Interpretable Graph Spectral Processing and Analysis for Geometric Data and Beyond

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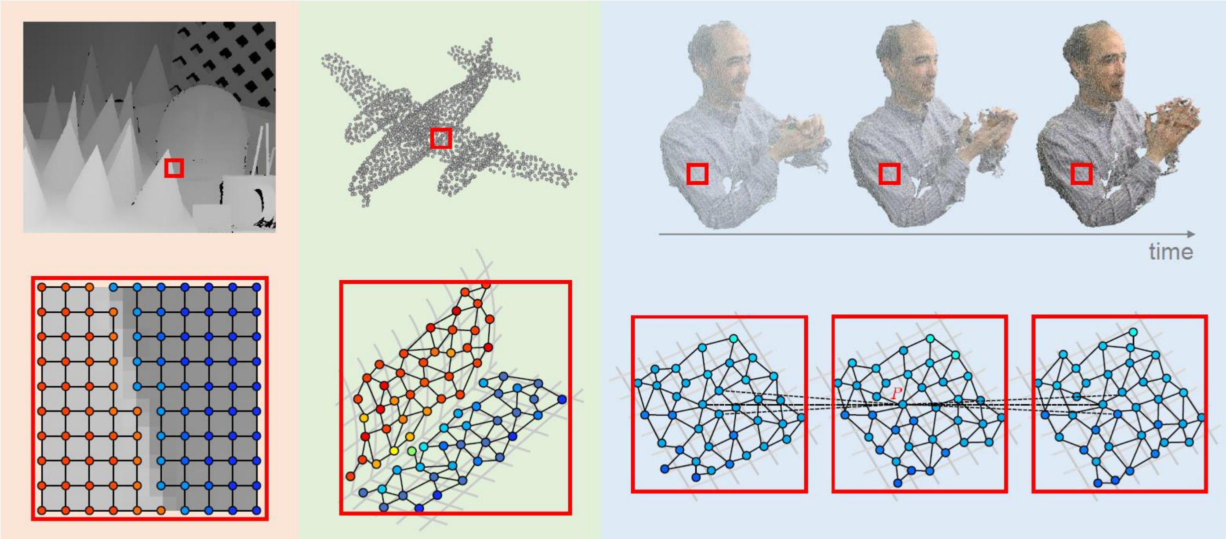
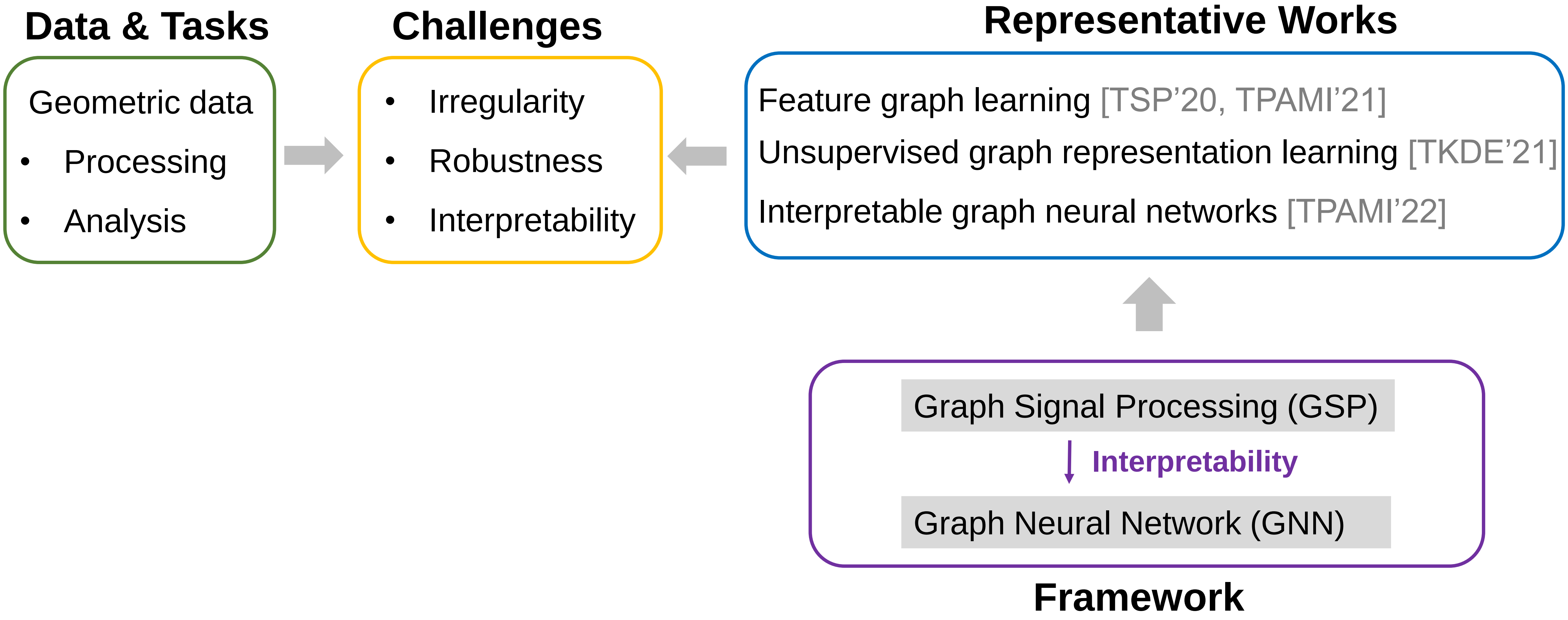


(a) 2D Depth Map (b) 3D Point Cloud (c) 4D Dynamic Point Cloud

Outline



Data & Tasks

Geometric data

- Processing
- Analysis

Challenges

- Irregularity
- Robustness
- Interpretability

Representative Works

Feature graph learning [TSP'20, TPAMI'21]

Unsupervised graph representation learning [TKDE'21]

Interpretable graph neural networks [TPAMI'22]

Framework

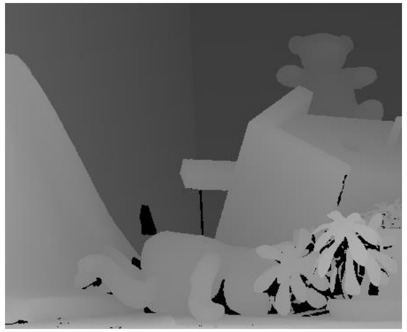
Graph Signal Processing (GSP)

Interpretability

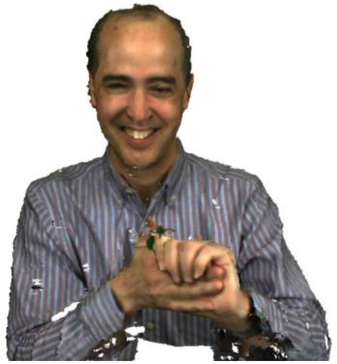
Graph Neural Network (GNN)

Geometric Data

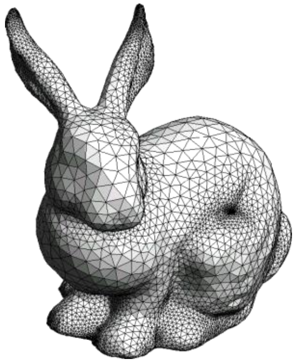
- Describe the geometry of the 3D world



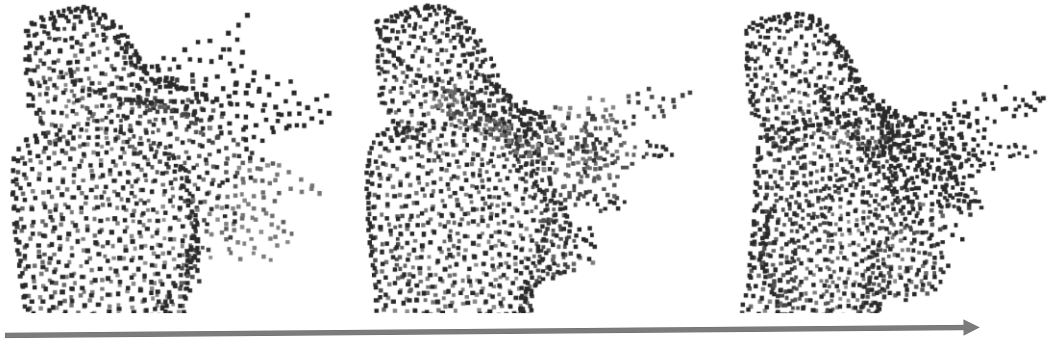
2D depth map



3D Point Cloud



3D Mesh



4D Dynamic Point Cloud

- Acquired by depth sensing, laser scanning or image processing

Microsoft Kinect

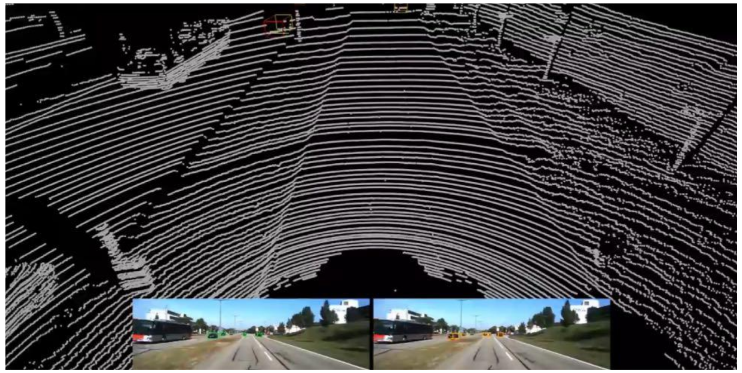
Intel RealSense

Velodyne LiDAR

LiDAR scanner of
Apple iPad Pro

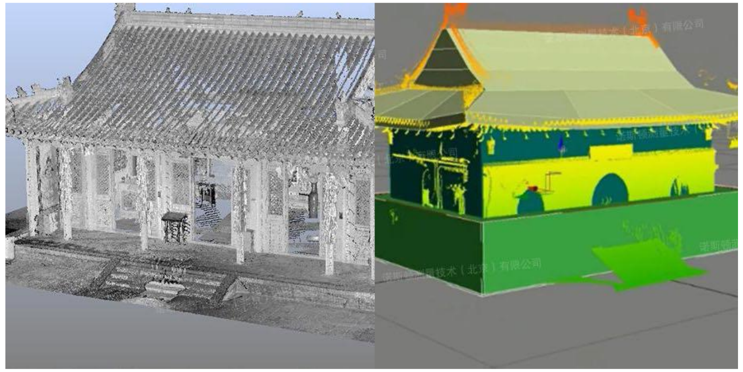
Geometric Data

- Central to a wide range of applications



Navigation in Autonomous Driving

Augmented/Virtual Reality



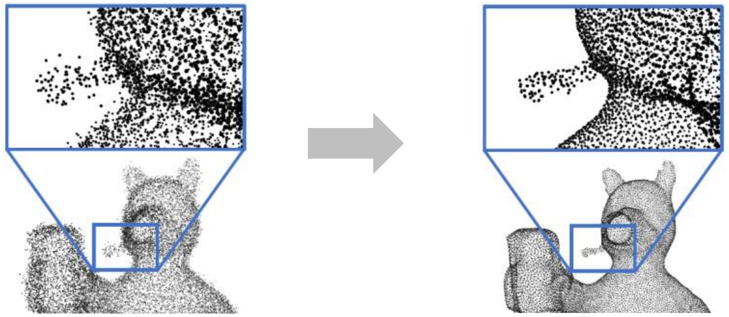
Heritage Protection

Free-viewpoint Video

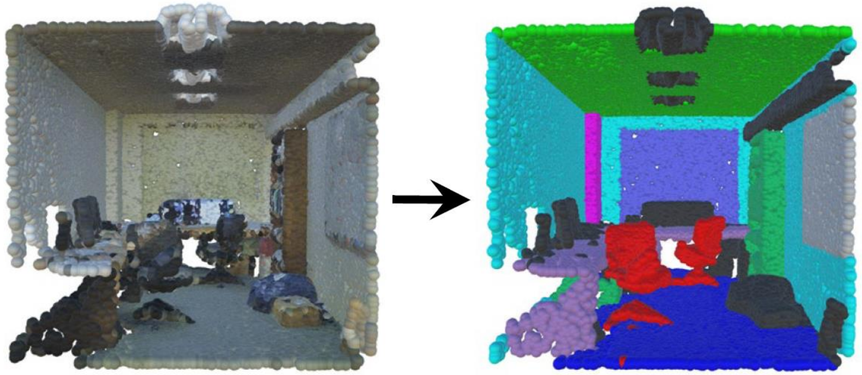
Introduction to geometric data processing and analysis

Tasks

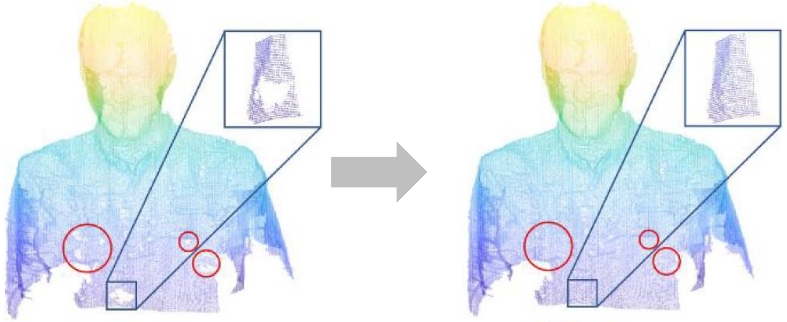
- **Processing**: denoising, inpainting, super-resolution, resampling, etc.
- **Analysis**: classification, segmentation, detection, etc.



