## Deep Learning on Meshes and Point Clouds

Ruben Wiersma SGP 2025 Graduate School, Bilbao





# Who are you?







#### Goal

- Provide a 'map' of deep learning on 3D shapes
- Outcome
  - Applying deep learning to 3D tasks
  - Developing deep learning techniques for 3D tasks
- Audience
  - Some familiarity with optimization or machine learning





# Why are we interested?





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From Bronstein









Understanding and Improving Features Learned in Deep Functional Maps, Attaiki and Ovsjanikov (2023)









Automated morphological phenotyping [...], O. Thomas et al. (2023)







Mesh Neural Networks for SE(3)-Equivariant Hemodynamics Estimation of the Artery Wall, Suk et al. (2022)







Fully Convolutional Graph Neural Networks for Parametric Virtual Try-On, Vidaurre et al. (2020)





#### Why are we interested?

- Classification
- Segmentation
- Registration, correspondence
- Surface reconstruction
- Speeding up classical geometry tasks (i.e., smart lookup table)
- Generative modeling





#### What's the difference?







### **Chapter 1: Basics**





#### Deep learning is a machine learning method



#### "Classic" approaches







#### Deep learning is a machine learning method







#### Deep learning is a machine learning method







#### Machine learning basics







X'

#### Deep learning basics

 $\theta^* = \operatorname{argmin}_{\theta} \sum_{i}^{N} ||f_{\theta}(x_i) - y_i||_2^2$   $\operatorname{Training} \text{Loss}$ 

- $f_{\theta}(x)$  is non-linear  $\rightarrow$  numerical optimization
- $\theta$  is high-dimensional  $\rightarrow$  gradient descent (instead of higher order methods)
- N is large  $\rightarrow$  stochastic gradient descent (only a few x, y pairs at a time)





#### Characterization of deep learning







#### Is deep learning all you need?







#### Is deep learning all you need?









#### "It's all about the data" – Alexei Efros

e.g., https://www.youtube.com/watch?v=M1VHu1d4sGQ









#### Characterization of deep learning







### **Typical models**

#### MLP – Multi-layer perceptron

• The Perceptron: A Probabilistic Model For Information Storage And Organization in the Brain – Rosenblatt (**1958**)

#### CNN – Convolutional Neural Network

- Gradient-based learning applied to document recognition Lecun et al. (1998)
- Transformer (Attention)
  - Attention Is All You Need Vaswani et al. (**2017**), attention was around before that





#### **Multi-Layer Perceptron (geometric perspective)**

 $\rightarrow$  Separate these points

- Distance to line/plane  $\vec{x} \cdot \vec{n} d$
- Step function

$$y = \sigma(\vec{x} \cdot \vec{n} - d)$$



https://medium.com/@shrutijadon/survey-on-activation-functions-for-deep-learning-9689331ba092





#### Multi-Layer Perceptron (geometric perspective)

 $\rightarrow$  Separate these points

- Distance to line/plane  $\vec{w}^T \vec{x} + b$
- Step function  $y = \sigma(\vec{w}^T \vec{x} + b)$
- Weights, biases
- $\sigma$  activation function
  - Non-linear!



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#### Multi-Layer Perceptron

$$y = \sigma(\vec{w}^T \vec{x} + b)$$

$\rightarrow$ Multiple outputs?	"Channels"
$\vec{y} = \sigma(\mathbf{W}\vec{x} + \vec{b})$	
$\rightarrow$ Not linearly separable?	"Layers"
$\vec{y} = \sigma(W_1\vec{x} + \vec{b}_1)$	







#### **Multi-Layer Perceptron Notes**

- Examples in 2D, but  $\vec{x}$  can be of any dimension
- Interpretation: cutting up space with halfspaces
- "Multilayer Feedforward Networks [MLPs] are Universal Approximators"
  - Hornik, Stinchcombe and White (1989)
  - Non-linearity is necessary!
  - Compare, e.g., Fourier transform
- Higher complexity, more risk of overfitting





