Introduction to Geometric Deep Learning

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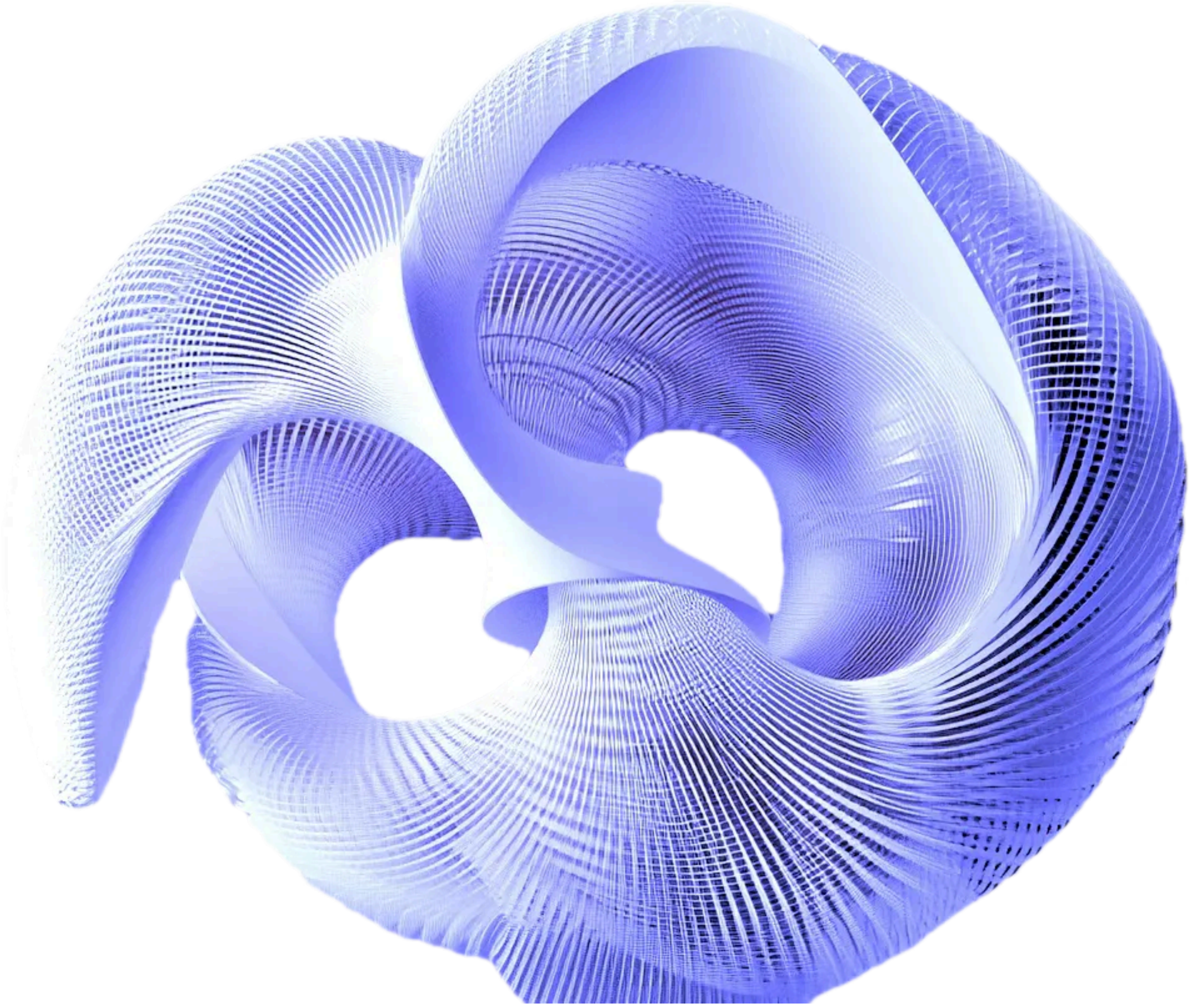
Facing challenges with high-dimensional, densely packed but limited data, and complex distributions? **Geometric Deep Learning** (GDL) offers a solution by ena data scientists to grasp the true shape and distribution of data. This newsletter explores the diverse techniques and frameworks shaping the field of Geometric I Learning.