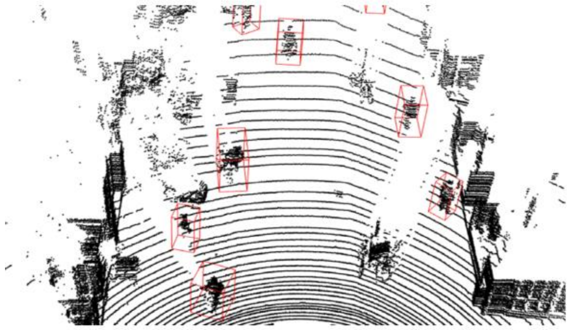
Point Cloud Denoising



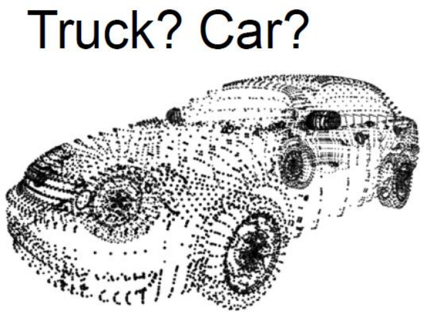
Point Cloud Segmentation



Point Cloud Inpainting

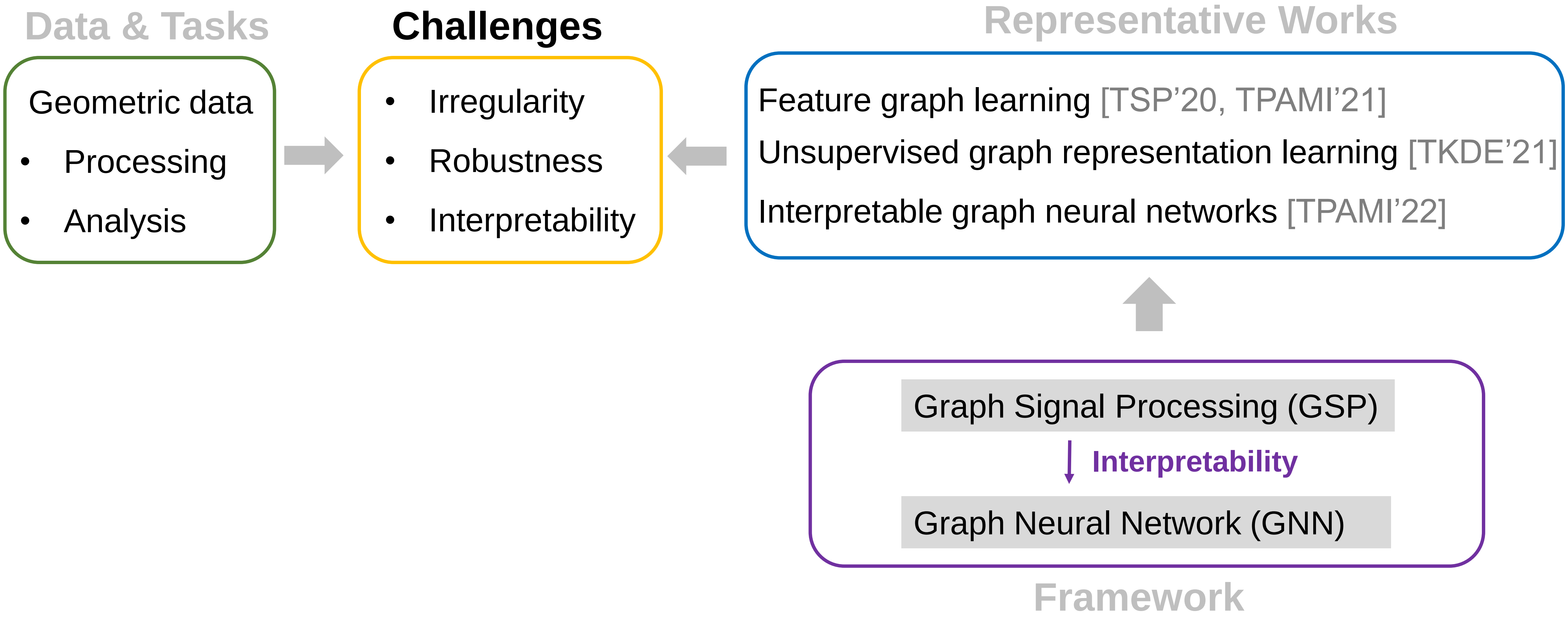


Point Cloud Detection



Point Cloud Classification

Outline



Data & Tasks

Geometric data

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Challenges

- Irregularity
- Robustness
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Representative Works

Feature graph learning [TSP’20, TPAMI’21]

Unsupervised graph representation learning [TKDE’21]

Interpretable graph neural networks [TPAMI’22]

Graph Signal Processing (GSP)

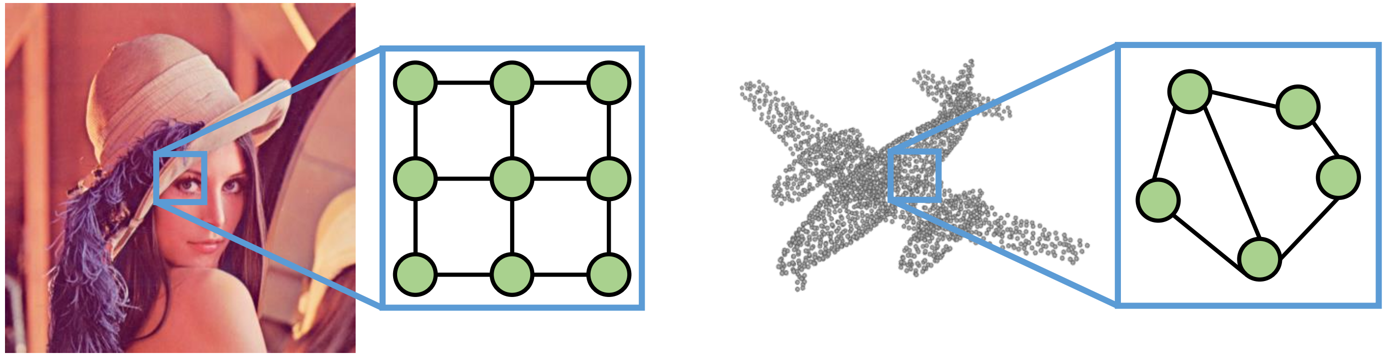
Interpretability

Graph Neural Network (GNN)

Framework

Challenges

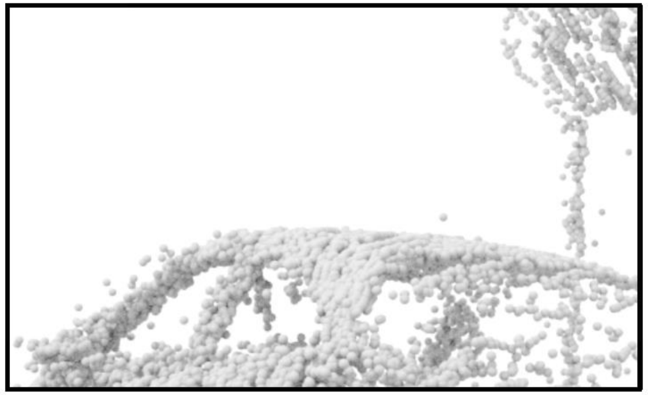
① Unlike images, a wide range of geometric data have **irregular sampling patterns**



Traditional image/video processing/analysis methods: assume sampling patterns over ***regular*** grids

② Real-world geometric data often suffer from noise, missing data, ….

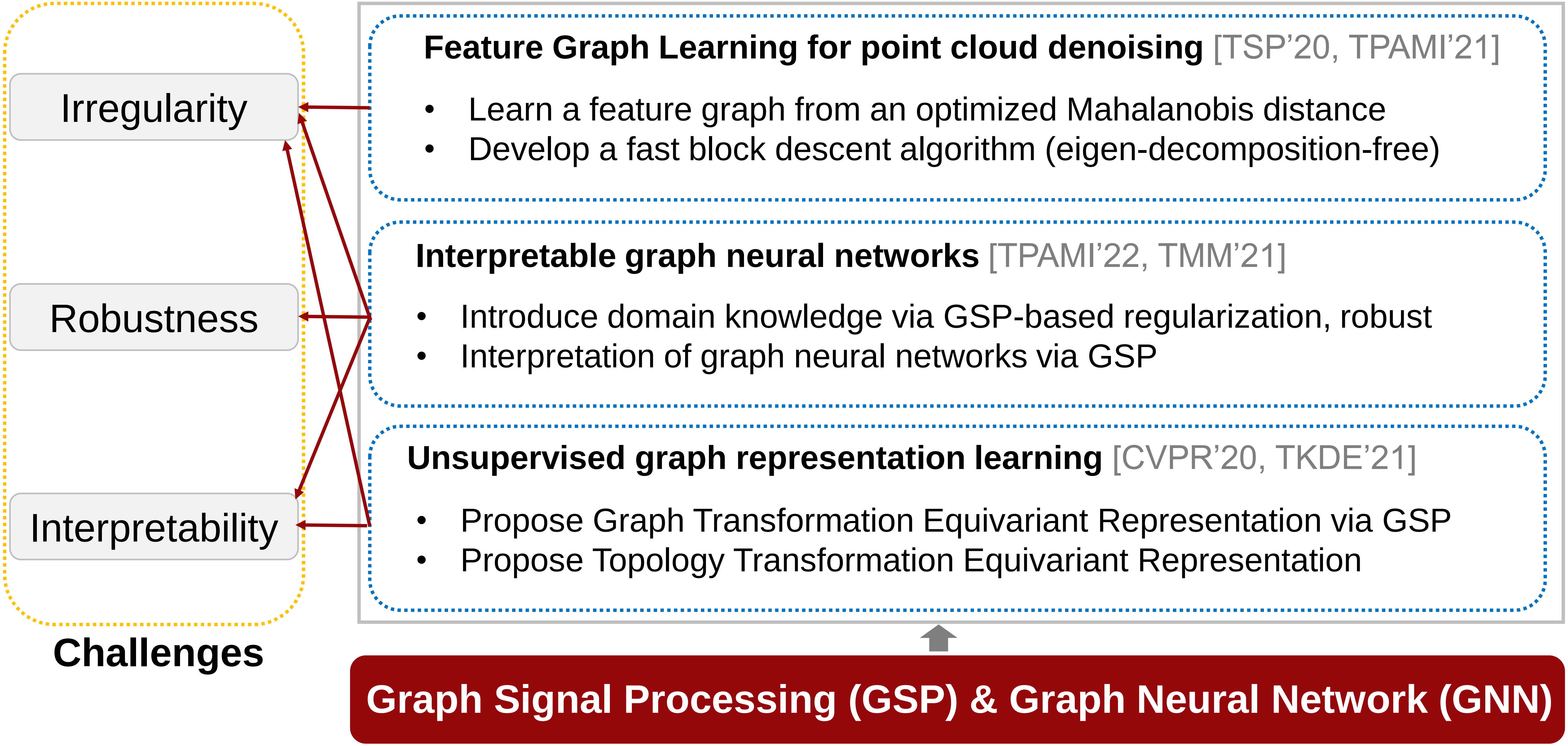
- ➢ Require **Robustness**



Paris-rue-Madame

③ Model **Interpretability** of geometric deep learning for analysis tasks

Contributions



Irregularity

Robustness

Interpretability

Challenges

Feature Graph Learning for point cloud denoising [TSP’20, TPAMI’21]

- Learn a feature graph from an optimized Mahalanobis distance
- Develop a fast block descent algorithm (eigen-decomposition-free)

Interpretable graph neural networks [TPAMI’22, TMM’21]