#### **MLP** on images









#### **MLP** on images







### **MLP** on images

- Stack all pixel values, feed into MLP
- Problem?
  - Not efficient ( $\vec{x}$  is of dimension width \* height)
  - Patterns can be anywhere in the image

x<sub>i</sub> are the pixel values






## **Convolutional Neural Network**







#### **Schematics**









#### **Schematics**







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# **Convolutional Neural Networks**



https://medium.com/data-science/u-net-explained-understanding-its-image-segmentation-architecture-56e4842e313a





#### **Hierarchies of Features in CNNs**



Edges (layer conv2d0)

Textures (layer mixed3a)

Patterns (layer mixed4a)

Parts (layers mixed4b & mixed4c)

Objects (layers mixed4d & mixed4e)

Feature Visualization, Olah, Mordvintsev, Schubert (2017) – https://distill.pub/2017/feature-visualization/





# **Convolutional Neural Networks Notes**

- Interpretation: MLP on patches
- Consistent pixel grid helps
  - Orientation
  - Maps to hardware well
- Downside (?) Template is fixed







# **Limitation of Convolution Kernels**







## **Limitation of Convolution Kernels**



Gaussian kernel g

$$x'_i = \sum_{j \in \mathcal{N}} g(\|p_j - p_i\|) x_j$$

Based on distance





#### Denoising with Gaussian filter vs. Bilateral filter

$$x'_i = \sum_{j \in \mathcal{N}_i} g(\|p_j - p_i\|) x_j$$



Isotropic blurring

$$x'_{i} = \sum_{j=0}^{N} f(||x_{j} - x_{i}||)g(||p_{j} - p_{i}||)x_{j}$$
  
Look at pixel value as well



Preserves features





# Self-attention (Transformers)

$$x'_{i} = \sum_{j=0}^{N} f(||x_{j} - x_{i}||) g(||p_{j} - p_{i}||) x_{j}$$

• Replace distance with cosine similarity

$$x'_i = \sum_{j=0}^N \left[ x_j^T x_i \right] x_j$$

• Add flexibility with weight matrices and make sure weight 'behaves'

$$x_i' = \sum_{j=0}^N \operatorname{softmax}\left(\left(\mathsf{W}_q x_j\right)^T \mathsf{W}_k x_i\right) \mathsf{W}_v x_j$$





#### Self-attention (Transformers)







# Self-attention (Transformers)

$$x'_{i} = \sum_{j=0}^{N} \operatorname{softmax}\left(\left(W_{q} x_{j}\right)^{T} W_{k} x_{i}\right) W_{\nu} x_{j}$$

- Transformers combine these blocks
- Positional encoding based on  $p_i p_i$
- Pro: Highly flexible, very effective (LLMs, Vision Transformers, etc.)
- Pro: 'Global' connections (vs. U-Net)
- Con: Computationally expensive (compared to CNN)
  - Solutions: work at coarse scale OR only apply locally





# Summary

#### Multi-Layer Perceptrons (MLP)

- Linear combination, followed by non-linearity, repeated
- Basic building block of Neural Networks

#### Convolutional Neural Network (CNN)

- Learn local kernel, convolve
- Weight sharing, translation invariance
- 'Constructs' localized features of increasing abstraction

#### Transformers

- Learn weights based on feature similarity
- Highly expressive, but expensive; current SOTA for many tasks





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# **Chapter 2: 3D Data**







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### **Deep learning for 3D data**



**'Philosophy':** Scaling (data, compute) beats algorithmic complexity







**3D Data** 

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Based on slides by Klaus Hildebrandt

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# What about implicit functions?

$$f: \mathbb{R}^3 \to \mathbb{R}$$

Value > 0 outside shape, < 0 inside

#### In deep learning

- Use MLP to represent *f*
- Rarely used as input to MLP
  - Convert to voxels/mesh/point cloud



Based on slides by Olga Sorkine-Hornung





# **Point Cloud**

• Set of points in d-dimensional space

$$P \in \mathbb{R}^3$$









#### Mesh

- 'Complements' point cloud
  - connectivity and surface given by V, E, F
- Geometry can be on points, edges, etc. •









#### **Datasets**

- ShapeNet (meshes, point clouds) segmentation, classification
- ModelNet40 (meshes) classification
- ScanNet (v2, v3) (RGB-D + reconstructions) segmentation
- S3DIS (point clouds) segmentation
- Thingi10k (meshes) n/a
- **ABC** (meshes) n/a
- Consider ethics, copyright!
  - E.g., <a href="https://huggingface.co/datasets/allenai/objaverse/discussions/18">https://huggingface.co/datasets/allenai/objaverse/discussions/18</a>