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Why this Matters

Purpose: Introduction to **Geometric Deep Learning** and how it addresses the limitations of current machine learning models.

Audience: Anyone with some basic understandings of artificial intelligence and machine learning.

Value: Learning about **Geometric Deep Learning** and **Graph Neural Networks** unlocks the ability to model complex, structured, and relational data, enabling advanced problem-solving in areas like social networks, molecular science, desig optimization, and transportation systems.

Limitations of Current Models

Deep Learning

Data scientists face challenges when building deep learning models that can be addressed by **geometric**, **non-Euclidean representation** of data. Those challenge [ref ***1***]:

- **High dimensionality**: Models related to computer vision or images deal witl high-dimensional data, such as images or videos, which can make training n difficult due to the curse of dimensionality.
- **Availability of quality data**: The quality and quantity of training data signifi affect the model's ability to generate realistic samples. Insufficient or biased can lead to overfitting or poor generalization.
- **Underfitting or overfitting**: Balancing the model's ability to generalize well avoiding overfitting to the training data is a critical challenge. Models that c may generate high-quality outputs that are too similar to the training data, l novelty.
- **Embedding physics law or geometric constraints**: Incorporating domain constraints such as boundary conditions or differential equations model s ve challenging for high-dimensional data.
- **Representation dependence**: The performance of many learning algorithms very sensitive to the choice of representation (i.e. z-normalization impact on predictors).

Generative Models

Generative modeling includes techniques such as auto-encoders, generative adversarial networks (GANs), Markov chains, transformers, and their various derivatives.

Creating generative models presents several specific challenges beyond plain va deep learning models for data scientists and engineers, primarily due to the complexity of modeling and generating data that accurately reflects real-world distributions [ref ***2***]. The challenges that can be addressed with **differential geom** include:

- **Performance evaluation**: Unlike supervised learning models, assessing the performance of generative models is not straightforward. ***Traditional metrics accuracy do not apply,*** leading to the development of alternative metrics such Frechet Inception Distance (FID) or Inception Score, which have their limita
- **Latent space interpretability**: Understanding and interpreting the latent sp generative models, where the model learns a ***compressed representation of the can be challenging*** but is crucial for controlling and improving the generation process.

What is Geometric Deep Learning

Geometric Deep Learning has been introduced by *M. Bronstein*, *J. Bruna*, *Y. LeCu* *Szlam* and *P. Vandergheynst* in 2017 [ref ***3***]. Readers can explore the topic further t a tutorial by *M. Bronstein* [ref ***4***].