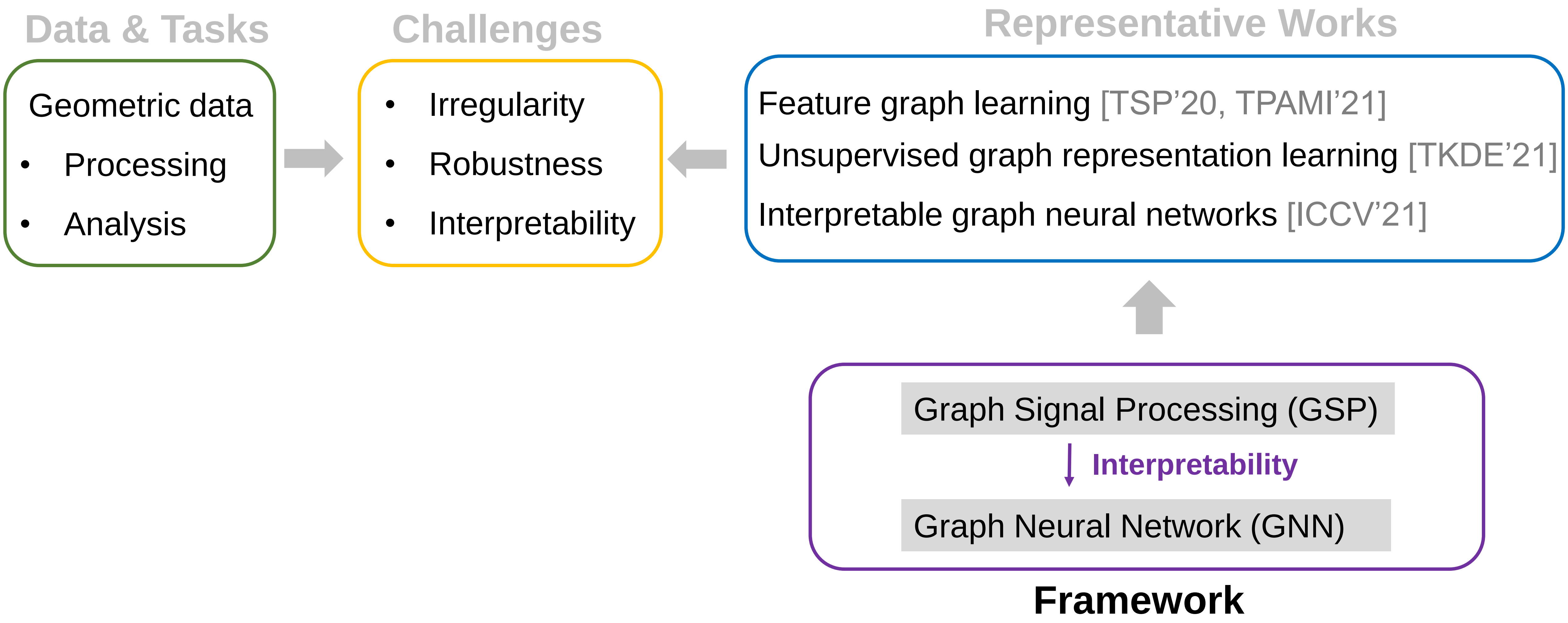
- Introduce domain knowledge via GSP-based regularization, robust
- Interpretation of graph neural networks via GSP

Unsupervised graph representation learning [CVPR’20, TKDE’21]

- Propose Graph Transformation Equivariant Representation via GSP
- Propose Topology Transformation Equivariant Representation

Graph Signal Processing (GSP) & Graph Neural Network (GNN)

Outline



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Interpretable graph neural networks [ICCV’21]

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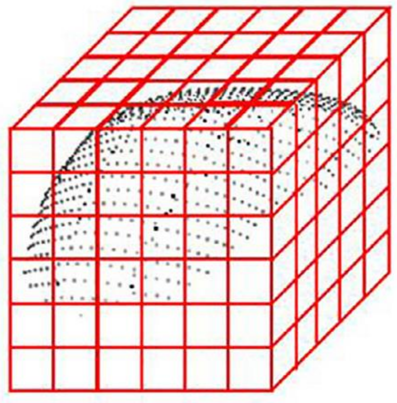
Framework

Why Graph Representation?

Non-Graph representations of irregular geometric data

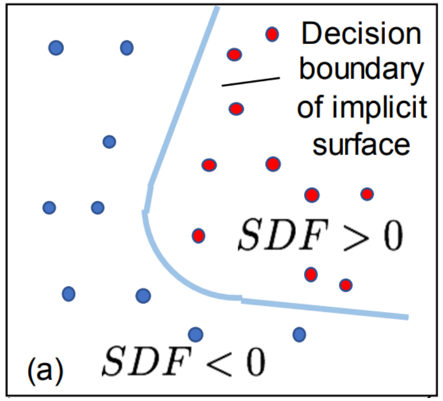
- Quantization-based representations



Quantize onto regular voxel grids

Project onto multiple viewpoints

- Implicit functions



Signed Distance Function

☺ Amenable to existing methods for Euclidean data

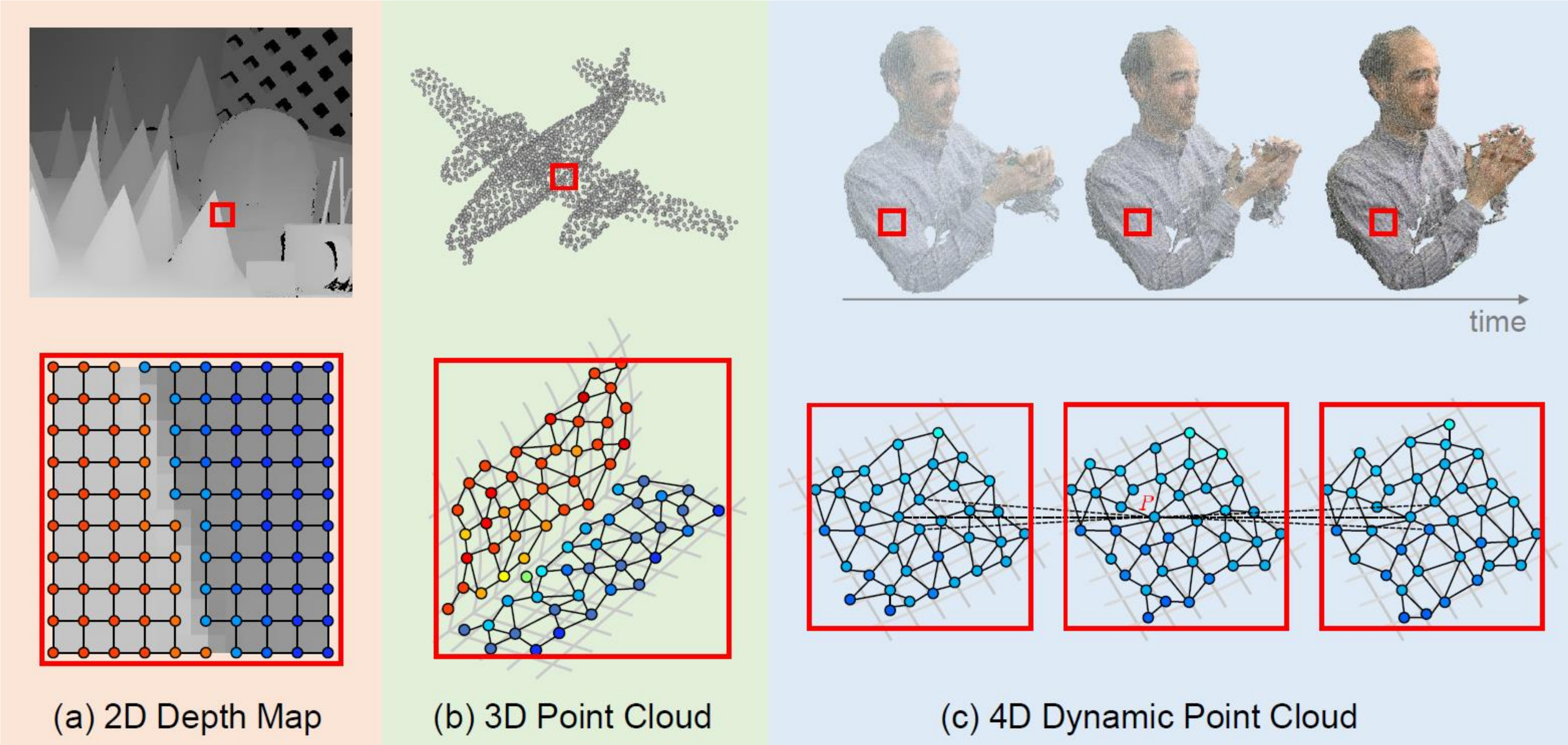
☹ Often deficient in capturing the geometric ***structure*** explicitly

☹ Sometimes inaccurate

☹ Sometimes redundant

Why Graph Representation?

- Graphs provide ***structure-adaptive***, ***accurate***, and ***compact*** representations for geometric data



Background in GSP & GNN

Graph Signal Processing (GSP)

- Extend classical signal processing to the graph domain
- Principled mathematical models
- **Theoretical** guarantee

Tools: **Graph filter**, Graph Fourier Transform, graph wavelets, etc.

Graph Neural Network (GNN)

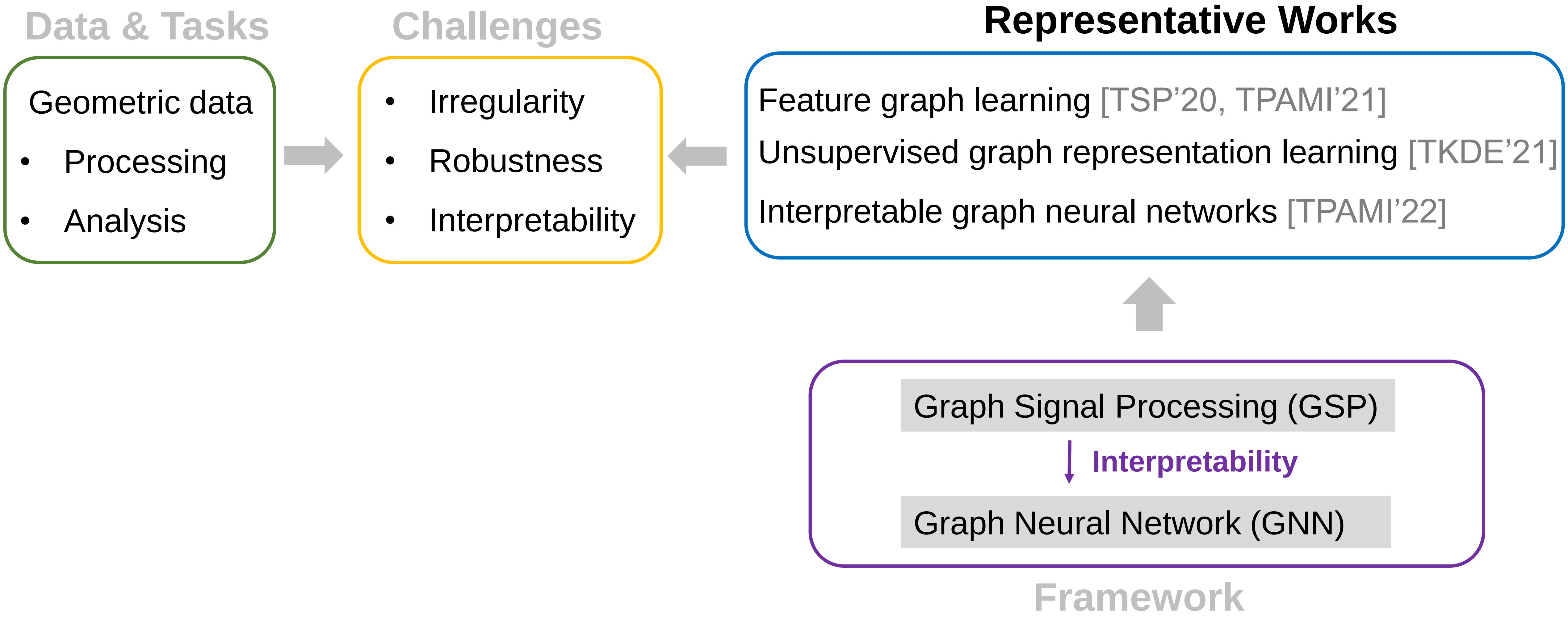
- Extend deep learning techniques to the graph domain
- Data-driven models
- **Empirical** performance

Tools: **Graph convolution**, graph attention, graph pooling, etc.

- **Interpretability** (e.g., interpretation of graph convolution)
- **Introduce GSP-based domain knowledge into GNNs**

Wei Hu, Jiahao Pang, Xianming Liu, Dong Tian, Chia-Wen Lin, Anthony Vetro, “Graph Signal Processing for Geometric Data and Beyond: Theory and Applications,” accepted to TMM, 2021.