## More exotic inputs and outputs: simulation

- Input: positions, distance to loops
- **Output:** tangent vector at each vertex



Mesh Neural Networks for SE(3)-Equivariant Hemodynamics Estimation of the Artery Wall, Suk et al. (2022)







# More exotic inputs and outputs: simulation

- Stage 1
  - Input: Garment parameters
  - **Output:** Mesh positions on mean shape
- Optimize topology
- Stage 2
  - Input: Mesh positions, target shape parameters
  - Output: Smooth mesh positions
- Stage 3
  - Input: Smooth mesh positions
  - Output: Fine mesh positions (wrinkles, etc.)



Fully Convolutional Graph Neural Networks for Parametric Virtual Try-On, Vidaurre et al. (2020)





#### More exotic inputs and outputs: Jacobians

- Neural Jacobian Fields
  - Input: Per-triangle centroid + global code
  - **Output:** Jacobian matrix
  - Model: MLP
- Post-proces:
  - Restrict Jac
  - Solve Poiss



Neural Jacobian Fields: Learning Intrinsic Mappings of Arbitrary Meshes, Aigerman et al. (2022)



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# What if I have data, but no labels?

- Unsupervised learning
- For example: auto-encoders







# What if I have data, but no labels?

- Unsupervised learning
- For example: auto-encoders







# Chapter 3: 3D Deep Learning Models





### **Deep learning for 3D data**



**'Philosophy':** Scaling (data, compute) beats algorithmic complexity





# Let's start simple







MLP



Stack all points?

Which order?



"Bunny"





# **PointNet**

- MLP on each point
- Maximum over all points

 $y = \max_{j \in P} f_{\theta}(x_j)$ 

Cannot learn from neighborhoods



PointNet: Deep Learning on Point Sets for 3D Classification and Segmentation, Qi, Su, Mo, Guibas (2016)



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### PointNet++

- MLP on each point
- Maximum over neighborhood
  - kNN homogeneous
  - Radius more robust to sampling
    - Geodesic/Euclidean?

$$x'_i = \max_{j \in N_i} f_{\theta}(x_j, p_j - p_i)$$

• Hierarchies with maximum pooling (like CNN)

PointNet++: Deep Hierarchical Feature Learning on Point Sets in a Metric Space, Qi, Yi, Su, Guibas (2017)







# Taking a step back





#### Surface as a graph

• Vertices or points are nodes







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## Surface as a graph

- Vertices or points are nodes
- Edges connect nearby points (radius graph, k-NN graph)
- For meshes: use mesh edges

- What can meshes help with?
  - Geodesic neighborhoods (we know connectivity)
  - Encode geometry (e.g., MeshCNN)



## Message passing

- 1. Compute 'message' on each node
- 2. Aggregate messages over edges



Neural Message Passing for Quantum Chemistry, Gilmer, Schoenholz, Riley, Vinayls, Dahl (2017)

https://pytorch-geometric.readthedocs.io/en/latest/tutorial/create\_gnn.html







#### **PointNet++ as Message Passing**

- 1. **Message:** MLP on features + relative location
- 2. **Passing:** Maximum over neighbors

$$x'_i = \max_{j \in N_i} f_\theta(x_j, p_j - p_i)$$

PointNet++: Deep Hierarchical Feature Learning on Point Sets in a Metric Space, Qi, Yi, Su, Guibas (2017)






### EdgeConv as Message Passing

- 1. **Message:** MLP on 'relative features' (edges)
- 2. **Passing:** Maximum over neighbors

$$x'_i = \max_{j \in N_i} f_{\theta}(x_i, x_j - x_i)$$

Dynamic Graph CNN for Learning on Point Clouds, Wang, Sun, Liu, Sarma, Bronstein, Solomon (2019)





### **GCN as Message Passing**

1. **Message:** Linear transformation of features

2. Passing: Weight by degree, average

$$x'_i = \sigma(\mathsf{W}_0 x_i + \sum_{j \in N_i} \frac{1}{c_{ij}} \mathsf{W}_1 x_j)$$