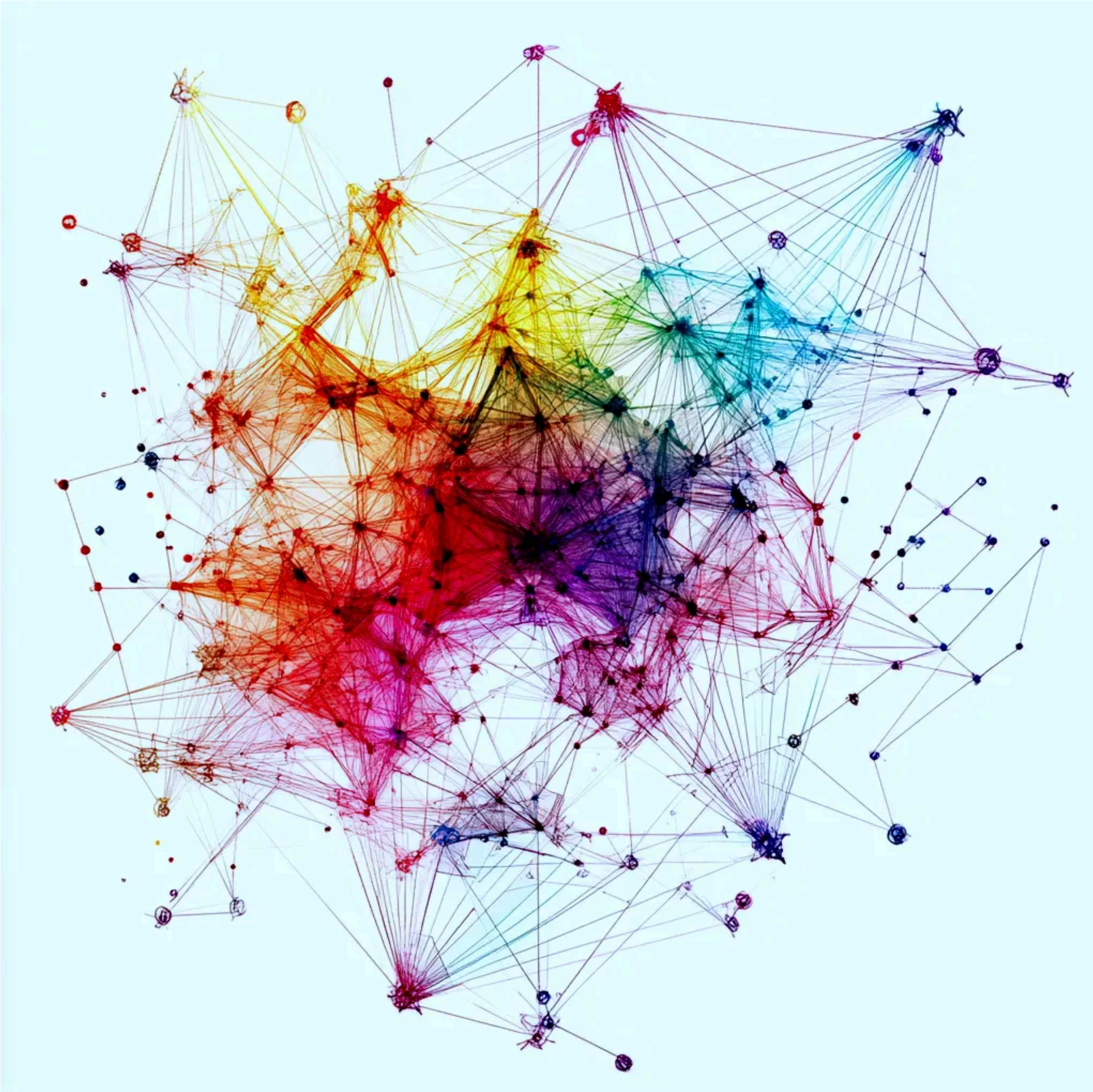
Geometric Deep Learning (GDL) is a branch of machine learning dedicated to extending deep learning techniques to non-Euclidean data structures. Currently, is no universally agreed-upon, well defined scope for Geometric Deep Learning, interpretation varies among authors.

Here's a somewhat arbitrary breakdown:

- **Graphs**: Represent relationships between entities (nodes/vertices and edges), as social networks, knowledge graphs, and molecular structures. **Graph Neu Networks** (**GNNs**) are widely used models that leverage graph-based representations.
- **Topological Domains**: Encode higher-level relationships between entities ir scientific datasets using structures like hypergraphs, simplicial complexes, c complexes. **Topological Data Analysis** (TDA) and **Topological Deep Learnir** address limitations of Graph Neural Networks by capturing non-local prope and dependencies.
- **Manifolds**: Utilize differential and Riemannian geometry to represent low-dimensional, continuous, curved spaces or embeddings within higher-dimer Euclidean spaces. **Manifold learning** and **manifold neural networks** are des to extract intrinsic data representations.
- **Point Clouds**: Represent 3D data often processed through **mesh-based** or **gr based models**, enabling effective analysis of spatial structures.

Graph Neural Networks

Data on manifolds can often be represented as a graph, where the manifold's loc structure is approximated by connections between nearby points. GNNs and the variants (like Graph Convolutional Networks (GCNs)) extend neural networks to process data on non-Euclidean domains by leveraging the graph structure, whicl approximate the underlying manifold [ref ***5***, ***6***, ***7***]



Types of Graph Neural Networks

- **Graph Convolutional Networks** (GCNs): GCNs generalize the concept of convolution from grids (e.g., images) to graphs. They aggregate information node's neighbors using normalized adjacency matrices and apply transforma to learn node embeddings.
- **Graph Attention Networks** (GATs): GATs use attention mechanisms to lear importance of neighboring nodes dynamically. Each edge is assigned a learn weight during aggregation.
- **GraphSAGE** (Graph Sample and Aggregate):It learns node embeddings by sampling and aggregating features from a fixed-size neighborhood of each n

enabling scalable learning on large graphs.