Outline



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Graph Signal Processing (GSP)

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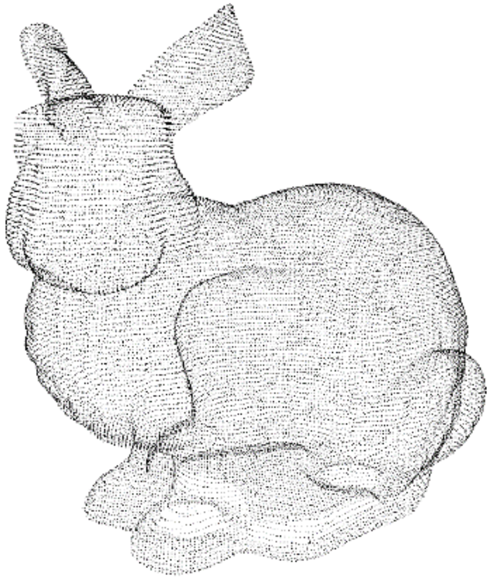
Framework

Problem Statement - Feature graph learning

- **Problem:** The graph is often unavailable over geometric data

- **Previous works:**
  - ➢ Previous graph learning methods often require *multiple observations*

- **Contributions:**
  - ➢ Given **feature vector** per node, we propose feature graph learning from only **a single or even partial signal observation**
  - ➢ Develop a fast algorithm (eigen-decomposition-free)



Wei Hu, Xiang Gao, Gene Cheung, Zongming Guo, "Feature Graph Learning for 3D Point Cloud Denoising," *IEEE Transactions on Signal Processing (TSP)*, vol. 68, pp.2841-2856, March 2020.

Cheng Yang, Gene Cheung, **Wei Hu**, "Signed Graph Metric Learning via Gershgorin Disc Alignment," accepted to *IEEE Transactions on Pattern Analysis and Machine Intelligence (TPAMI)*, 2021.

Key Idea - Feature graph learning

- Given **a single or partial observation** with relevant **feature vector** $\mathbf{f}_i$, compute the *Mahalanobis distance*: $$\delta_{i,j} = (\mathbf{f}_i - \mathbf{f}_j)^\top \mathbf{M} (\mathbf{f}_i - \mathbf{f}_j)$$ ↖ PD **metric matrix**

- **Edge weight** $w_{i,j}$ of **feature graph** is $w_{i,j} = \exp\{-\delta_{i,j}\}$ ⟵ feature distance

- Minimize **Graph Laplacian Regularizer** (GLR):

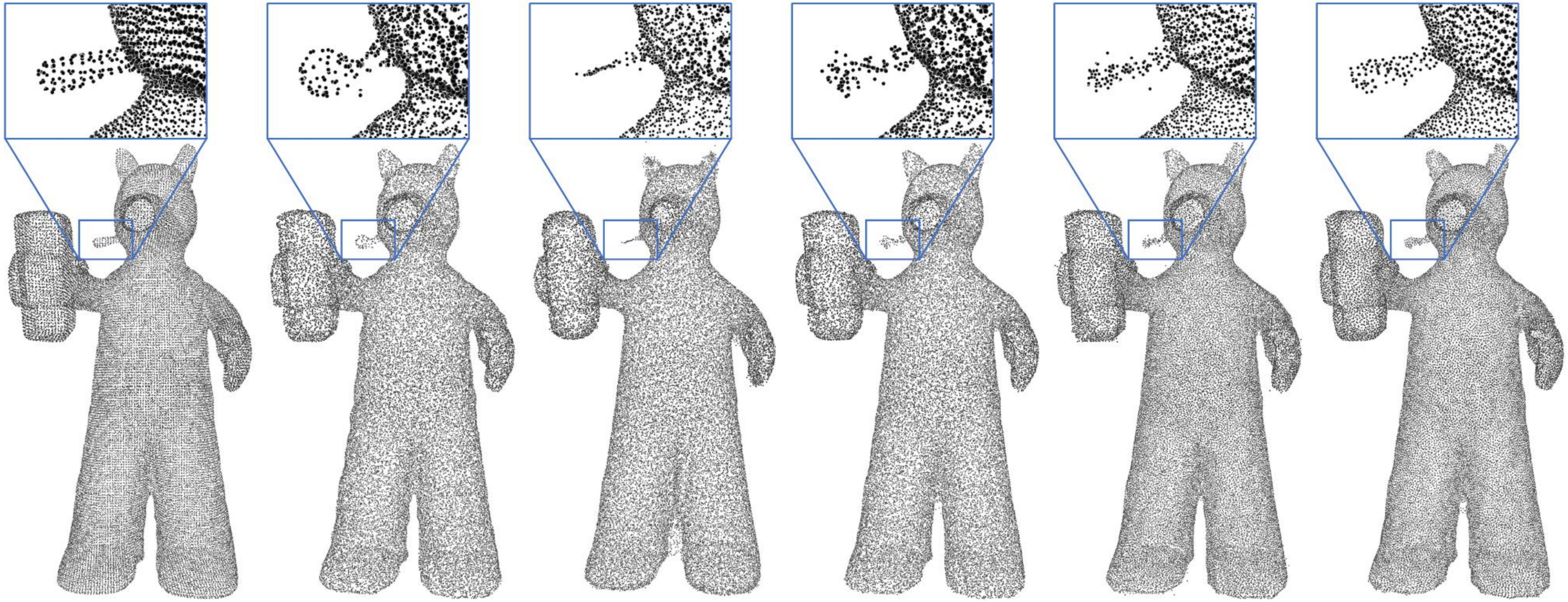
$$\min_{\mathbf{M}} \boxed{\mathbf{x}^\top \mathbf{L} \mathbf{x} = \sum_{i,j} w_{i,j}(x_i - x_j)^2} = \sum_{i,j} \exp\{-(\mathbf{f}_i - \mathbf{f}_j)^\top \mathbf{M} (\mathbf{f}_i - \mathbf{f}_j)\} d_{i,j}$$

$$\text{s.t.} \quad \mathbf{M} \succ 0; \quad \operatorname{tr}(\mathbf{M}) \le C.$$

Minimizing GLR makes the graph adapt to the signal structure

➢ Solved via our proposed **eigen-decomposition-free** block-coordinate descent algorithm

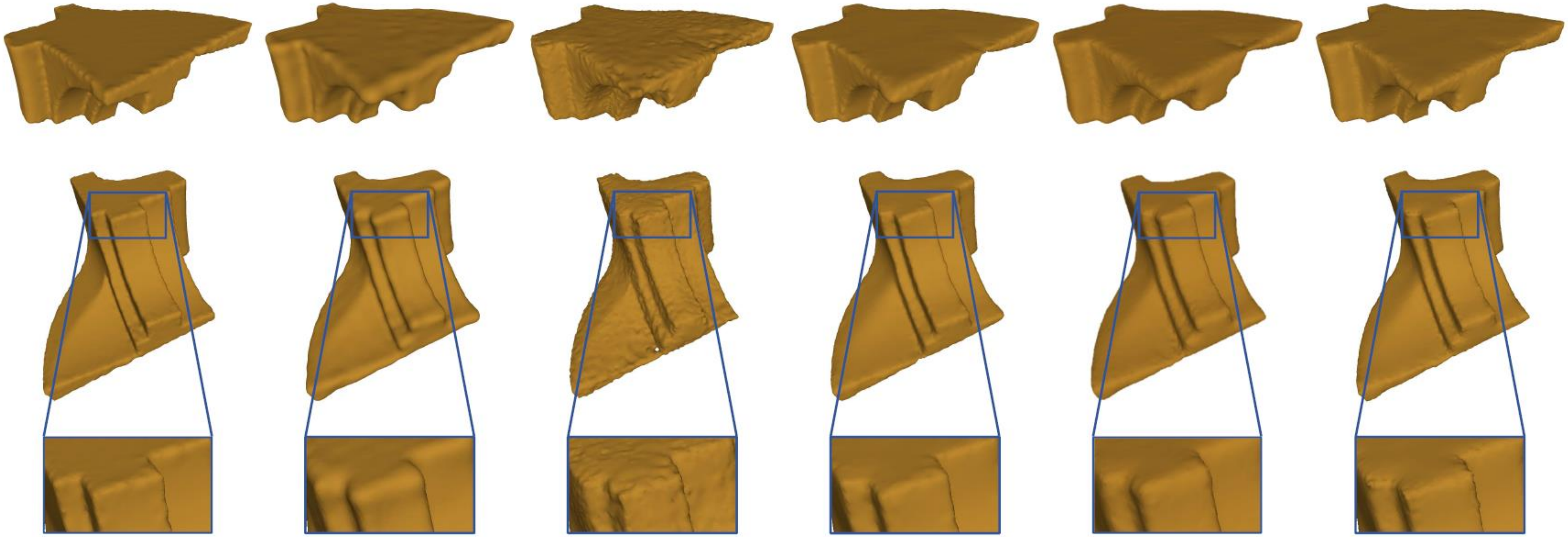
Results: 3D Point Cloud Denoising



(a) Ground-truth (b) APSS (c) AWLOP (d) MRPCA (e) GLR (f) Ours

Wei Hu, Xiang Gao, Gene Cheung, Zongming Guo, “Feature Graph Learning for 3D Point Cloud Denoising,” *IEEE Transactions on Signal Processing (TSP)*, vol. 68, pp.2841-2856, March 2020.

Results: 3D Point Cloud Denoising



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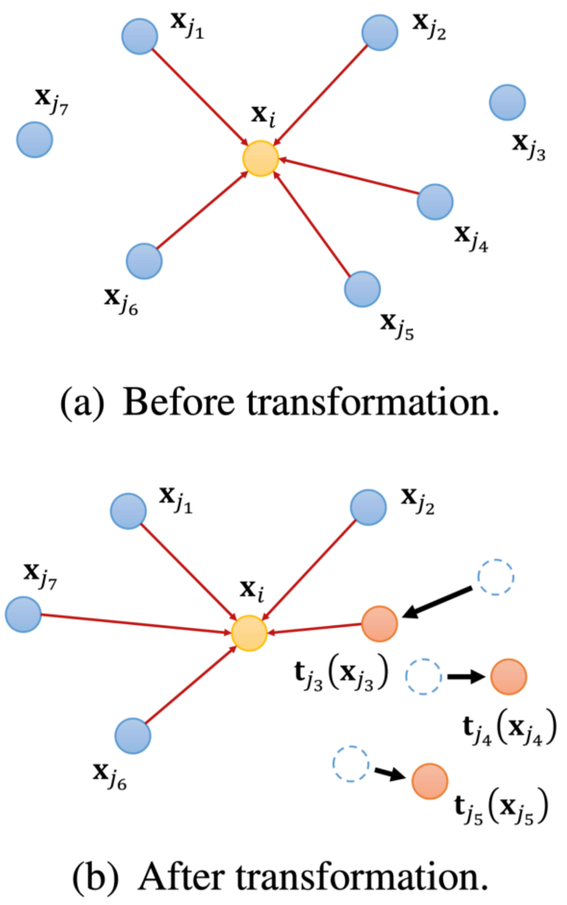
Problem Statement – Unsupervised GraphTER learning

- **Problem:** Existing GNNs are mostly trained in a (semi-)supervised manner, requiring **a large amount of labeled data**
- **Previous works: Transformation Equivariant Representation**
  - **Assumption**: representations equivarying to transformations are able to encode the intrinsic structures of data
  - **Limitation**: focus on Euclidean data such as images, which cannot be directly extended to graphs
- **Contributions:**
  - Define generic graph signal transformations
  - Propose **Graph Transformation Equivariant Representation** (GraphTER) learning in an **unsupervised** manner



(a) Before transformation.

