



Computer Aided Topological Design

—Applications of computational topology in geometric design and processing

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Nov. 22, 2024



- 1. Introduction to computational topology**
- 2. Applications in geometric design**
- 3. Porous retrieval, design, and printing**
- 4. Interpretability of DNN**
- 5. Applications in computational psychology**
- 6. Conclusion**

Brief History

- **Computational Topology** is first presented in:
Dey T K, Edelsbrunner H, Guha S. Computational topology. Contemporary mathematics, 1999, 223: 109-144.
- **Computational Geometry** → **Computational Topology**
- **Topological Data Analysis**: Proposed in 2009
Carlsson G. Topology and Data. Bulletin of the American Mathematical Society, 2009, 46(2): 255-308.
- **Computer Aided Geometric Design** → **Computer Aided Topological Design**

1.2 创始人介绍

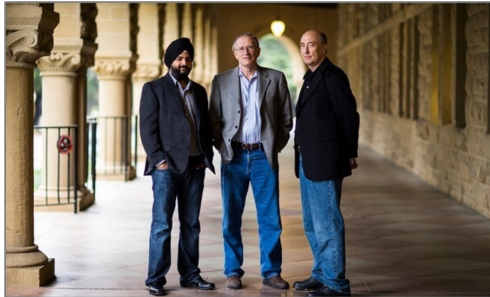
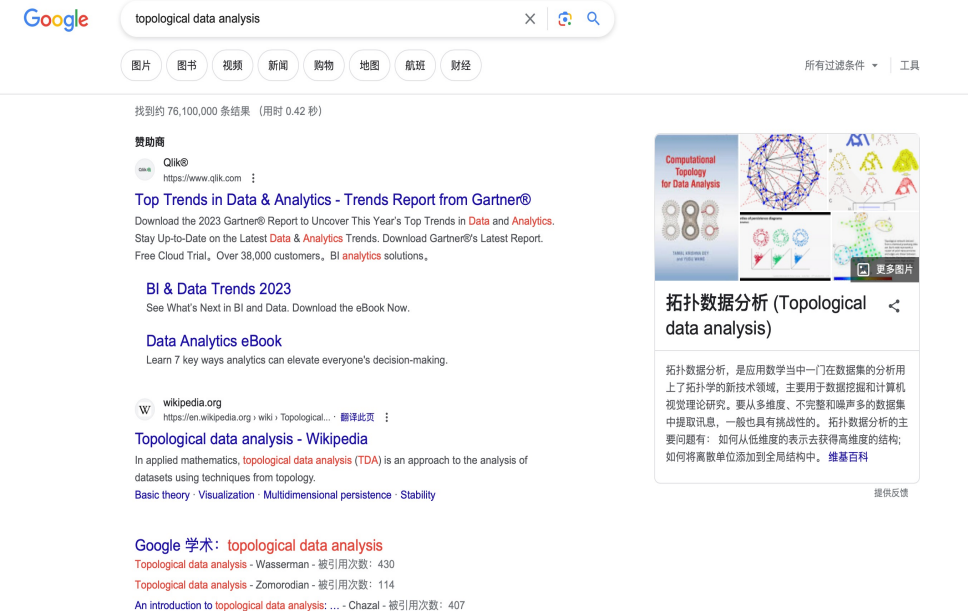


图: Ayasdi创始人Gurjeet Singh, Gunnar Carlsson, Harlan Sexton (从左往右)

2008年, Gunnar Carlsson、Gurjeet Singh和Harlan Sexton在斯坦福大学进行了12年的研发工作后联合成立了Ayasdi公司。在斯坦福大学研究期间,三位创始人获得了美国国防部高级研究计划局(DARPA)和美国情报高级研究计划署(IARPA)的资助,用于“高风险、高回报”的研究项目。2012年, Ayasdi获得了由Floodgate Capital和Khosla Ventures牵头的1025万美元的首轮融资,就此这家高精技术公司开启了它的征程。

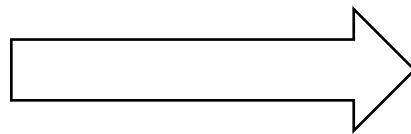
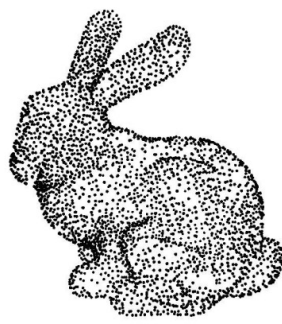
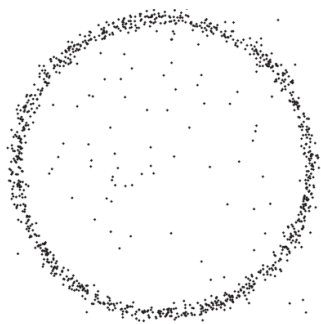
公司总顾问Gunnar Carlsson是世界上最著名的数学家之一,他拥有哈佛大学的本科学位和斯坦福大学的博士学位,在过去的35年里,先后在芝加哥大学、加州大学、普林斯顿大学任教。自1991年以来, Gunnar一直在斯坦福大学担任数学教授,他是斯坦福大学数学领域里拓扑学的思想领袖。在21世纪初,这项工作获得了美国国家科学基金会(NSF)和美国国防部高级研究计划局(DARPA)1000万美元的研究拨款,用于研究拓扑数据分析技术(TDA)在美国政府关切问题上的应用。