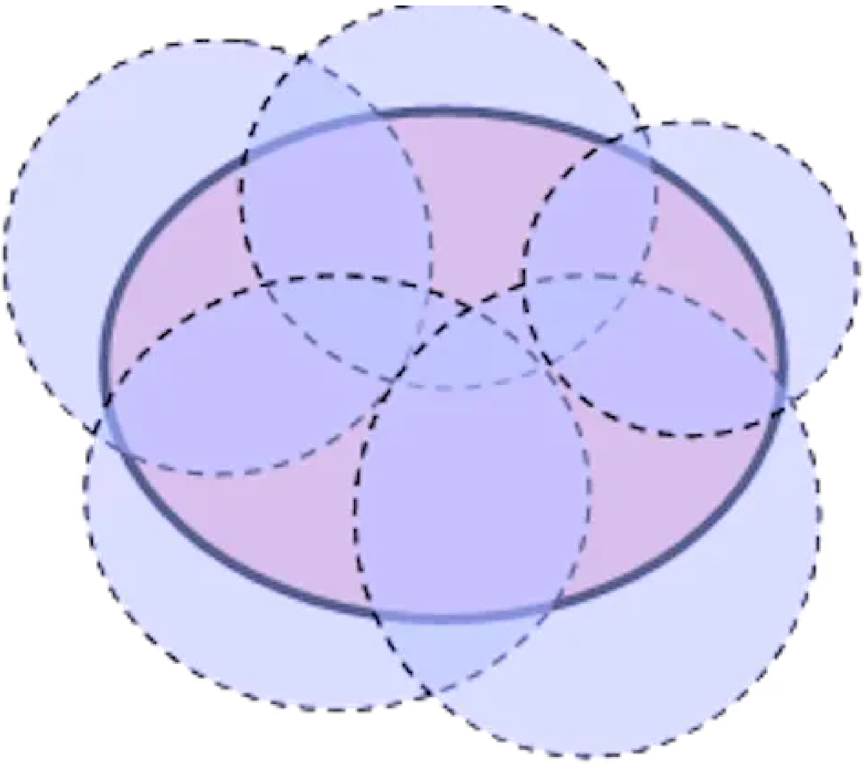
- **Graph Isomorphism Networks** (**GINs**): GINs are designed to be as powerful Weisfeiler-Lehman (WL) graph isomorphism test, distinguishing graph stru more effectively.
- **Spectral Graph Neural Networks** (**SGNN**): These networks operate in the sp domain using the graph Laplacian. They use eigenvectors of the Laplacian fo convolution-like operations.
- **Graph Pooling Networks**: They summarize graph information into a smalle representation, similar to pooling in CNNs. They can be categorized into Gl and hierarchical pooling
- **Hyperbolic Graph Neural Networks**: These networks operate in hyperbolic which is well-suited for representing hierarchical or tree-like graph structur
- **Dynamic Graph Neural Networks**: These networks are designed to handle temporal graphs, where nodes and edges evolve over time.
- **Relational Graph Convolutional Networks** (**R-GCN**s):R-GCNs extend GCN handle heterogeneous graphs with different types of nodes and edges.
- **Graph Transformers:** They adapt the Transformer architecture to graph-structured data using attention mechanisms and global context.
- **Graph Autoencoders**: These are used for unsupervised learning on graphs, a to reconstruct graph structure and node features.
- **Diffusion-Based GNNs**: These networks use graph diffusion processes to propagate information.

PyTorch Geometric [ref *8*] is a widely used library for implementing, training, a evaluating Graph Neural Networks. This library will discussed in a future article

Note: *Future articles will cover Graph Neural Network architecture and theory, along w hands-on applications implemented using Torch Geometric.*

Topological Data Analysis

Topological Data Analysis (**TDA**) is a methodology that applies concepts from algebraic topology and computational geometry to analyze and extract meaningf patterns from complex datasets. It provides a geometric and topological perspec study the shape and structure of data. TDA seeks to develop rigorous mathemati statistical, and algorithmic techniques to infer, analyze, and leverage the intricat topological and geometric structures underlying data, often represented as point clouds in Euclidean or more general metric spaces. [ref ***9***].



