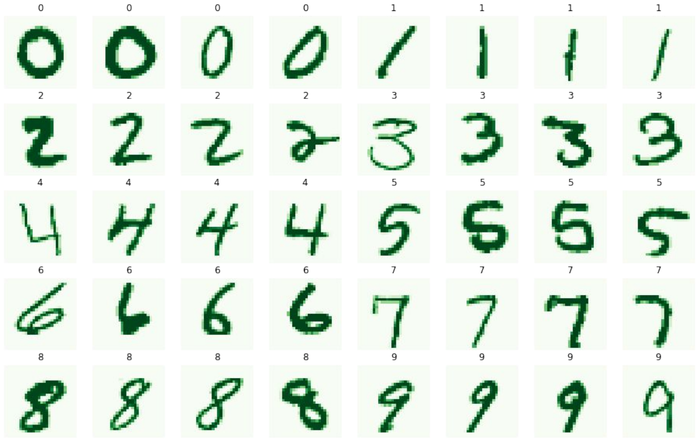
Learned Representation	Gaussian	Student-T	Identity	Graph Kernel Weights	Uniform over K-Neighbors	Uniform over Positive Pairs	Cross-Modal Pairs	Uniform over Classes	Data-Label Pairs
Gaussian	SNE [Hinton 2002] X-Sample CL [Sobal 2025]	Dual t-SNE		SNE Graph Embeddings	SNE with Uniform Affinities LGSimCLR [El Banani 2023]	InfoNCE [Bachman 2019] SimCLR [Chen 2020] MoCoV3 [Chen 2021]	CLIP [Radford 2021] CMC [Tian 2020]	SupCon [Khosla 2020]	Cross Entropy [Good 1963]
Gaussian $\sigma \to \infty$			PCA [Pearson 1901]			VI-Reg [Bardes 2021]	Average Margin CLIP	Average Margin SupCon	
Gaussian $\sigma \to 0$						Triplet Loss [Schultz 2004]	Triplet CLIP	Triplet SupCon	Error rate
Student-T	t-SNE [Van der Maaten 2008]	Doubly t-SNE		t-SNE Graph Embedding	t-SNE with Uniform Affinities	t-SimCNE [Böhm 2023] t-SimCLR [Hu 2023]	t-CLIP	t-SupCon	Harmonic Loss [Baek 2025]
Cluster Probabilities	K-Means [Macqueen 1967]	t K-Means		Normalized Cuts [Shi 2000]	DCD [Yang 2012]	InfoNCE Clustering [Ours]		Supervised Clustering	

Dimensionality Reduction · Cluster Learning · Unimodal SSL · Multimodal SSL · Supervised Learning · Interpretation of Gaps

https://openreview.net/forum?id=WfaQrKCr4X

MNIST: Convolutional Neural Networks (aka Grid Learning)

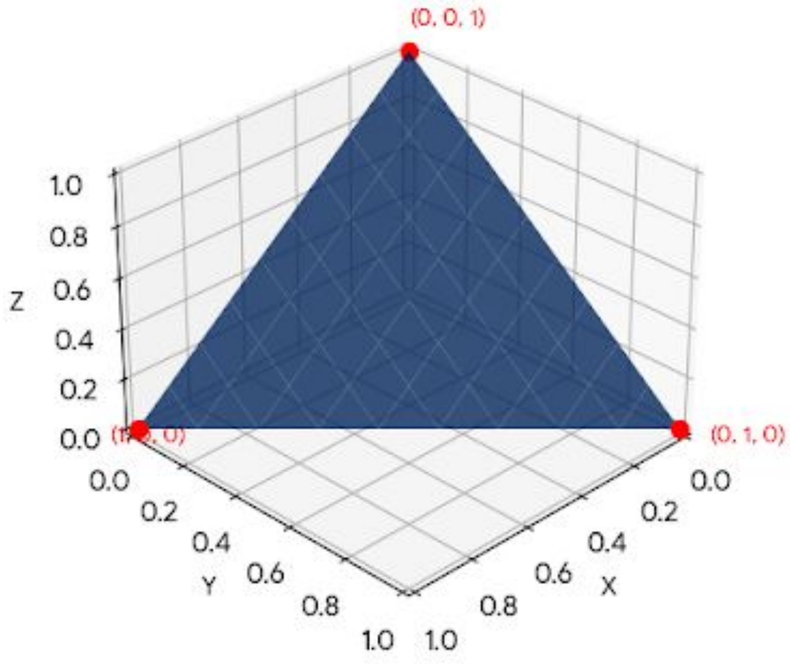
Input images (28 by 28)