Google search results for "topological data analysis". The search bar shows "topological data analysis" with a search button. Below the search bar are filters for "图片", "图书", "视频", "新闻", "购物", "地图", "航班", "财经". The search results show approximately 76,100,000 results in 0.42 seconds. The first result is from Qlik, titled "Top Trends in Data & Analytics - Trends Report from Gartner®". The second result is from Wikipedia, titled "Topological data analysis - Wikipedia". The sidebar on the right shows a preview of a presentation titled "Computational Topology for Data Analysis" and a search result for "拓扑数据分析 (Topological data analysis)".

<https://www.weiyangx.com/379809.html>

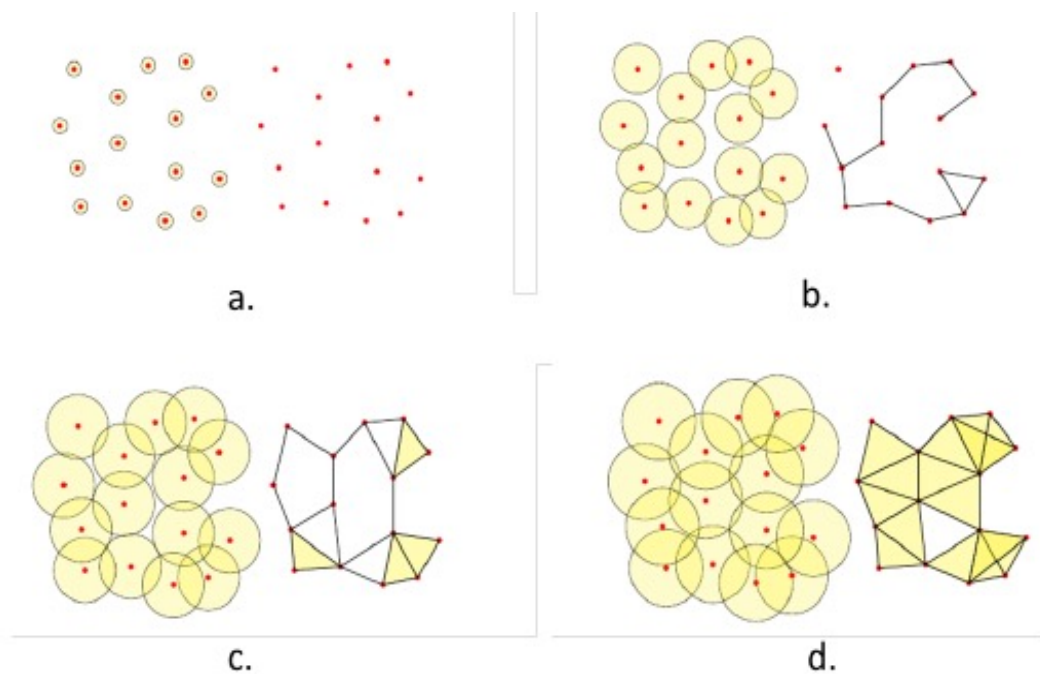
TDA已经成功应用于金融、生物、医学、药物设计、人工智能、脑神经科学等领域



Topological Inference for
point cloud data

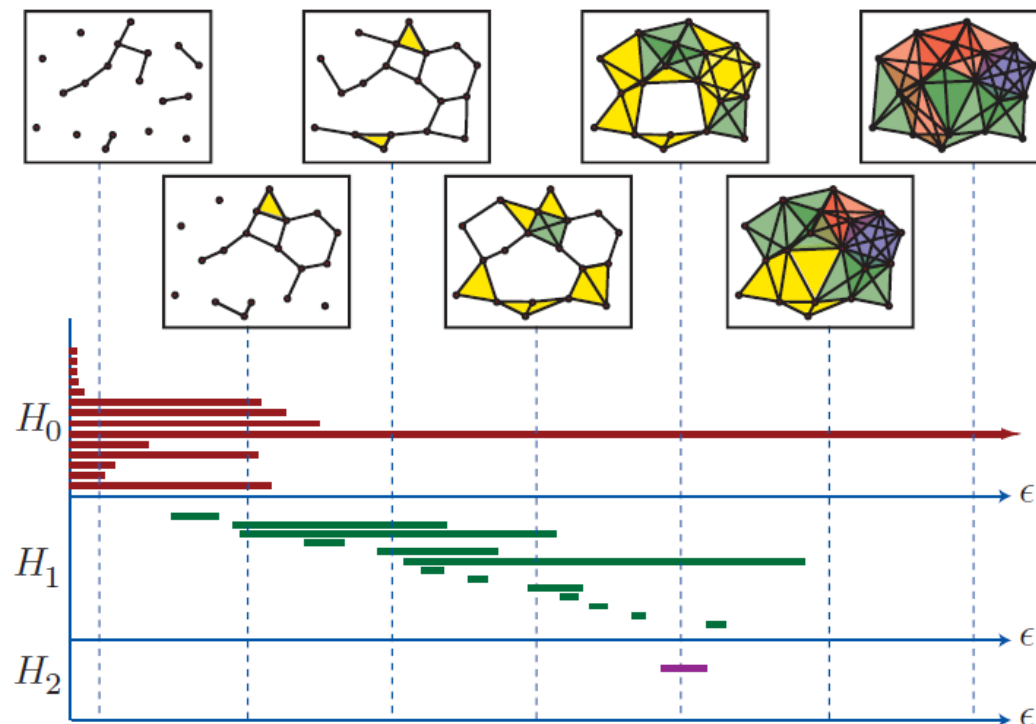
- How to **infer** the **essential topological features** of a hidden shape?
 - To extract components, loops, voids and higher dimensional features
 - To measure their importance
 - Stable with respect of small perturbations
- Mathematical Background
 - Algebraic Topology (Homology Theory)
 - Statistics
 - Geometry
- A promising bridge between topology and geometry in the view of computation