Features

- **Understand data shape**: TDA focuses on capturing the "shape" or structure data, including patterns, clusters, loops, and voids that traditional methods miss.
- **Reduce dimension**: It enables the extraction of features that summarize the properties of high-dimensional data while preserving important topological characteristics.
- **Discount noise**: TDA methods are designed to distinguish signal from noise effectively, providing stable and meaningful insights even in noisy datasets.

- **Quantify global properties**: TDA quantifies global and intrinsic properties c datasets, such as connectedness, holes, or higher-dimensional features.

Benefits

- **Insight into Complex Structures:** TDA can reveal features like clusters, loop voids in data that are not immediately apparent using standard statistical or machine learning techniques.
- **Versatility**: It can be applied to any dataset, regardless of the domain, and w effectively on structured, unstructured, and graph-based data.
- **Improved Noise Tolerance**: Topological features are stable and robust to sm perturbations in data, making TDA especially valuable for noisy or incomple datasets.
- **Enhancing Machine Learning**: TDA features can be combined with machin learning models to improve predictions, clustering, and classification, espec in tasks where geometry and relationships between data points matter.
- **Nonlinearity Detection**: TDA captures nonlinear patterns and relationships may be missed by linear methods like PCA or linear regression.

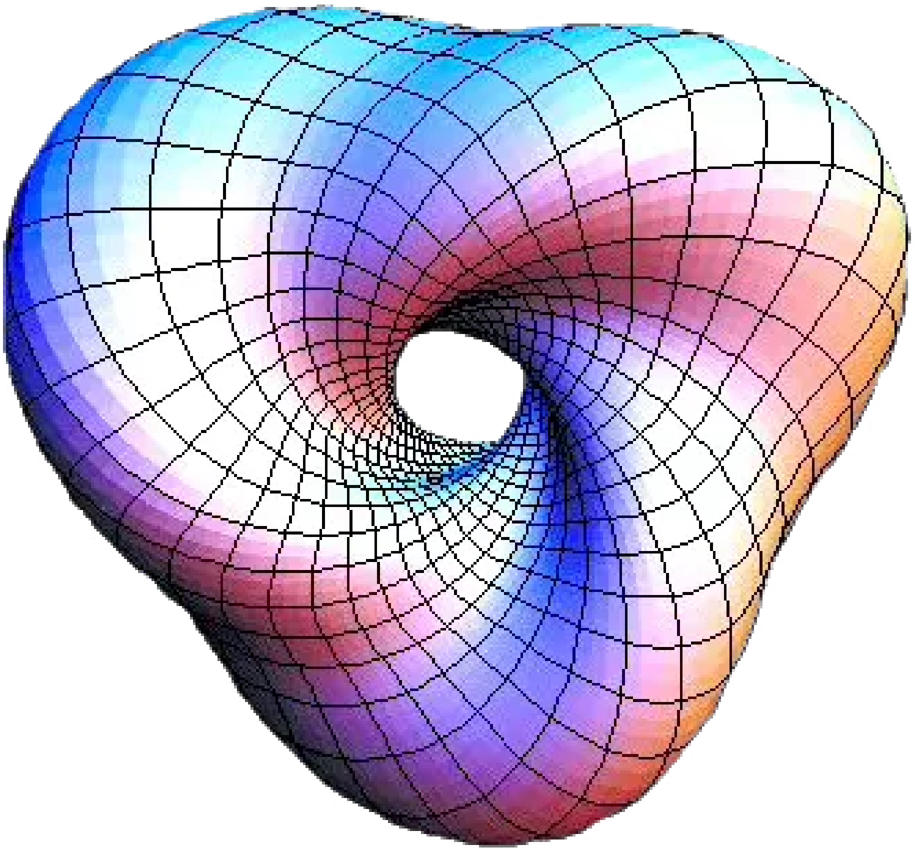
Recently, TDA has evolved into **Topology Deep Learning** that encompasses extr high level abstraction and hierarchical representation from data. For instance, **Topological neural networks** enable the processing of data, for example via high order message-passing schemes on a topological space [ref ***10***].

Note: *The most common data structures and algorithms for TDA as implemented in GU library, with C++ implementation and Python interfaces [ref* ***11***].