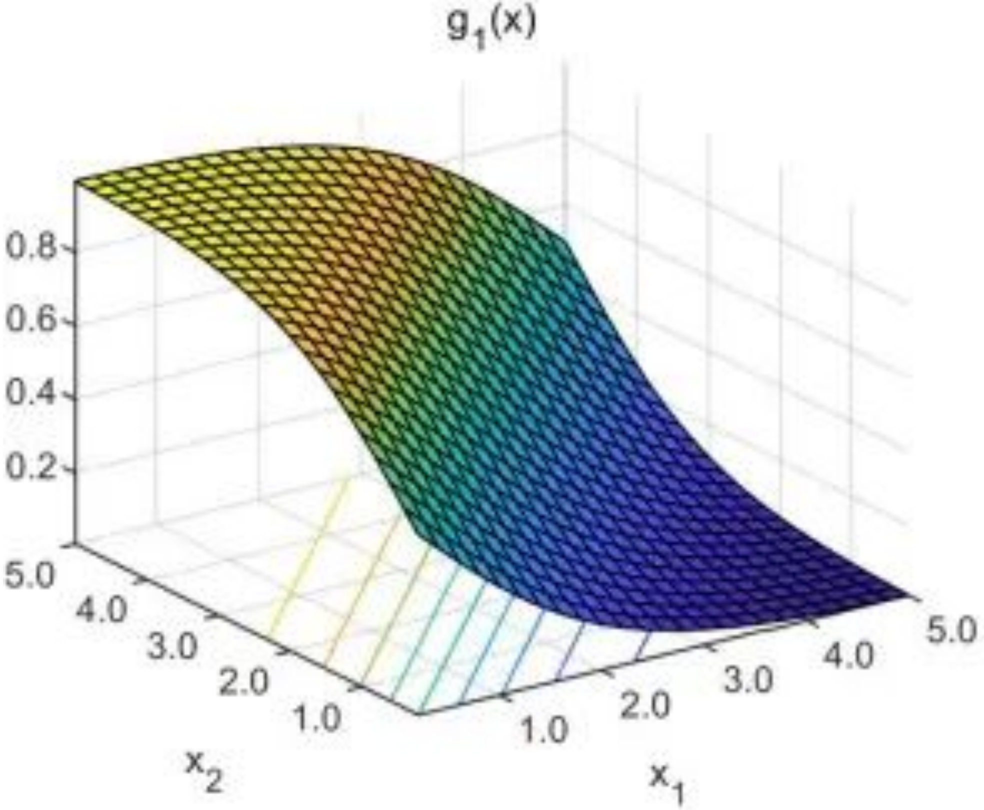


https://www.kaggle.com/code/gpreda/simple-introduction-to-cnn-for-mnist-99-37

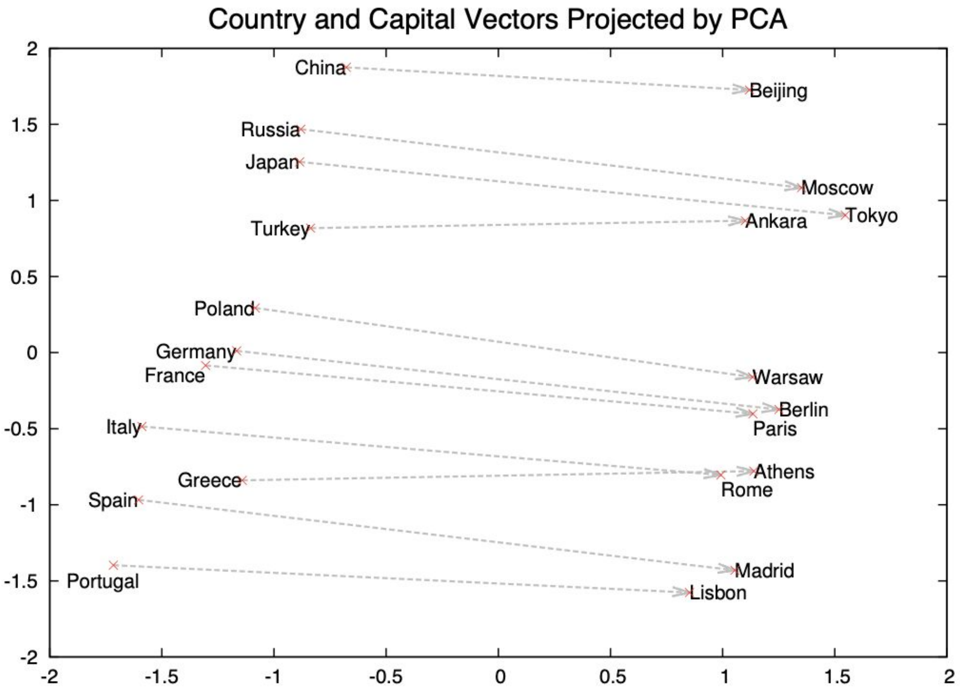
```
_________________________________________________________________
Layer (type)                 Output Shape              Param #
=================================================================
conv2d (Conv2D)              (None, 28, 28, 32)        320
batch_normalization (BatchNo (None, 28, 28, 32)        128
conv2d_1 (Conv2D)            (None, 26, 26, 32)        9248
batch_normalization_1 (Batch (None, 26, 26, 32)        128
conv2d_2 (Conv2D)            (None, 13, 13, 32)        25632
max_pooling2d (MaxPooling2D) (None, 6, 6, 32)          0
batch_normalization_2 (Batch (None, 6, 6, 32)          128
dropout (Dropout)            (None, 6, 6, 32)          0
conv2d_3 (Conv2D)            (None, 3, 3, 64)          18496