Filtration, Persistent Homology



Filtration (Čech complex)

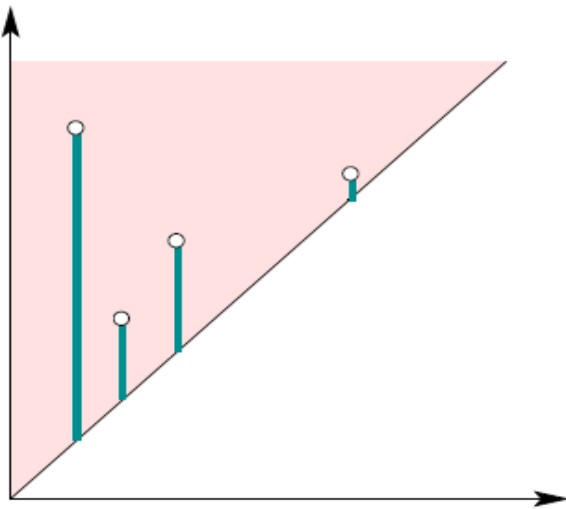
As the radii of open balls grow, the **simplicial complex** can be constructed on point cloud data, which gives a nested complex sequence, a **filtration**.



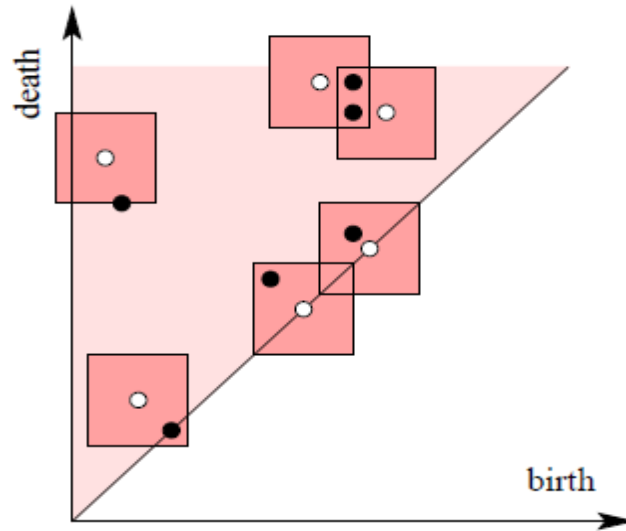
Barcode

- As time goes by, the radii of open balls grow
- New k -holes are **born**
- Some k -holes are destroyed by higher-dimensional simplex and **die**