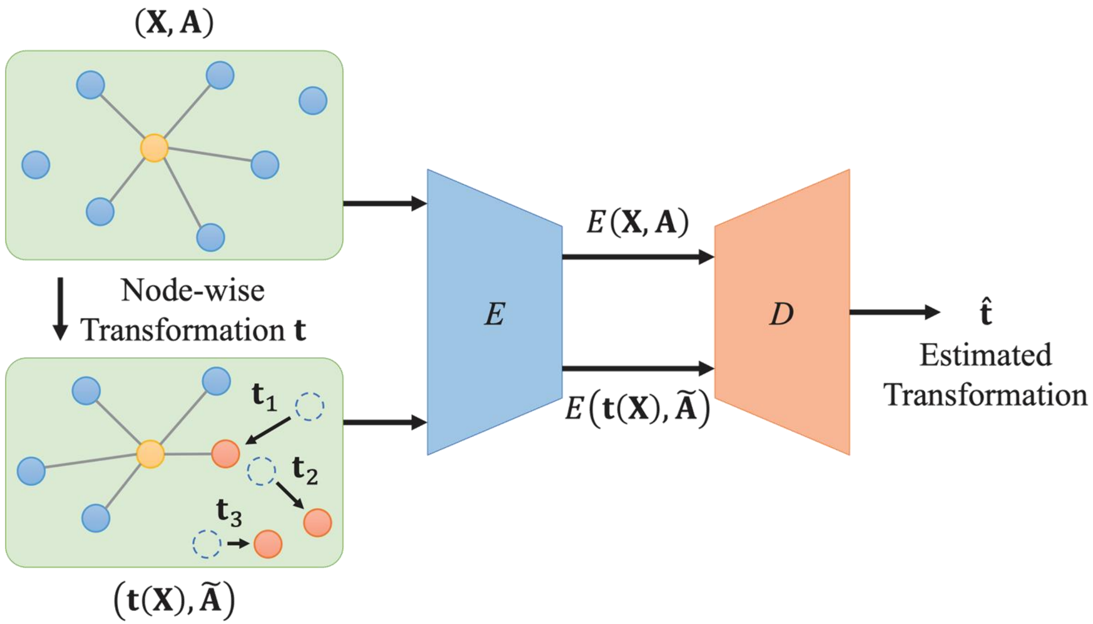
$\mathbf{x}_{j_1}$
$\mathbf{x}_{j_2}$
$\mathbf{x}_{j_7}$
$\mathbf{x}_i$
$\mathbf{t}_{j_3}(\mathbf{x}_{j_3})$
$\mathbf{t}_{j_4}(\mathbf{x}_{j_4})$
$\mathbf{x}_{j_6}$
$\mathbf{t}_{j_5}(\mathbf{x}_{j_5})$

(b) After transformation.

Xiang Gao, **Wei Hu**, Guo-Jun Qi, “GraphTER: Unsupervised Learning of Graph Transformation Equivariant Representations via Auto-Encoding Node-wise Transformations,” IEEE CVPR, 2020.

Key Idea - Unsupervised GraphTER learning

- Define a generic **graph signal transformation** on the signal $\mathbf{X}$ as **node-wise graph filtering** on $\mathbf{X}$, e.g.,
  - Low-pass graph filtering (averaging connected nodes)
  - Node-independent graph filtering


$(\mathbf{X}, \mathbf{A})$
Node-wise Transformation $\mathbf{t}$
$\mathbf{t}_1$
$\mathbf{t}_2$
$\mathbf{t}_3$
$(\mathbf{t}(\mathbf{X}), \tilde{\mathbf{A}})$
E
$E(\mathbf{X}, \mathbf{A})$
$E(\mathbf{t}(\mathbf{X}), \tilde{\mathbf{A}})$
D
$\hat{\mathbf{t}}$
Estimated Transformation

- A function $E(\cdot)$ is transformation equivariant if

$$E\left(\underset{\downarrow}{\mathbf{t}}(\mathbf{X}), f\left(\mathbf{t}(\mathbf{X})\right)\right) = \underset{\downarrow}{\rho(\mathbf{t})}[E(\mathbf{X}, \mathbf{A})]$$

node-wise transformation

homomorphism transformation of t

The function $E(\cdot)$ extracts equivariant representations of graph signal $\mathbf{X}$

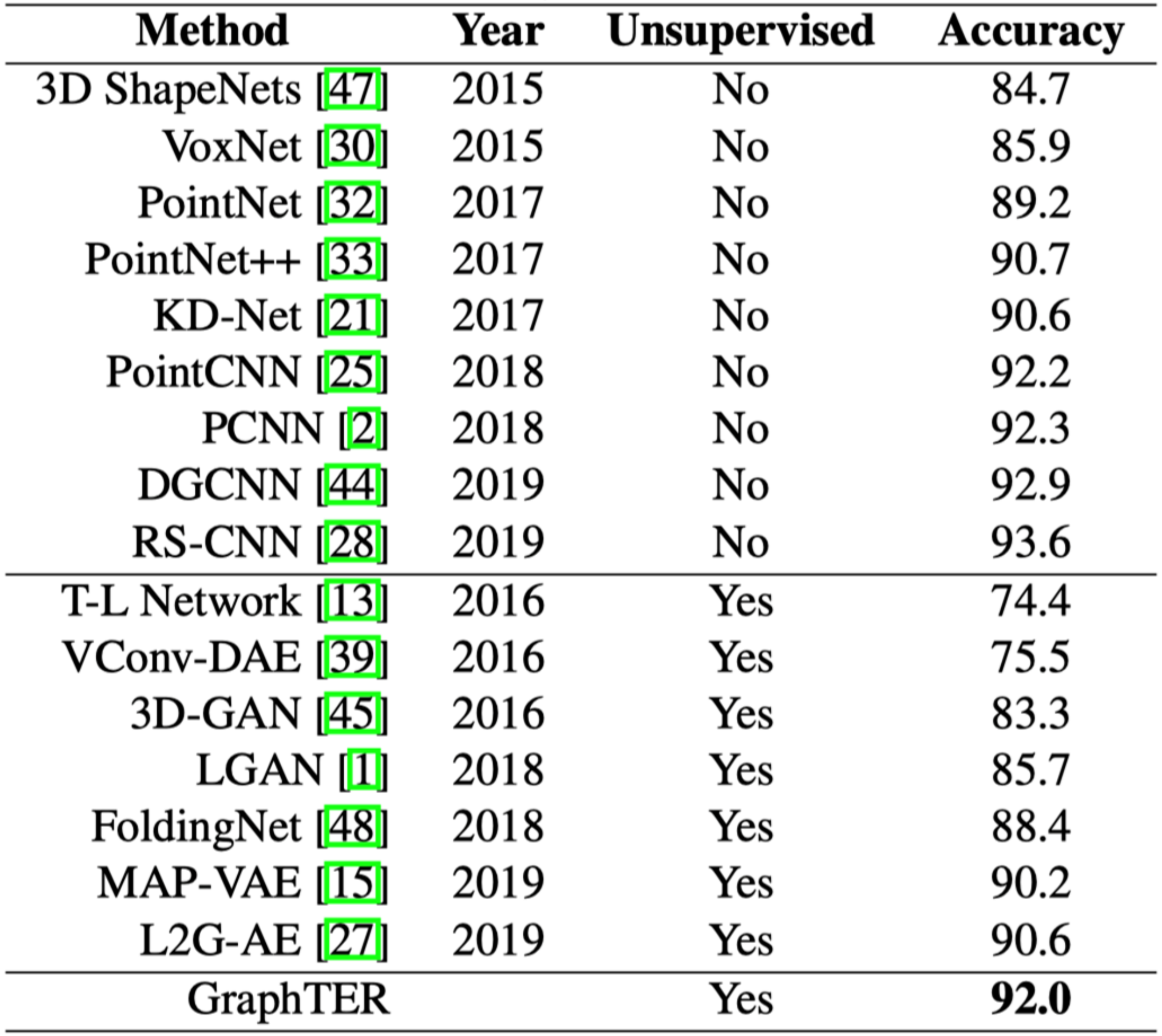
Xiang Gao, **Wei Hu**, Guo-Jun Qi, "GraphTER: Unsupervised Learning of Graph Transformation Equivariant Representations via Auto-Encoding Node-wise Transformations," IEEE CVPR, 2020.

Results: unsupervised point cloud learning

3D Point Cloud Classification

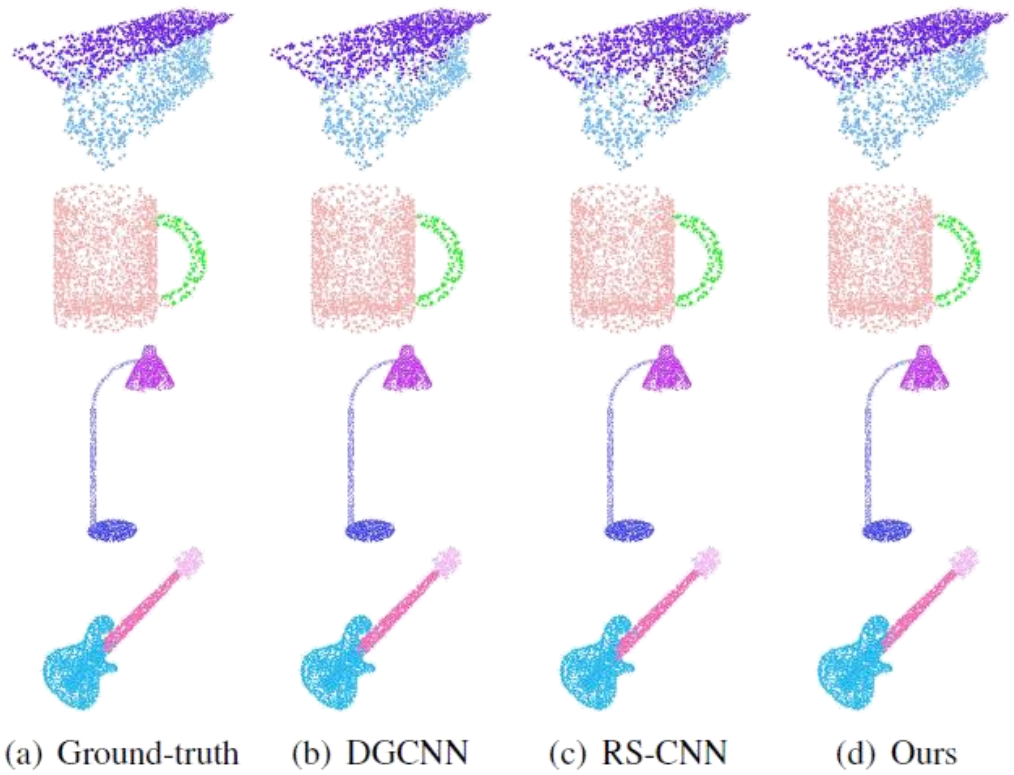
- Dataset: ModelNet40
- Metric: Accuracy (%)

Approach the upper bound set by the fully supervised counterparts

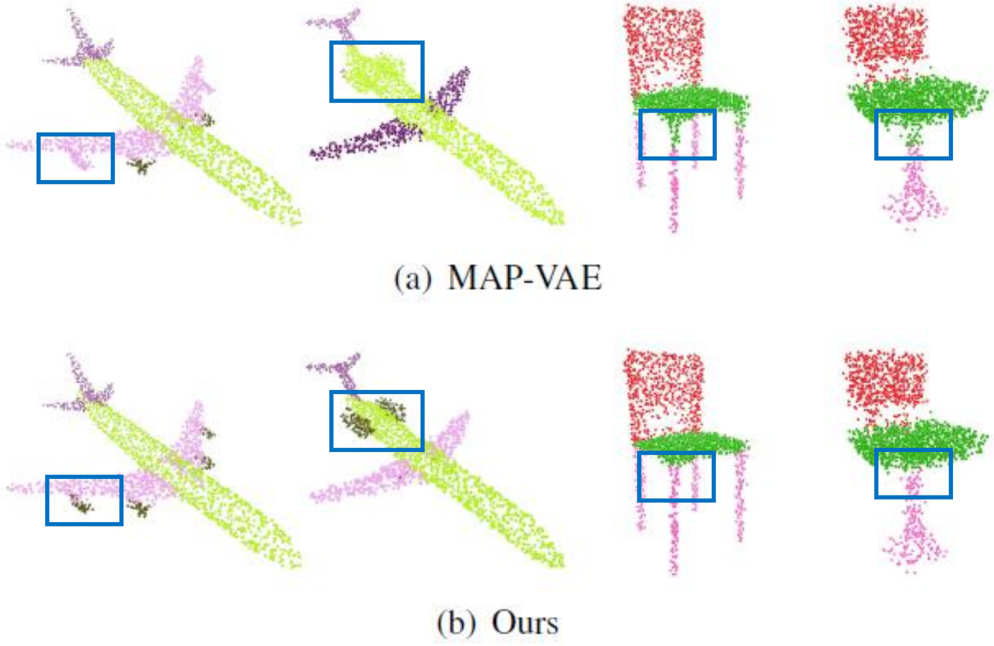


Method	Year	Unsupervised	Accuracy
3D ShapeNets [47]	2015	No	84.7
VoxNet [30]	2015	No	85.9
PointNet [32]	2017	No	89.2
PointNet++ [33]	2017	No	90.7
KD-Net [21]	2017	No	90.6
PointCNN [25]	2018	No	92.2
PCNN [2]	2018	No	92.3
DGCNN [44]	2019	No	92.9
RS-CNN [28]	2019	No	93.6
T-L Network [13]	2016	Yes	74.4
VConv-DAE [39]	2016	Yes	75.5
3D-GAN [45]	2016	Yes	83.3
LGAN [1]	2018	Yes	85.7
FoldingNet [48]	2018	Yes	88.4
MAP-VAE [15]	2019	Yes	90.2
L2G-AE [27]	2019	Yes	90.6
GraphTER		Yes	**92.0**