max_pooling2d_1 (MaxPooling2 (None, 1, 1, 64)          0
batch_normalization_3 (Batch (None, 1, 1, 64)          256
conv2d_4 (Conv2D)            (None, 1, 1, 64)          36928
dropout_1 (Dropout)          (None, 1, 1, 64)          0
flatten (Flatten)            (None, 64)                0
dense (Dense)                (None, 128)               8320
dropout_2 (Dropout)          (None, 128)               0
dense_1 (Dense)              (None, 10)                1290
=================================================================
Total params: 100,874
Trainable params: 100,554
Non-trainable params: 320
```

Softmax function for multiclass classification problems





Everything is a vector space (but not a Euclidean one)



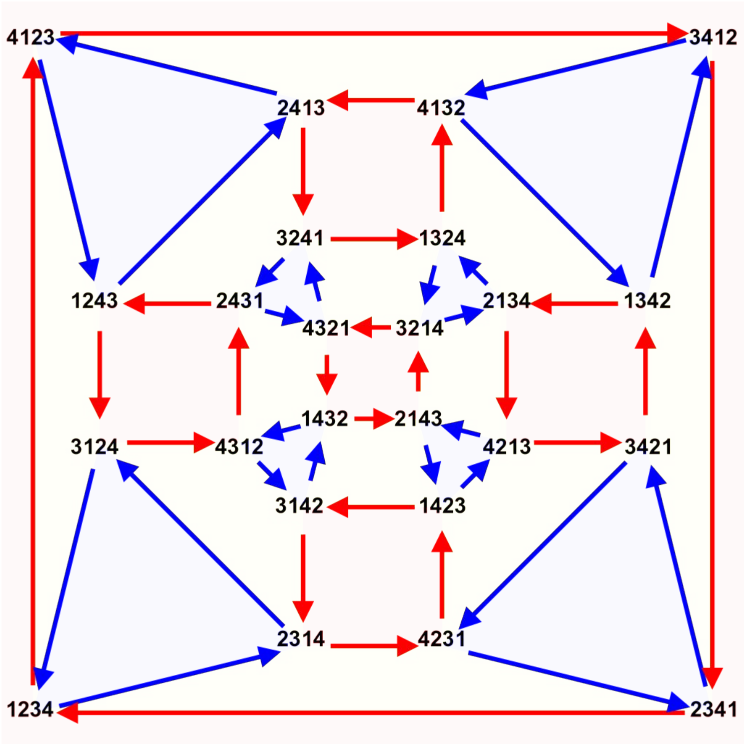
https://proceedings.neurips.cc/paper_files/paper/2013/file/9aa42b31882ec039965f3c4923ce901b-Paper.pdf