Data Manifolds

Machine learning models based on manifolds leverage differential geometry [ref **manifold** is essentially a space that, around every point, looks like Euclidean spa created from a collection of maps (or charts) called an atlas, which belongs to Euclidean space. **Differential** (or **smooth**) **manifolds** have a tangent space at eacl point, consisting of vectors. **Riemannian manifolds** are a type of differential mai equipped with a metric to measure curvature, gradient, and divergence [ref ***13***].

In deep learning, the manifolds of interest are typically Riemannian due to these properties.



It is important to keep in mind that the goal of any machine learning or deep lea model is to predict **p**(**y**) from **p**(**y**|**x**) for observed features **y** given latent features **x**.

$$p(y) = \int_{\Omega} p(y|x).\, p(x) dx$$

The latent space x can be defined as a differential manifold embedding in the da space (number of features of the input data).

Given a differentiable function **f** on a domain a manifold **M** of dimension **d** is de by:

$$M = f(\Omega) \quad with\ f : \Omega \subset \mathbb{R}^d \rightarrow \mathbb{R}^d$$

In a Riemannian manifold, the metric can be used to

- Estimate kernel density
- Approximate the encoder function of an auto-encoder
- Represent the vector space defined by classes/labels in a classifier

Studying data that reside on manifolds can often be done without the need for Riemannian Geometry, yet opting to perform data analysis on manifolds present three key advantages:

- By analyzing data directly on its residing manifold, you can simplify the syst reducing its degrees of freedom. This simplification not only makes calculat easier but also results in findings that are more straightforward to understar interpret.
- Understanding the specific manifold to which a dataset belongs enhances yc comprehension of how the data evolves over time.
- Being aware of the manifold on which a dataset exists enhances your ability predict future data points. This knowledge allows for more effective signal extraction from datasets that are either noisy or contain limited data points.

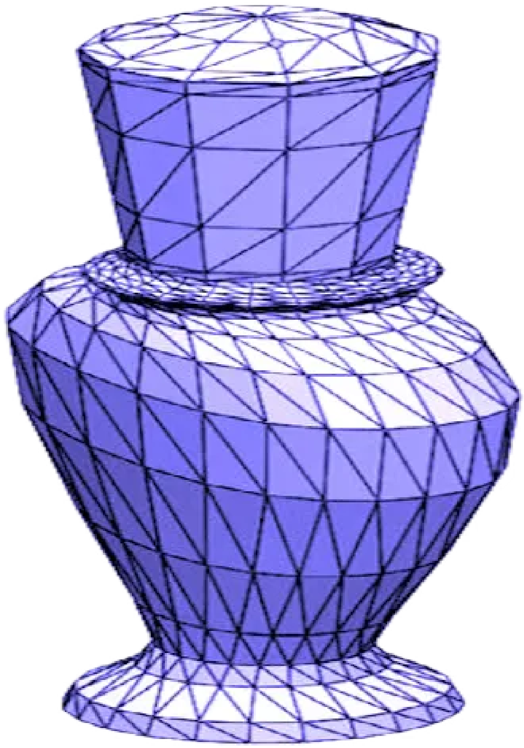
Geomstats [ref *14*] and Py**Torch Geometric** [ref *8*] are among the most widely use Python libraries for machine learning on data manifolds.

Note: *Future articles will cover topics such as application of differential geometry, deep learning models on manifolds along with hands-on applications and information geome*

Mesh & Grid Based Models

These models are a special cases of Graph Neural Networks and Geometric Deep Learning applied to 3D spaces.

A **mesh** is a collection of vertices, edges, and faces that define the shape of a 3D (Mesh-based learning focuses on directly processing these structures. A **grid** repr data in a structured, regular manner, such as a 2D/3D pixel or voxel grid.



Mesh-based learning models use triangular, quadrilateral, or polygonal meshes t represent surfaces. It preserves **topology** and **local geometric structure** and idea **irregular surfaces**, such as 3D scans, medical imaging, and CAD models [ref ***15***].

The common designs are

- **GNN on meshes** for which mesh is treated as a graph
- **Spectral** models that use the Laplacian of the mesh
- **Geometric Deep Learning** methods that apply message passing the mesh.

A **grid** represents data in a structured, regular manner, such as a 2D/3D pixel or v grid. It uses uniform grids and is suitable for applications where data is naturally aligned with a regular grid.

The common designs are

- **Voxel-based Neural Networks** converting 3D objects into voxel grids and ap 3D CNNs.
- **Implicit Representations** representing surfaces as signed distance functions
- **Physics-Based Learning** simulating physical interactions within a grid.