Persistence Diagram, Distance and Stability



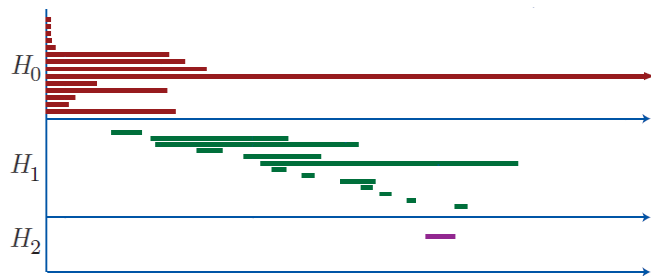
Persistence Diagram



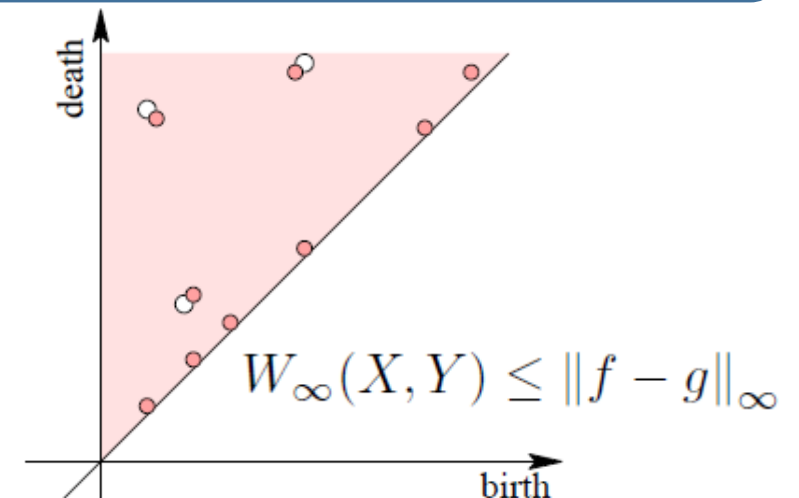
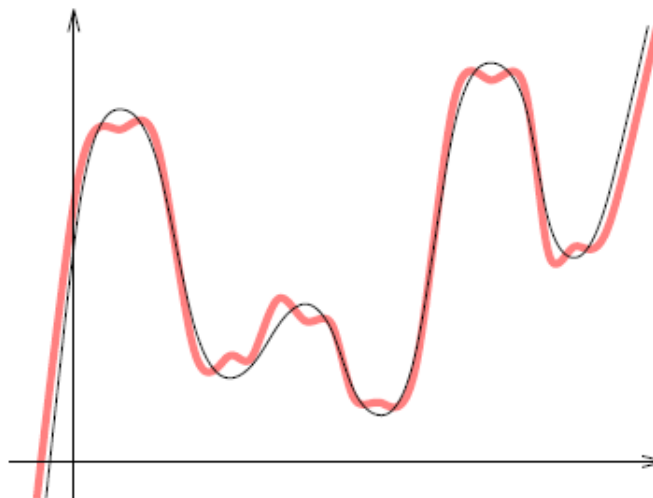
$$W_\infty(X, Y) = \inf_{\eta: X \rightarrow Y} \sup_{x \in X} \|x - \eta(x)\|_\infty$$

Wasserstein Distance

Stability: The *Wasserstein distance* of two persistence diagrams is controlled by the small perturbations on the tame function f

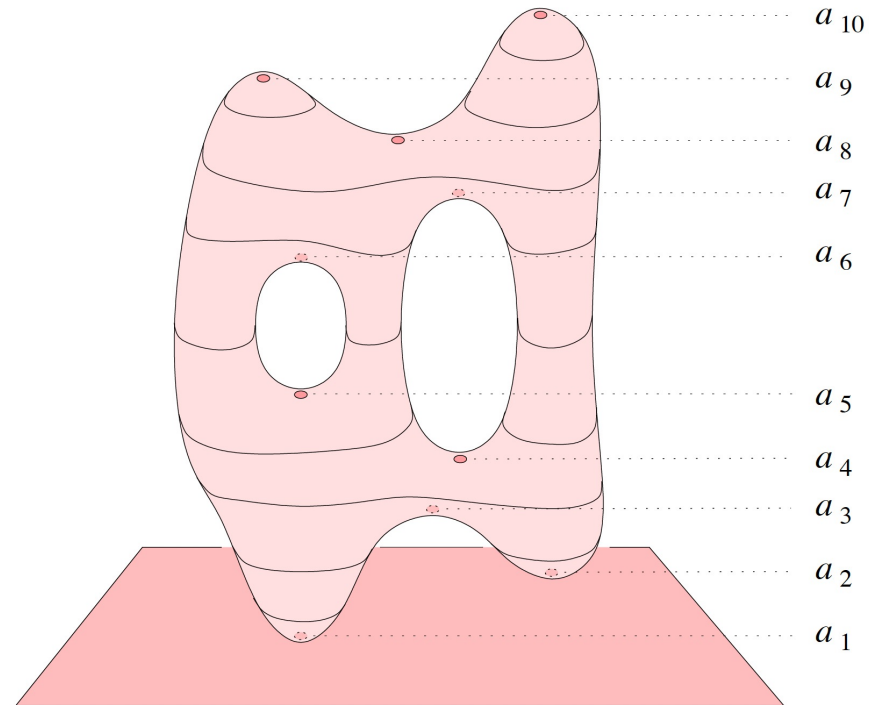


Barcode



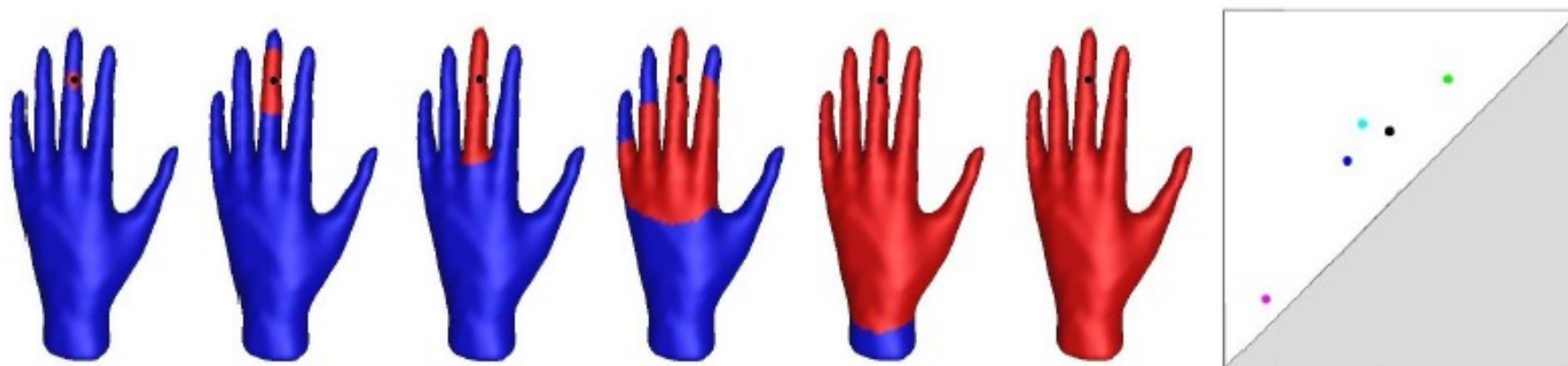
$$W_\infty(X, Y) \leq \|f - g\|_\infty$$