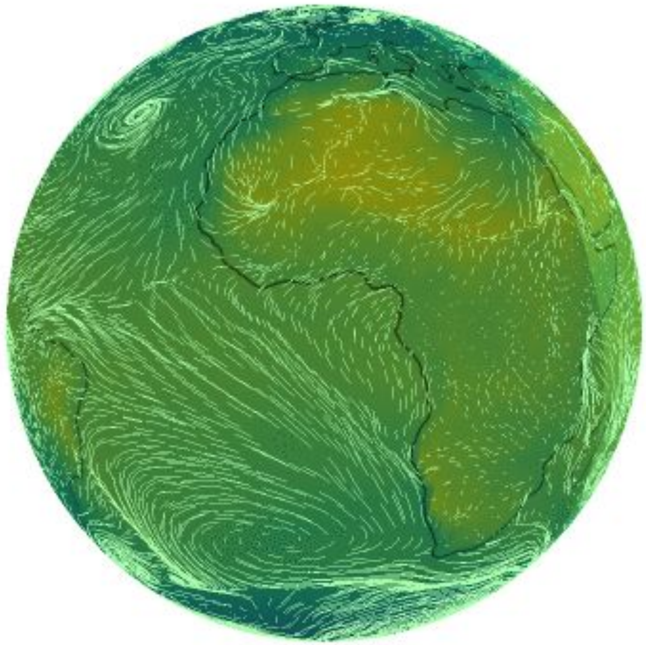
Closeness to the "gender" vector

$\overrightarrow{\text{she}}-\overrightarrow{\text{he}}$	92%
$\overrightarrow{\text{her}}-\overrightarrow{\text{his}}$	84%
$\overrightarrow{\text{woman}}-\overrightarrow{\text{man}}$	90%
$\overrightarrow{\text{Mary}}-\overrightarrow{\text{John}}$	75%
$\overrightarrow{\text{herself}}-\overrightarrow{\text{himself}}$	93%
$\overrightarrow{\text{gal}}-\overrightarrow{\text{guy}}$	85%
$\overrightarrow{\text{girl}}-\overrightarrow{\text{boy}}$	90%
$\overrightarrow{\text{female}}-\overrightarrow{\text{male}}$	84%

https://arxiv.org/pdf/1607.06520

Deep Learning on Symmetric non-Euclidean Spaces





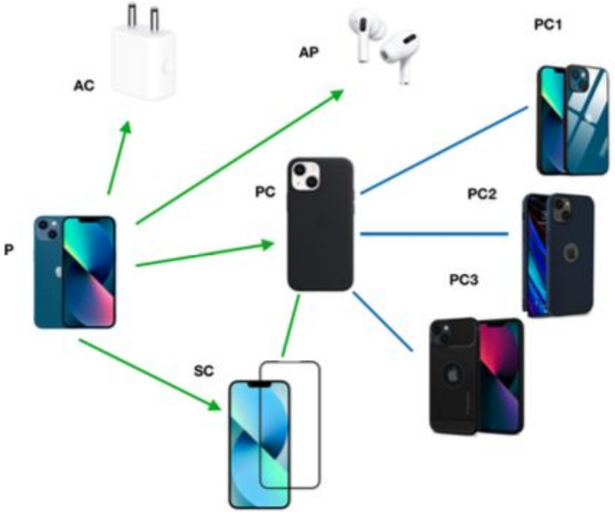
https://en.wikiversity.org/wiki/Symmetric_group_S4#/media/File:Symmetric_group_4;_Cayley_graph_4,9.svg

https://research.google/blog/scalable-spherical-cnns-for-scientific-applications/