Feature	Mesh-Based Learning	Grid-Based Learning
Structure	Irregular (vertices, edges, faces)	Regular (grids, voxels)
Flexibility	Adapts to curved surfaces	Limited to structured data
Computational Cost	More efficient storage	Higher memory requirement
Common Use Cases	3D modeling, simulations, GNNs	Image processing, volumetric learning

Applications

Classifying applications based on their association with specific models can be challenging, as multiple approaches may offer accurate representations and relia predictions. Here are some examples:

- **Community detection**: Identify clusters or communities in social networks (*Neural Networks*).
- **Recommendations**: Suggest products, services or connection using graph-ba similarity (*Graph Neural Networks*).
- **Drug Discovery:** Predict molecular properties, drug-target interactions, or generate novel compounds (*Graph Neural Networks*).
- **Protein Structure Prediction:** Model amino acid interactions to predict 3D protein folding and stability (*Graph Neural Networks*).
- **Gene Networks:** Analyze gene regulatory interactions or detect disease path (*Graph Neural Networks*).
- **3D Shape Analysis:** Analyze and process point clouds or 3D meshes (*3D Mes model*),
- **Action Recognition:** Use graphs to model relationships between body joints objects in video sequences (*Graph Neural Networks*).

- **Fraud Detection:** Detect fraudulent activities by modeling transaction netw (*Graph Neural Networks*).
- **Portfolio Optimization:** Represent and analyze stock correlations using gra (*Graph Neural Networks*).
- **Electronic Circuit Design:** Optimize circuit layouts represented as graphs (*Neural Networks*).
- **Risk Management:** Model credit risk and customer relationships in financia networks (*Graph Neural Networks*).
- **Disease Prediction:** Model patient similarities and interactions for personal medicine (*Graph Neural Networks*).
- **Patient Care Networks:** Represent patient-doctor or hospital networks to optimize care pathways (*Graph Neural Networks*).
- **Drug Repurposing:** Identify new therapeutic uses for existing drugs using g based analysis (*Graph Neural Networks*).
- **Physics-Informed Learning:** Modeling physical systems using graphs and manifolds (*Manifold learning*).
- **Disease Prediction:** Model patient similarities and interactions for personal medicine (*Graph Neural Networks*).
- **Patient Care Networks:** Represent patient-doctor or hospital networks to optimize care pathways (*Graph Neural Networks*).
- **Drug Repurposing:** Identify new therapeutic uses for existing drugs using g based analysis (*Graph Neural Networks*).
- **Knowledge Graphs:** Improve semantic search, question answering, and reas by embedding nodes and edges (*Graph Neural Networks*).
- **Collaboration Networks:** Model co-authorship or citation networks for anal research trends (*Graph Neural Networks*).
- **Astronomy:** Analyze large-scale cosmic networks and galaxy clusters (*Graph Neural Networks*).

- **Power Grid Management:** Monitor and optimize energy distribution networ (*Graph Neural Networks*).
- **Text Classification:** Represent relationships between words, sentences, or documents as graphs for classification (*Graph Neural Networks*).
- **Trajectory Optimization:** Manifold learning helps model and optimize robo trajectories, especially in constrained spaces like joints or environments (*Ma learning*).
- **Pose Estimation:** Manifold models are used to represent rotations, translati and orientations in 3D space (e.g., SO(3), SE(3) groups) (*Manifold learning*).
- **3D Shape Analysis:** Used for **shape recognition**, **segmentation**, and **alignme** (*Manifold learning*).
- **Physics Simulations:** Manifolds represent physical systems like fluid dynam electromagnetic fields for improved simulation and understanding (*Manifold learning*).
- **Manifold-based Data Augmentation:** Generative models use learned manif create augmented data samples that adhere to the original data distribution (*Manifold learning*).
- **Brain Signal Analysis:** EEG/MEG data is modeled on manifolds to uncover l patterns related to neurological states (*Manifold learning*).
- **Matrix Factorization:** Manifold-based optimization is applied to problems l low-rank matrix approximation in recommendation systems (*Manifold learni*
- **Topology and Geometry Analysis:** Persistent homology and topological data analysis rely on manifold representations for analyzing complex data structu (*Topological data analysis*).
- **Manifold-Aware Transformers:** Emerging methods adapt transformer architectures to manifold-structured data (*Topological data analysis*).
- **Hyperbolic Embeddings:** Effective for modeling hierarchical or tree-like da structures (e.g., taxonomies, organizational hierarchies) (*Topological data ana*