- Distance definition and computation
- Stability
- Representation
- Extended persistence
- Zigzag persistence
- Multiparameter persistence
- Persistence Module
- ...





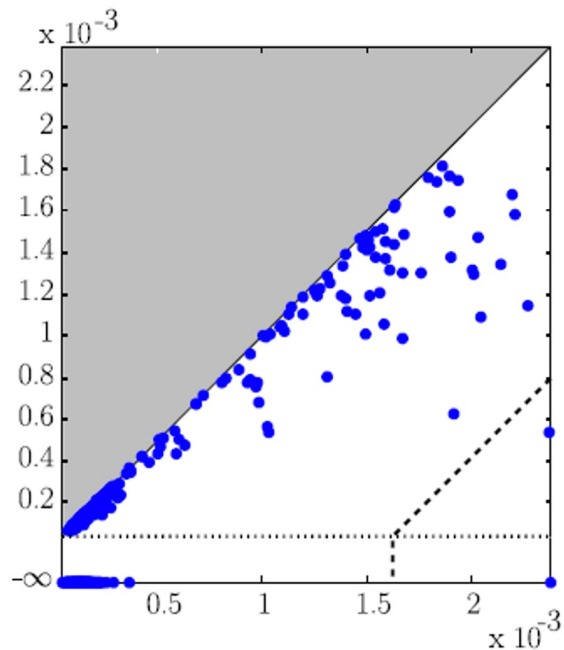
1. Introduction to computational topology
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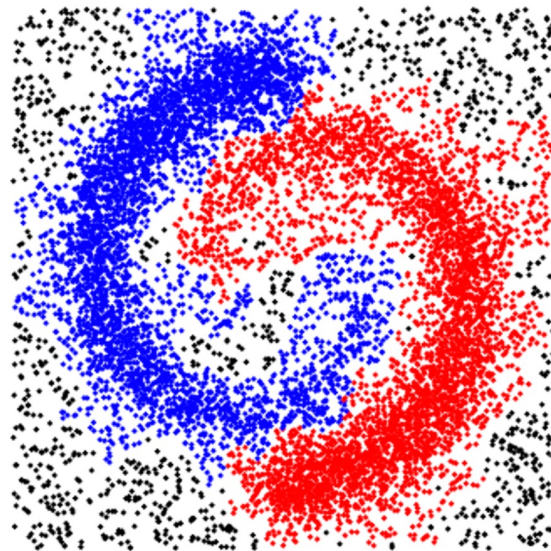
- The **persistence diagram** corresponding to this family is shown in the right
- The pink, blue, light blue, black and green points correspond to the middle, index, ring, pinky and thumb respectively

Carrière M, Oudot S Y, Ovsjanikov M. Stable topological signatures for points on 3d shapes. Computer graphics forum. 2015, 34(5): 1-12.

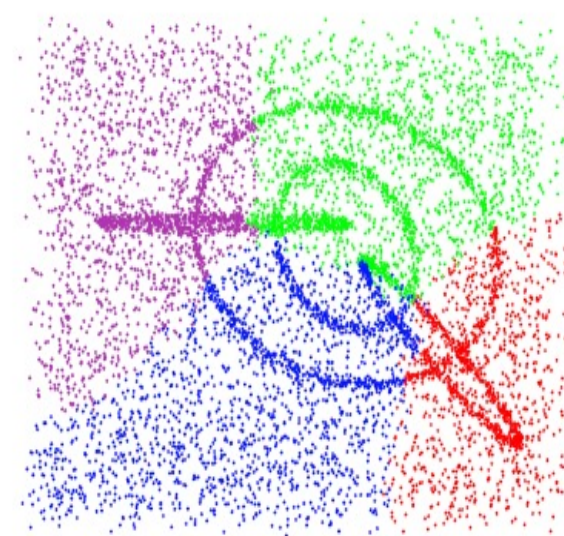
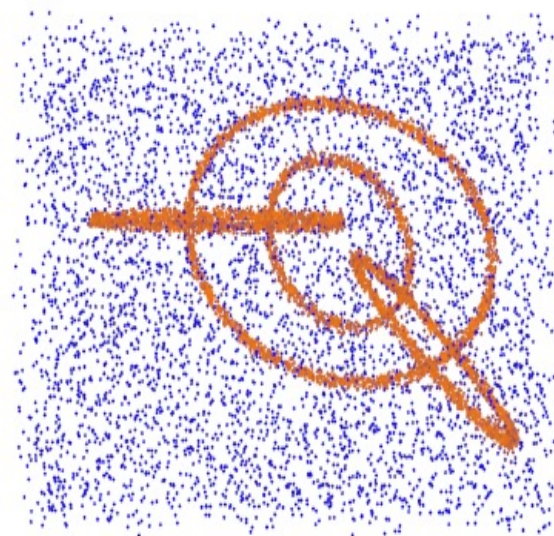
Applications: Clustering of Point Clouds