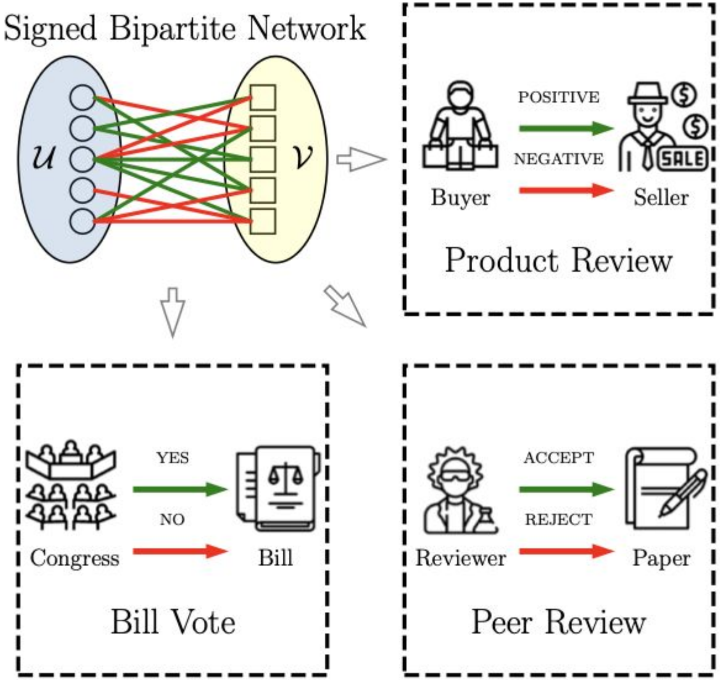
Graph Neural Networks

Molecular Analysis

Product Recommendation

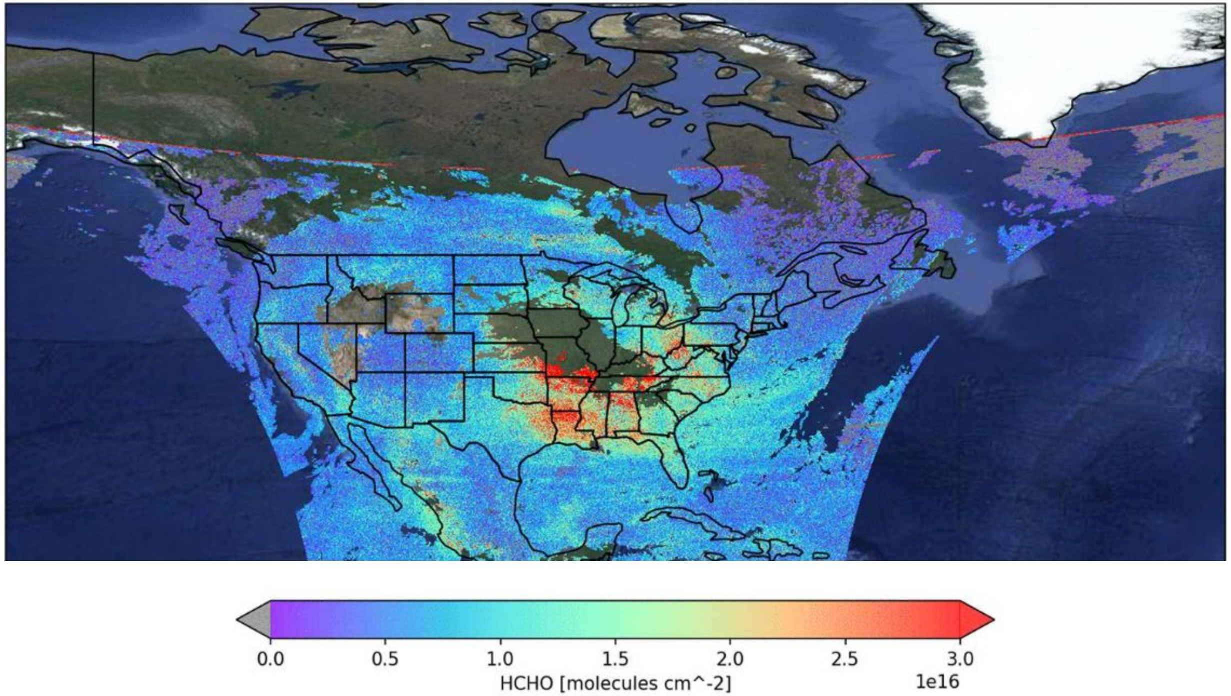


https://arxiv.org/abs/2211.11583



https://arxiv.org/abs/2108.09638

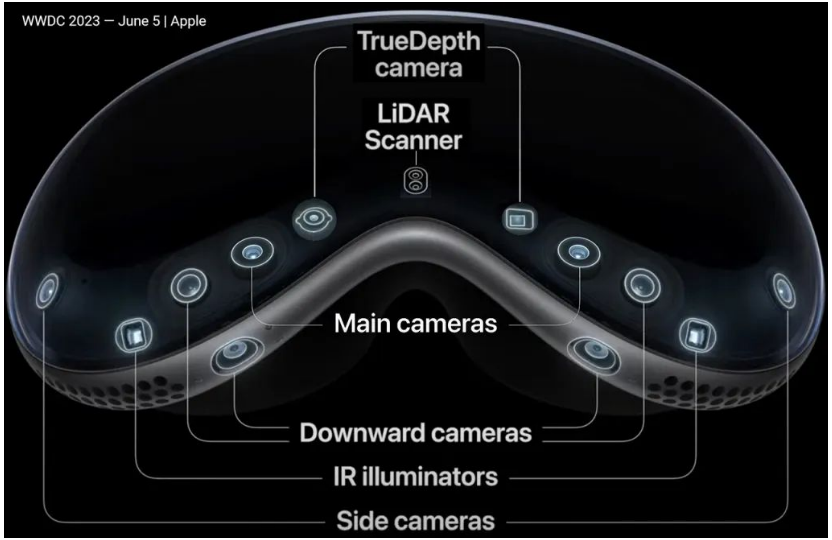
Example of Geodesics and Gauges: Satellite Data



https://ceos.org/document_management/Virtual_Constellations/AC-VC/Meetings/AC-VC-19/presentations/Presentations%20PDF/2.%20Wed%2025%20Oct%202023%20-%20TRACE%20GASES%20AND%20AEROSOLS%20AIR%20QUALITY/We-01_Liu_TEMPO_v1.pdf

Example of Geodesics and Gauges: Apple Vision Pro

The Vision Pro looks down to capture mouth movements but shows forward angle



Thoughts? Questions?

Next Meeting (September 1)

Introduction https://geometricdeeplearning.com/book/introduction.html
Lecture: “ICLR 2021 Keynote: GDL: The Erlangen Programme of ML by M Bronstein”
https://www.youtube.com/watch?v=w6Pw4MOzMuo

To present, fill out this form:
https://docs.google.com/forms/d/e/1FAIpQLSfjuvRWuHfQ9M11uz9PUnq_3j_trOAcTyDG2a5yPoMvMWgfLQ/viewform?usp=header

Additional Reference:
Mathematical Foundations of Geometric Deep Learning by Borde and Bronstein
https://www.arxiv.org/abs/2508.02723
Introduction to Geometric Deep Learning by Patrick Nicolas
https://patricknicolas.substack.com/p/introduction-to-geometric-deep-learning