Frameworks & Libraries

There are numerous open-source Python libraries available, with a variety of foc not exclusively tied to machine learning or generative modeling:

- **diffgeom**: A PyPi project aimed at symbolic differential geometry. Detailed information is available at PyPi Diffgeom.
- **SymPy**: A more comprehensive library for symbolic mathematics, useful for studying topology and differential geometry. Documentation is accessible at SymPy
- **Geomstats**: Designed for performing computations and statistical analysis o nonlinear (Riemannian) manifolds (Github Geomstats).
- **PyG**: PyTorch Geometric is a library built on PyTorch dedicated to geometri deep learning and graph neural networks (Pytorch Geometric).
- **PyRiemann**: A package based on scikit-learn provides a high-level interface processing and classification of multivariate data through the Riemannian geometry of symmetric positive definite matrices (pyRiemann: Machine lear for multivariate data with Riemannian geometry).
- **PyManOpt**: A library for optimization and automatic differentiation on Riemannian manifolds (PyManOpt).
- **GUDHI**: The library is a generic open source C++ library with a Python inte for Topological Data Analysis and Higher Dimensional Geometry Understar (GUDHI - Geometry Understanding in Higher Dimensions).

Takeaways

- Geometric Deep Learning (GDL) tackles key limitations of traditional deep learning models, including overfitting, representation dependency, and interpretability challenges.

- GDL methods fall into several categories: Graph Neural Networks, Topologi Data Analysis, data manifold models, and mesh/grid-based models.
- Applications leveraging GDL are beginning to emerge, supported by various Python libraries, with **Geomstats** and **PyTorch Geometric** being among the widely used.
- This newsletter explores the diverse techniques and frameworks shaping the of Geometric Deep Learning.

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Exercises

- **Q1**: What are the two most widely used Python libraries for Geometric Deep Learning?
- **Q2**: Can you name four different types of Graph Neural Networks?
- **Q3**: What are the advantages of using Topological Data Analysis?
- **Q4**: How does a differential (smooth) manifold differ from a Riemannian manifold?
- **Q5**: Between mesh-based and grid-based learning models, which has the hig computational cost?

Exercises Answers

News & Reviews

This section focuses on news and reviews of papers pertaining to geometric deep learning and its related disciplines.

Paper review Intrinsic and extrinsic deep learning on manifolds **Y. Fang, i. Ohh, Gupta, L. Lin 2023**

This paper introduces two types of general deep neural network architecture on manifolds:

Extrinsic deep neural network on manifolds

This architecture maintains the geometric characteristics of manifolds by emplo an *equivariant embeddings* of a manifold into the Euclidean space.

This method is applied in regression models or *Gaussian processes on manifolds*, w the idea is to construct the neural network based on the manifold's representatic after embedding, while still maintaining its geometric properties. By adopting th strategy, it becomes possible to utilize stochastic gradient descent and backpropagation techniques from Euclidean space. This results in enhanced acc compared to conventional machine learning algorithms like SVM, random forest

Intrinsic deep neural network on manifolds

The objective is to embed the inherent geometric nature of Riemannian manifol using e*xponential and logarithmic maps*. This framework, which projects localized points from a Riemannian manifold onto a single tangent space, proves benefici when embeddings cannot be determined. Each localized tangent space (or chart) mapped (via exp/log functions) onto a neural network. This architectural approac achieves higher accuracy compared to deep models in Euclidean space and the Extrinsic architecture.

These two frameworks are assessed based on their performance in

1. Classifying health-related simulated datasets on a spherical manifold
2. Dealing with symmetric semi-positive definite matrices.

Patrick Nicolas has over 25 years of experience in software and data engineering, archit design and end-to-end deployment and support with extensive knowledge in machine le He has been director of data engineering at Aideo Technologies since 2017 and he is the author of "Scala for Machine Learning", Packt Publishing ISBN 978-1-78712-238-3 an [Geometric Learning in Python](#) Newsletter on LinkedIn.

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