Results: unsupervised point cloud learning



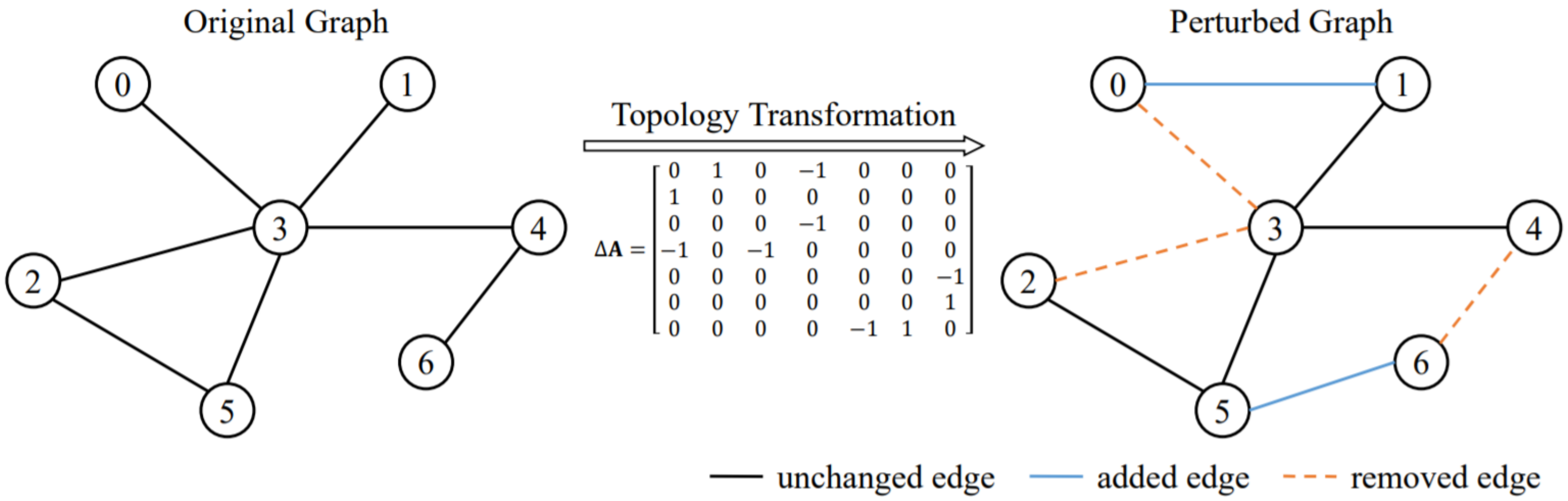
Visual comparison with
the **supervised** methods



Visual comparison with
the SOTA **unsupervised** method

Extension to Unsupervised TopoTER learning

Idea: maximize the mutual information between topology transformations & node representations before and after the transformations.



$$\Delta\mathbf{A}=\begin{bmatrix}0&1&0&-1&0&0&0\\1&0&0&0&0&0&0\\0&0&0&-1&0&0&0\\-1&0&-1&0&0&0&0\\0&0&0&0&0&0&-1\\0&0&0&0&0&0&1\\0&0&0&0&-1&1&0\end{bmatrix}$$

$$E\left(\mathbf{X},\widetilde{\mathbf{A}}\right)=E\left(\mathbf{X},\mathbf{t}(\mathbf{A})\right)=\rho(\mathbf{t})[E(\mathbf{X},\mathbf{A})]$$

Encoder $E:(\mathbf{X},\mathbf{A})\mapsto\mathbf{H},\left(\mathbf{X},\widetilde{\mathbf{A}}\right)\mapsto\widetilde{\mathbf{H}}$

Decoder $D:\left(\mathbf{H},\widetilde{\mathbf{H}}\right)\mapsto\widehat{\Delta\mathbf{A}}$

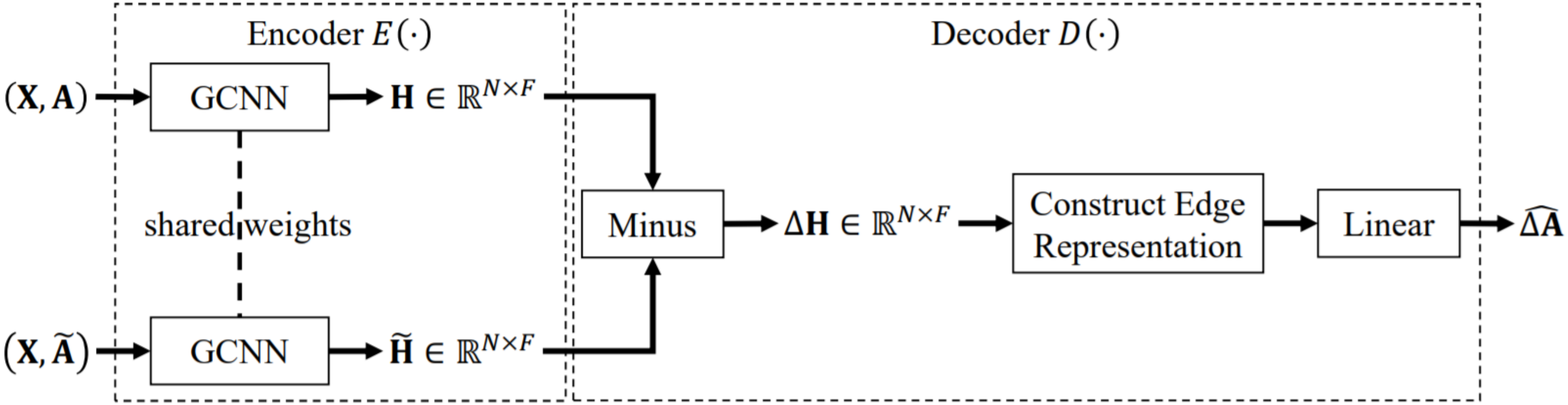
Xiang Gao, **Wei Hu**, Guo-Jun Qi, “Self-Supervised Graph Representation Learning via Topology Transformations,” accepted to IEEE TKDE, May, 2021.

Extension to Unsupervised TopoTER learning

Idea: maximize the mutual information between topology transformations & node representations before and after the transformations.

$$\max_{\theta} I\left(\mathbf{H}, \Delta\mathbf{A}; \widetilde{\mathbf{H}}\right)$$

$$\min_{\theta} H\left(p\left(\Delta\mathbf{A}, \widetilde{\mathbf{H}}, \mathbf{H}\right) \parallel q\left(\widehat{\Delta\mathbf{A}} \mid \widetilde{\mathbf{H}}, \mathbf{H}\right)\right) \triangleq - \underset{p\left(\Delta\mathbf{A}, \widetilde{\mathbf{H}}, \mathbf{H}\right)}{\mathbb{E}} \log q\left(\widehat{\Delta\mathbf{A}} \mid \widetilde{\mathbf{H}}, \mathbf{H}\right)$$

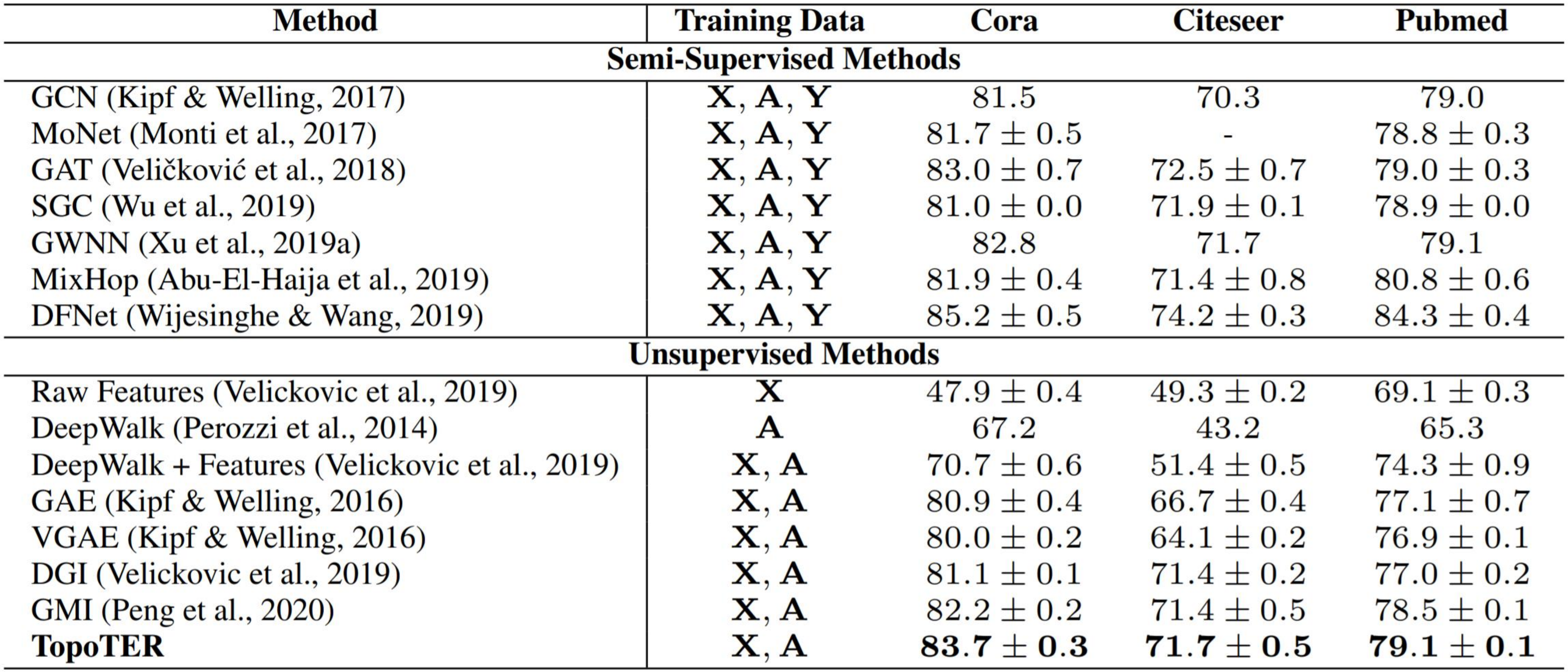


Encoder $E(\cdot)$
Decoder $D(\cdot)$
$(\mathbf{X}, \mathbf{A})$
GCNN
$\mathbf{H} \in \mathbb{R}^{N \times F}$
shared weights
$(\mathbf{X}, \widetilde{\mathbf{A}})$
GCNN
$\widetilde{\mathbf{H}} \in \mathbb{R}^{N \times F}$
Minus
$\Delta\mathbf{H} \in \mathbb{R}^{N \times F}$
Construct Edge Representation
Linear
$\widehat{\Delta\mathbf{A}}$

Xiang Gao, **Wei Hu**, Guo-Jun Qi, "Self-Supervised Graph Representation Learning via Topology Transformations," accepted to IEEE TKDE, May, 2021.