(a)



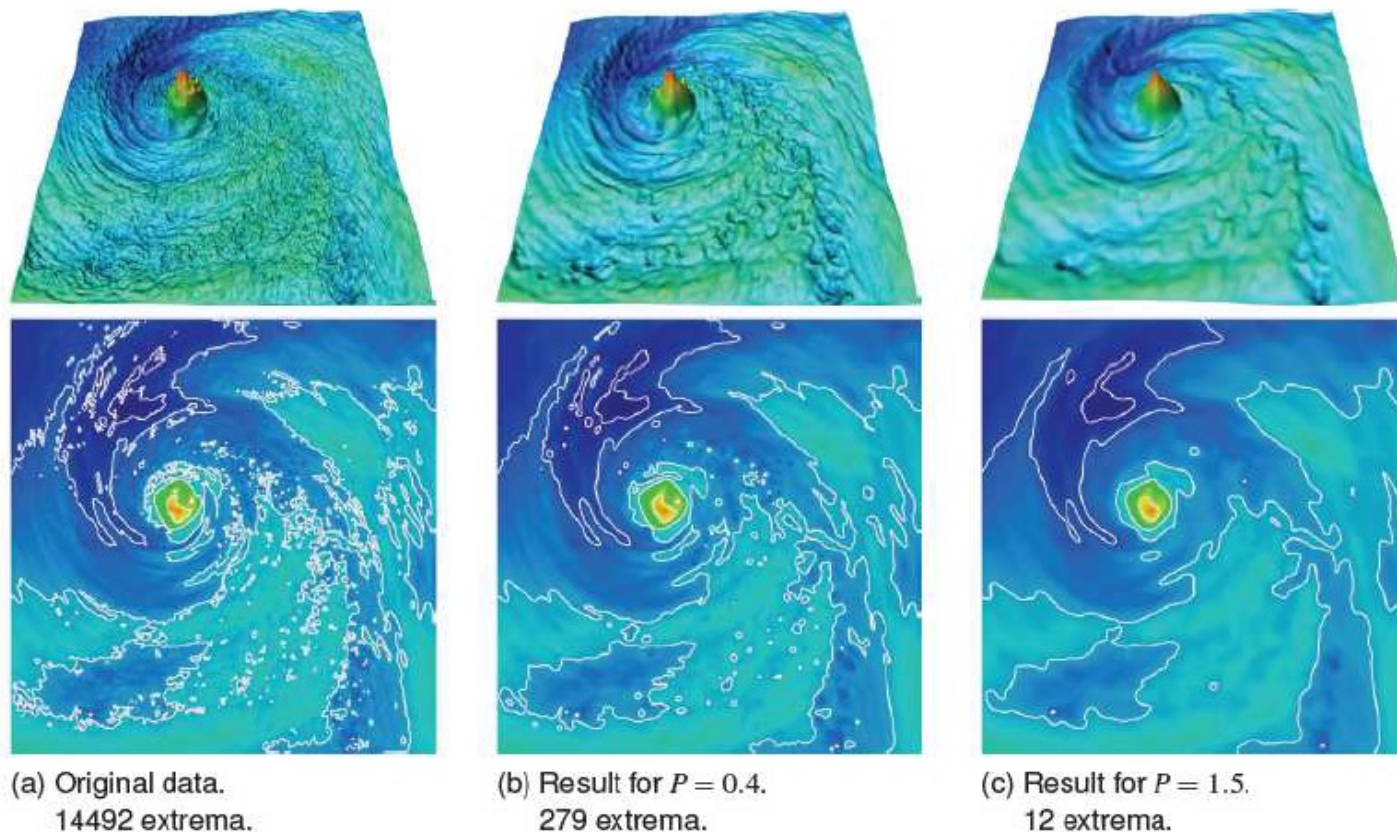
(b)



- The rings are detected by the clustering method with **persistence diagram** (left)
- Compared with the result obtained by spectral clustering (right)

Chazal F, Guibas L J, Oudot S Y, et al. Persistence-based clustering in Riemannian manifolds[J]. Journal of the ACM (JACM), 2013, 60(6): 1-38.

Applications: Topological Denoising



- Keep the salient features while denoising by **persistence-based filtering**

Figure 10. Temperature in the Hurricane Isabel data set (slice $z = 20$). Using persistence-based filtering, we create a hierarchy of scalar fields: with increasing persistence P , our method creates increasingly smoother versions of the data.