Graph Convolutional Networks, Kipf, Welling (2016)





### Laplacian in GCN and EdgeConv

- Laplacian: Sum of second derivatives
  - Discrete setting: Difference to average of neighbors







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# More geometry





### Why geometry?





Based on slides by Klaus Hildebrandt







### Why geometry?





DiffusionNet: Discretization Agnostic Learning on Surfaces, Sharp et al. 2022



### Why geometry?

Invariances







### Intrinsic operations can be beneficial

- + Robust to isometric deformations
- + 2D instead of 3D
- + No/less distortion or occlusion





### Why Geometry?

• Invariances within an invariance









## **Back to CNNs**







### **CNN on a Graph**

Single CNN layer with 3x3 filter



 $x_4' = \sigma(\sum W_i x_i)$ 





### **CNN on a Graph**

### Single CNN layer with 3x3 filter



$$x'_{4} = \sigma(\sum_{i} W_{i} x_{i})$$
  
Compare with GCN  
$$x'_{i} = \sigma(W_{0} x_{i} + \sum_{j \in N_{i}} \frac{1}{c_{ij}} W_{1} x_{j})$$





## **CNNs for 3D**

- Graph- and point based
  - GCN, PointNet++, EdgeConv
- 3D kernel (extrinsic)
  - KPConv, MinkowskiNet, SSCN



KPConv [Thomas et al. 2019]



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## **CNNs for 3D**

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- 2D kernels on surfaces (intrinsic)
  - GCNN, ACNN, MoNet, MDGCNN, HSN







## **CNNs for 3D**

- Graph- and point based
  - GCN, PointNet++, EdgeConv
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- 2D kernels on surfaces (intrinsic)
  - GCNN, ACNN, MoNet, MDGCNN, HSN
- Operator-based (e.g., Laplacian)
  - DeltaConv

#### Anisotropic operator







## **Transformers**







### **Attention on a Graph**

Single CNN layer with 3x3 filter







### **Transformers for 3D**

- PointTransformer Zhao et al. 2021
- Challenge: how to reduce cost?
  - Apply on local neighborhoods
  - Apply on serialized point clouds (space-filling curves, v3 2024)
- Challenge: positional encoding
  - PointNet++-like positional encoding,  $MLP(p_i p_i)$
  - Rotation invariance?







### **Current state-of-the-art**

- Many approaches, but PointNet++ still seems to work quite well
  - Due to tasks/benchmarks?
- Other options often seen
  - DGCNN (EdgeConv), PointTransformer v3, Sparse Voxel Convolutions
- Which one to use depends on your task
  - Do you expect the network to understand curvature? Maybe not PointNet++/DGCNN?
  - Do you want efficiency, simplicity? Try the simple networks first.





### Methods you should know, but we didn't cover

- MeshCNN (Hanocka et al. 2019)
  - Operates on mesh edges
  - Geometric features
    - dihedral angle, two inner angles and two edge-length ratios for each face
- DiffusionNet (Sharp et al. 2022)
  - Learning to diffuse
  - Accelerated in frequency domain (Eigenvectors of Laplacian)
  - Robust to discretizations (e.g., mesh → point cloud)





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## Rotation invariance, translation invariance?

- Data augmentation
  - Random rotation/translation
- 'Learn' the transformation
  - Spatial transformer, e.g., in PointNet
- Invariant input features
  - Heat-Kernel Signatures (DiffusionNet)
  - MeshCNN Edges, intrinsic features
- Encode features in local frames
  - Point difference, normals (translation-invariant)
  - Distances (translation-rotation-invariant)
- Rotation-equivariance
  - E.g., Tensor Field Networks (Thomas et al. 2018), Spherical Harmonics (Poulenard et al. 2019)







# Chapter 4: Hands-on with PyTorch Geometric





## **PyTorch Geometric**

https://pytorch-geometric.readthedocs.io/en/latest/

- Implementation of message-passing paradigm
- Supports many convolution types
- Many helpful utilities

- Alternatives
  - Kaolin, PyTorch3D, GraphGym









# Setting up the environment





## Dataset, loading and visualization





## Model





# Training







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