Extension to Unsupervised TopoTER learning

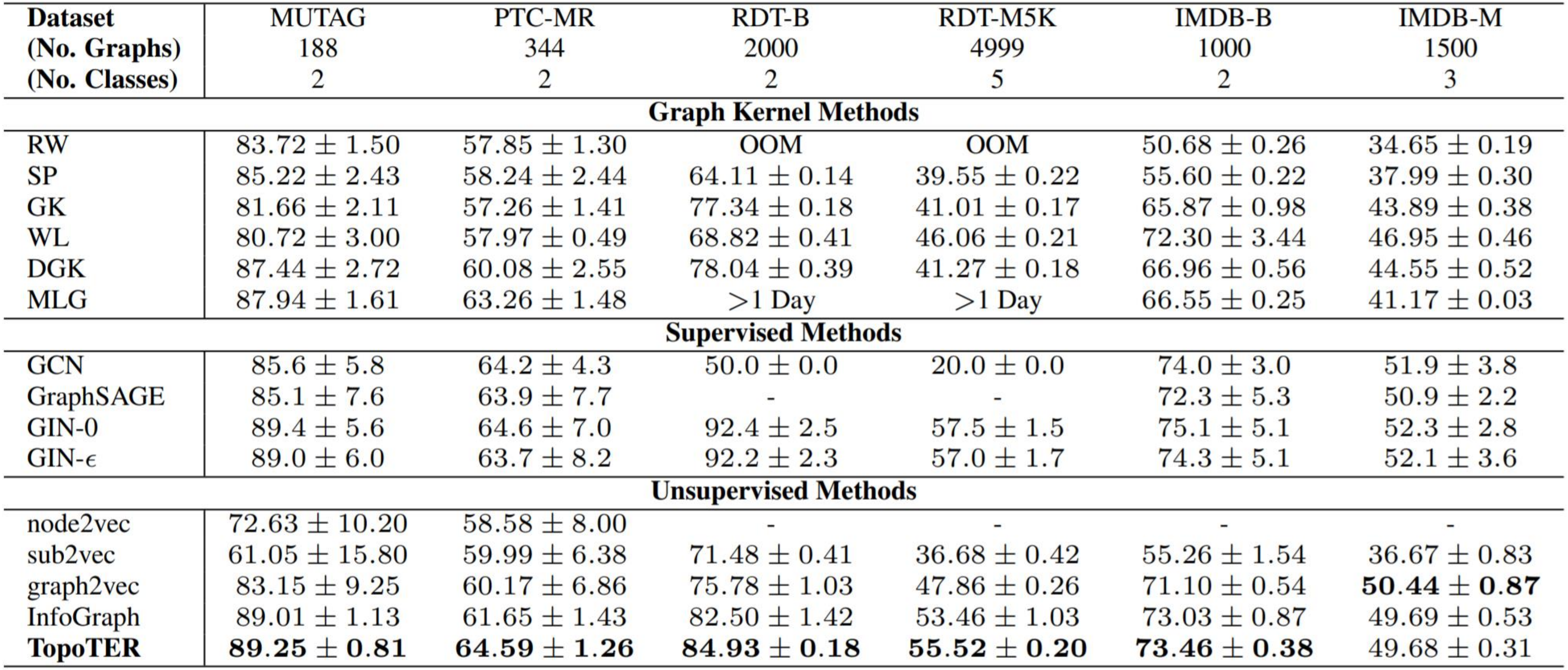
Results on node classification



Method	Training Data	Cora	Citeseer	Pubmed
Semi-Supervised Methods				
GCN (Kipf & Welling, 2017)	$\mathbf{X}, \mathbf{A}, \mathbf{Y}$	81.5	70.3	79.0
MoNet (Monti et al., 2017)	$\mathbf{X}, \mathbf{A}, \mathbf{Y}$	81.7 ± 0.5	-	78.8 ± 0.3
GAT (Veličković et al., 2018)	$\mathbf{X}, \mathbf{A}, \mathbf{Y}$	83.0 ± 0.7	72.5 ± 0.7	79.0 ± 0.3
SGC (Wu et al., 2019)	$\mathbf{X}, \mathbf{A}, \mathbf{Y}$	81.0 ± 0.0	71.9 ± 0.1	78.9 ± 0.0
GWNN (Xu et al., 2019a)	$\mathbf{X}, \mathbf{A}, \mathbf{Y}$	82.8	71.7	79.1
MixHop (Abu-El-Haija et al., 2019)	$\mathbf{X}, \mathbf{A}, \mathbf{Y}$	81.9 ± 0.4	71.4 ± 0.8	80.8 ± 0.6
DFNet (Wijesinghe & Wang, 2019)	$\mathbf{X}, \mathbf{A}, \mathbf{Y}$	85.2 ± 0.5	74.2 ± 0.3	84.3 ± 0.4
Unsupervised Methods				
Raw Features (Velickovic et al., 2019)	$\mathbf{X}$	47.9 ± 0.4	49.3 ± 0.2	69.1 ± 0.3
DeepWalk (Perozzi et al., 2014)	$\mathbf{A}$	67.2	43.2	65.3
DeepWalk + Features (Velickovic et al., 2019)	$\mathbf{X}, \mathbf{A}$	70.7 ± 0.6	51.4 ± 0.5	74.3 ± 0.9
GAE (Kipf & Welling, 2016)	$\mathbf{X}, \mathbf{A}$	80.9 ± 0.4	66.7 ± 0.4	77.1 ± 0.7
VGAE (Kipf & Welling, 2016)	$\mathbf{X}, \mathbf{A}$	80.0 ± 0.2	64.1 ± 0.2	76.9 ± 0.1
DGI (Velickovic et al., 2019)	$\mathbf{X}, \mathbf{A}$	81.1 ± 0.1	71.4 ± 0.2	77.0 ± 0.2
GMI (Peng et al., 2020)	$\mathbf{X}, \mathbf{A}$	82.2 ± 0.2	71.4 ± 0.5	78.5 ± 0.1
TopoTER	$\mathbf{X}, \mathbf{A}$	$\mathbf{83.7 \pm 0.3}$	$\mathbf{71.7 \pm 0.5}$	$\mathbf{79.1 \pm 0.1}$

Extension to Unsupervised TopoTER learning

Results on graph classification



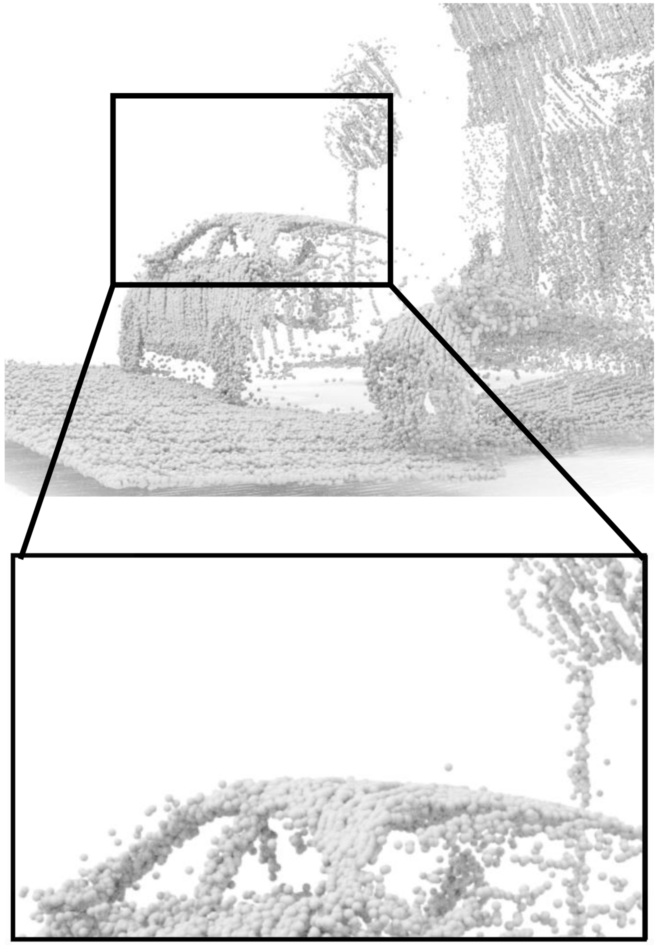
Dataset	MUTAG	PTC-MR	RDT-B	RDT-M5K	IMDB-B	IMDB-M
(No. Graphs)	188	344	2000	4999	1000	1500
(No. Classes)	2	2	2	5	2	3
Graph Kernel Methods						
RW	83.72 ± 1.50	57.85 ± 1.30	OOM	OOM	50.68 ± 0.26	34.65 ± 0.19
SP	85.22 ± 2.43	58.24 ± 2.44	64.11 ± 0.14	39.55 ± 0.22	55.60 ± 0.22	37.99 ± 0.30
GK	81.66 ± 2.11	57.26 ± 1.41	77.34 ± 0.18	41.01 ± 0.17	65.87 ± 0.98	43.89 ± 0.38
WL	80.72 ± 3.00	57.97 ± 0.49	68.82 ± 0.41	46.06 ± 0.21	72.30 ± 3.44	46.95 ± 0.46
DGK	87.44 ± 2.72	60.08 ± 2.55	78.04 ± 0.39	41.27 ± 0.18	66.96 ± 0.56	44.55 ± 0.52
MLG	87.94 ± 1.61	63.26 ± 1.48	>1 Day	>1 Day	66.55 ± 0.25	41.17 ± 0.03
Supervised Methods						
GCN	85.6 ± 5.8	64.2 ± 4.3	50.0 ± 0.0	20.0 ± 0.0	74.0 ± 3.0	51.9 ± 3.8
GraphSAGE	85.1 ± 7.6	63.9 ± 7.7	-	-	72.3 ± 5.3	50.9 ± 2.2
GIN-0	89.4 ± 5.6	64.6 ± 7.0	92.4 ± 2.5	57.5 ± 1.5	75.1 ± 5.1	52.3 ± 2.8
GIN-ϵ	89.0 ± 6.0	63.7 ± 8.2	92.2 ± 2.3	57.0 ± 1.7	74.3 ± 5.1	52.1 ± 3.6
Unsupervised Methods						
node2vec	72.63 ± 10.20	58.58 ± 8.00	-	-	-	-
sub2vec	61.05 ± 15.80	59.99 ± 6.38	71.48 ± 0.41	36.68 ± 0.42	55.26 ± 1.54	36.67 ± 0.83
graph2vec	83.15 ± 9.25	60.17 ± 6.86	75.78 ± 1.03	47.86 ± 0.26	71.10 ± 0.54	**50.44 ± 0.87**
InfoGraph	89.01 ± 1.13	61.65 ± 1.43	82.50 ± 1.42	53.46 ± 1.03	73.03 ± 0.87	49.69 ± 0.53
TopoTER	**89.25 ± 0.81**	**64.59 ± 1.26**	**84.93 ± 0.18**	**55.52 ± 0.20**	**73.46 ± 0.38**	49.68 ± 0.31

Problem Statement – Interpretable Graph Neural Networks

- **Problem:** Real-word data often suffer from **noise**, **missing data**…

- **Previous Works:**
  - Optimization-based approaches rely heavily on geometric priors
  - Deep learning methods often suffer from over-estimation or under-estimation of the displacement

- **Contributions:**
  - propose deep point set resampling for point cloud restoration, which models the distribution of degraded point clouds via **gradient fields** and converges points towards the underlying surface for restoration.



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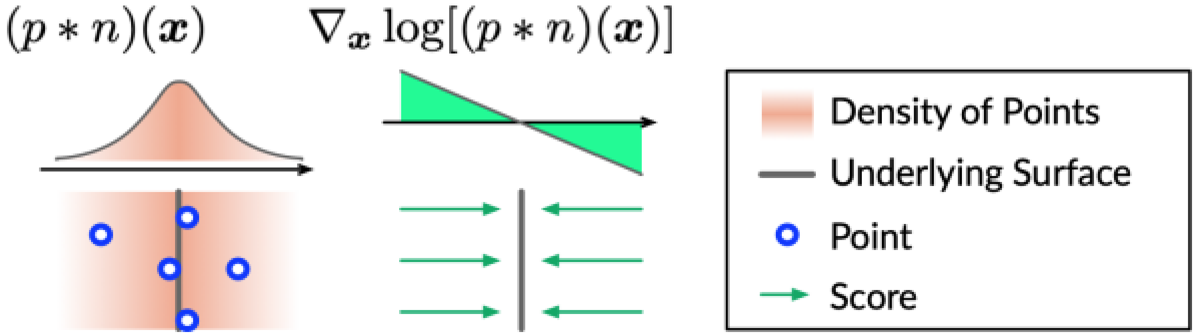
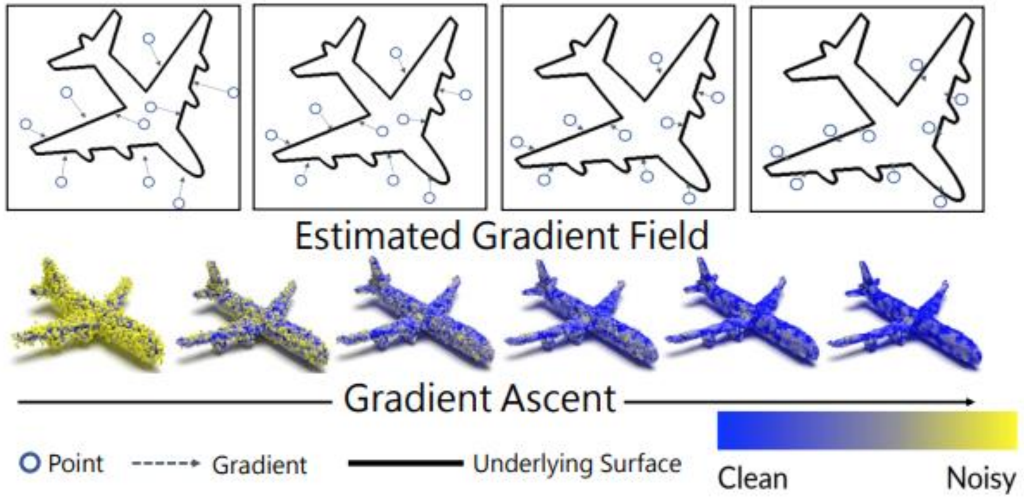
Shitong Luo, **Wei Hu**, "Score-Based Point Cloud Denoising," ICCV 2021.
Haolan Chen, Bi'an Du, Shitong Luo, **Wei Hu**, "Deep Point Set Resampling via Gradient Fields," accepted to TPAMI, 2022.