Günther D, Jacobson A, Reininghaus J, et al. Fast and memory-efficient topological denoising of 2D and 3D scalar fields. IEEE transactions on visualization and computer graphics, 2014, 20(12): 2585-2594.

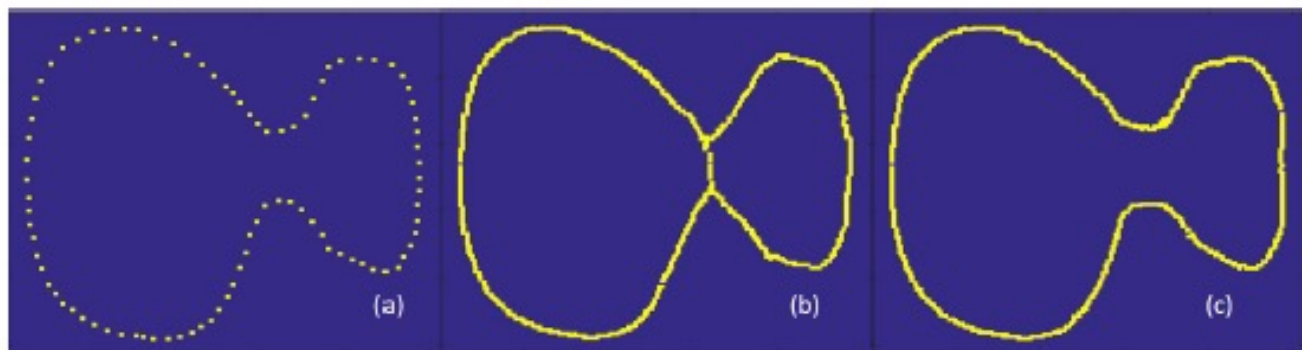
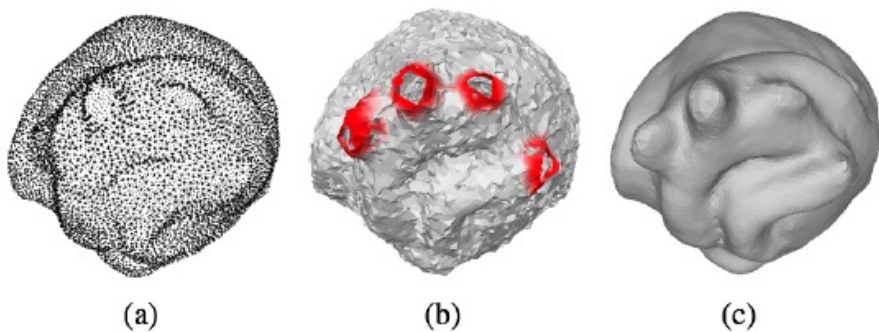
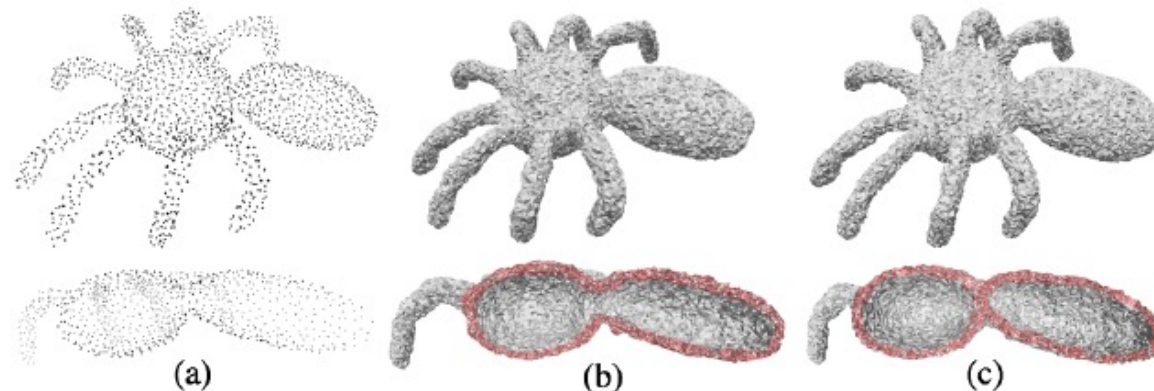
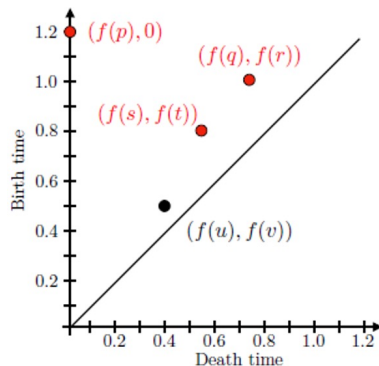
- Objective Function:**

$$-((d_1 - b_1)^2 - (d_2 - b_2)^2)$$

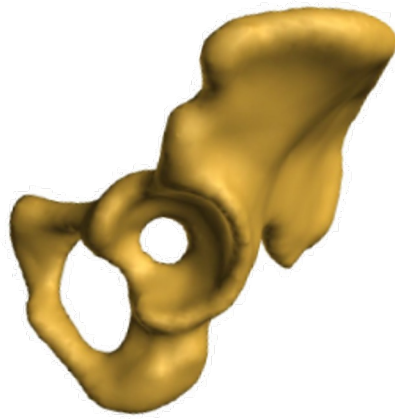
- The persistence of the first point is getting longer and longer
- The persistence of the other points are getting shorter and shorter.