Key Idea - Interpretable Graph Neural Networks

Key observation: the distribution of a noisy point cloud can be viewed as the distribution of noise-free points $p(\boldsymbol{x})$ convolved with some noise model n, leading to $(p * n)(\boldsymbol{x})$


$(p * n)(\boldsymbol{x})$
$\nabla_{\boldsymbol{x}} \log[(p * n)(\boldsymbol{x})]$
Density of Points
Underlying Surface
Point
Score



Perform gradient ascent on the log-probability function $\log[(p * n)(\boldsymbol{x})]$? $p * n$ is unknown!

- estimate the **gradient field** of the distribution: $\nabla_{\boldsymbol{x}} \log[(p * n)(\boldsymbol{x})]$,
- denoise the point cloud by gradient ascent to move noisy points towards the mode of $p * n$

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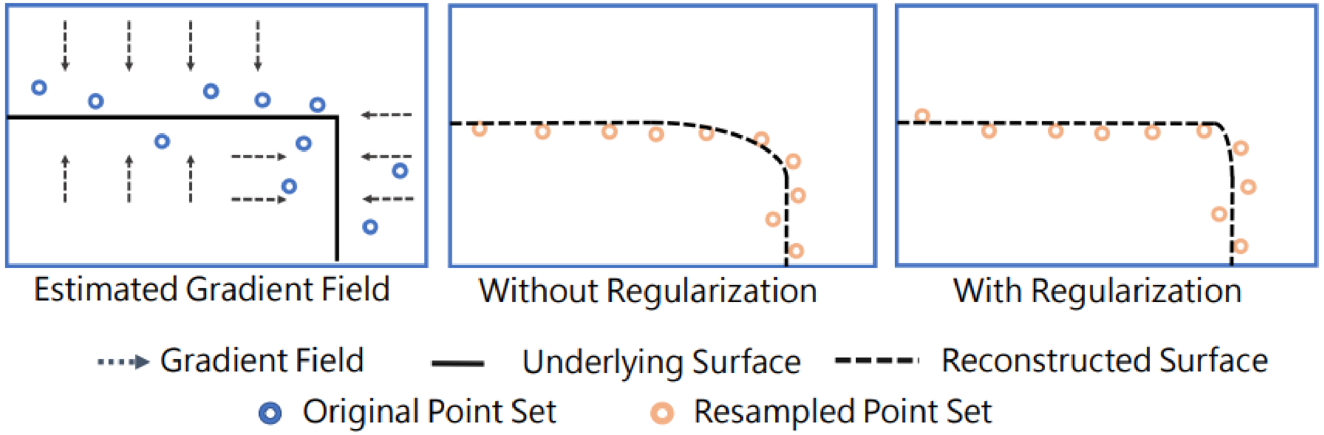
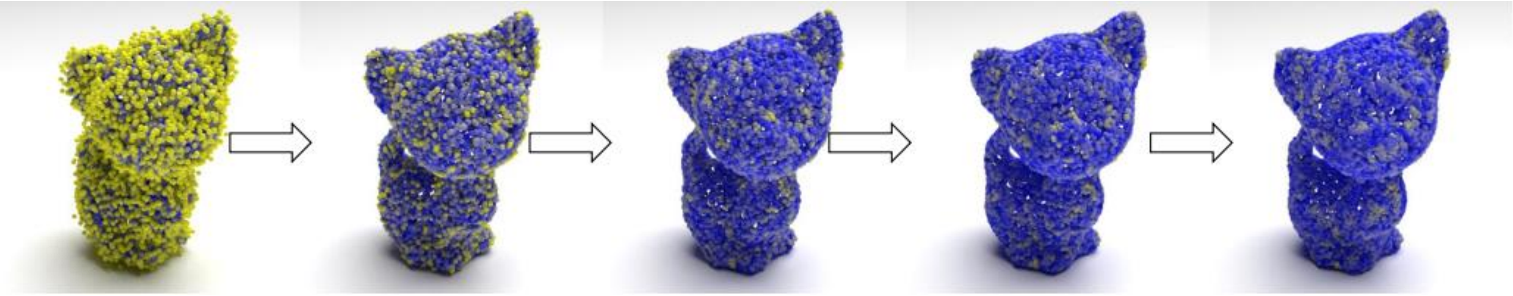
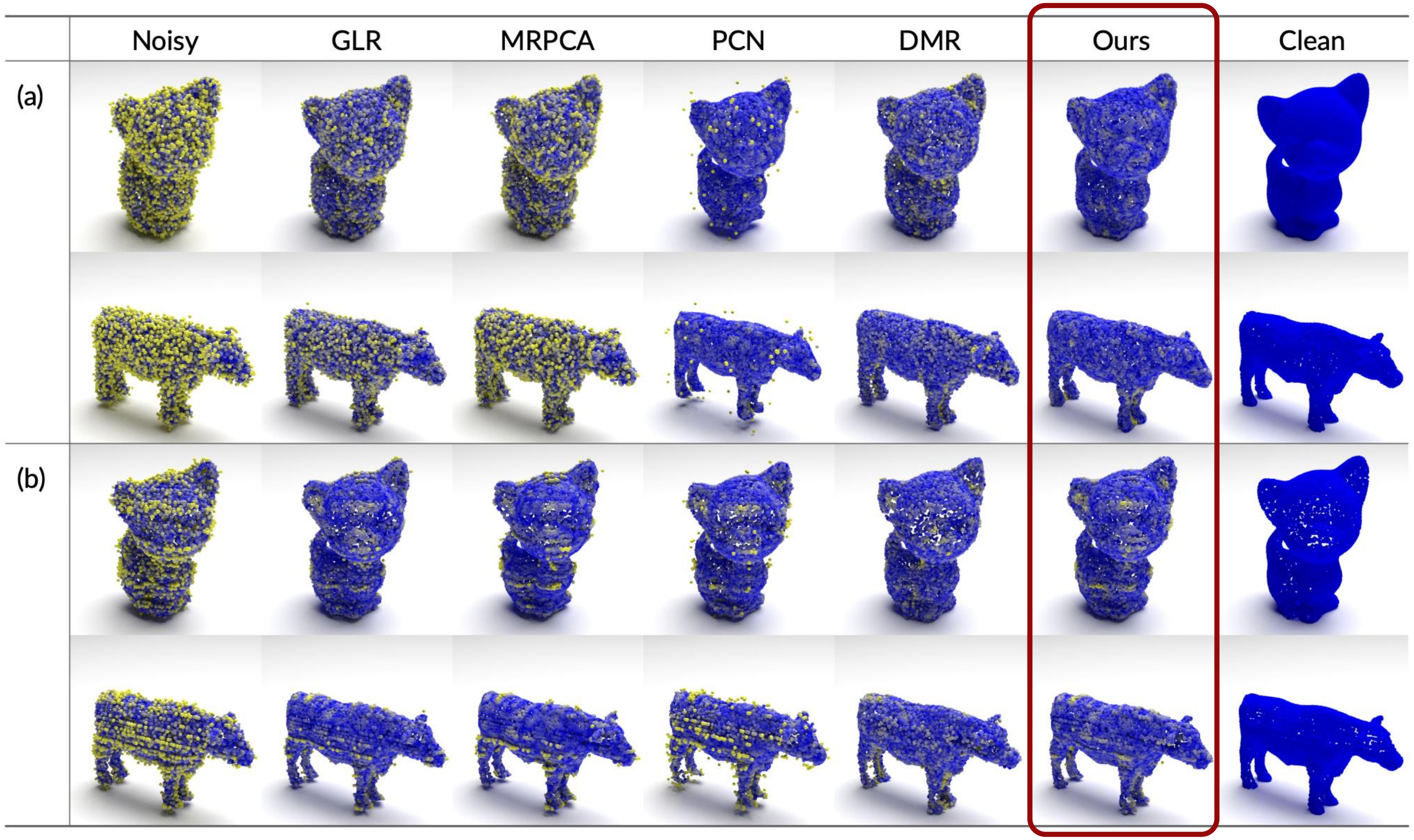


- introduce **regularization** (GLR, etc.) into the point set resampling process, to enhance the intermediate resampled point cloud iteratively **during the inference**
- more robust and interpretable

Results: Synthetic Point Cloud Denoising

A gradient ascent trajectory of our point cloud denoising every other 10 steps.



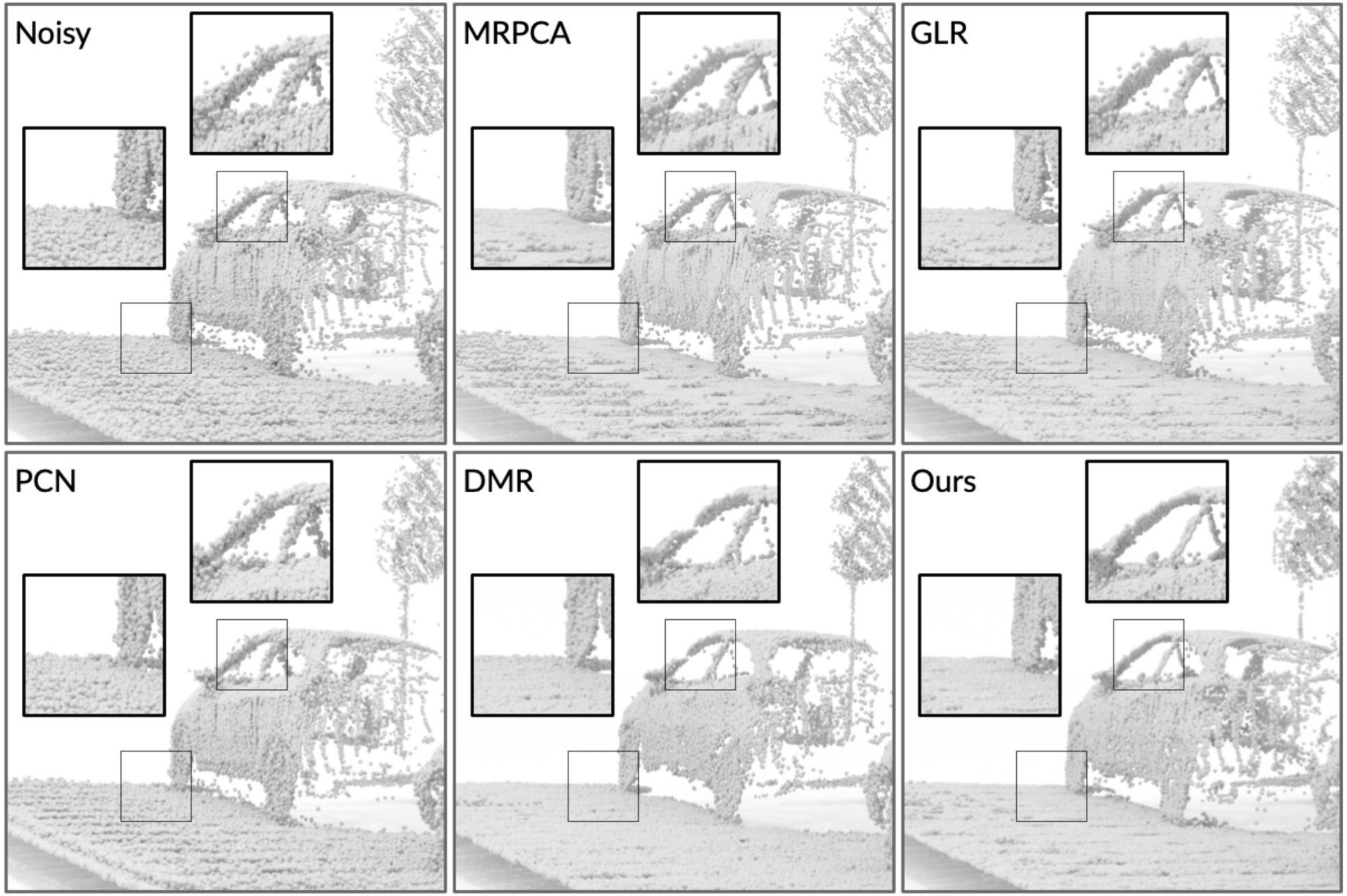


Comparison with other methods

(a) Gaussian noise

(b) Synthetic Lidar noise

Results: Real-world Point Cloud Denoising



Summary

- Graph is flexible abstraction of geometric data residing on **irregular** domains

- Propose graph spectral methods for **robust** & **interpretable** processing and analysis
  - Learn the underlying graph to infer the geometric data structure
  - Propose graph transformation equivariant representation learning for unsupervised & interpretable analysis
  - Introduce GSP-based prior knowledge for robust analysis

- Achieve efficient, robust and interpretable geometric data processing & analysis!

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Ongoing & Future Works

- GSP for enhancing model interpretability
  - ➢ e.g., the effect of graph sparsity on the depth of GNNs
- Model-based geometric deep learning
  - ➢ Systematic framework for combining knowledge and data
- Adversarial attacks on geometric data with interpretation
  - ➢ e.g., point cloud attacks with imperceptibility and transferability
- Functional brain network analysis with GSP & GNNs
  - ➢ e.g., neuron classification

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Thank you!

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