$$-((d_2 - b_2)^2 - (d_3 - b_3)^2)$$

- The persistence of the first two point is getting longer and longer
- The persistence of the other points are getting shorter and shorter



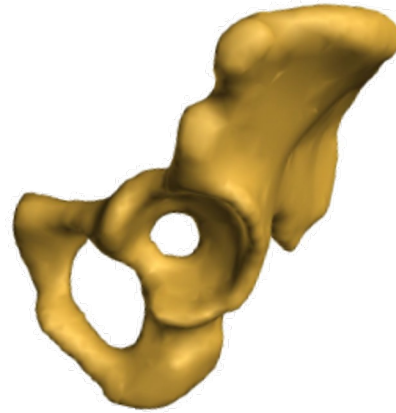
Brüel-Gabrielsson, Rickard, et al. Topology-Aware Surface Reconstruction for Point Clouds. *Computer Graphics Forum*. Vol. 39. No. 5. 2020.



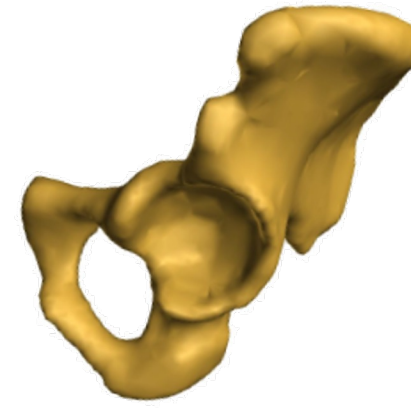
Original Shape



Input Point Cloud

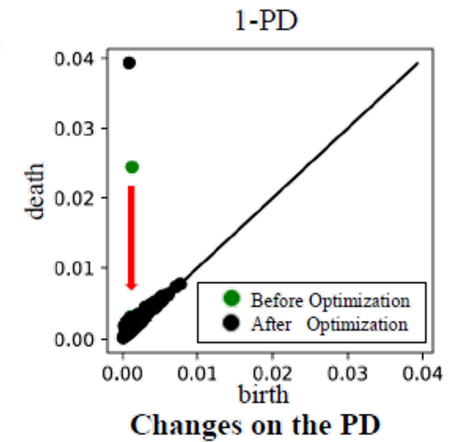


Before Optimization



After Optimization

(b) Hole removal.



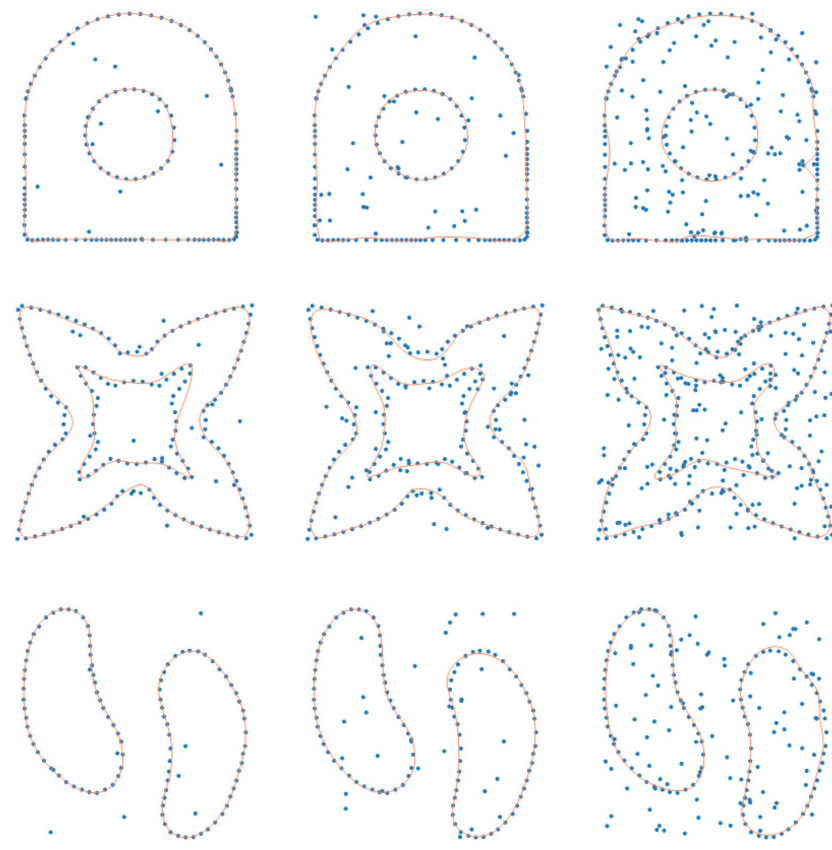
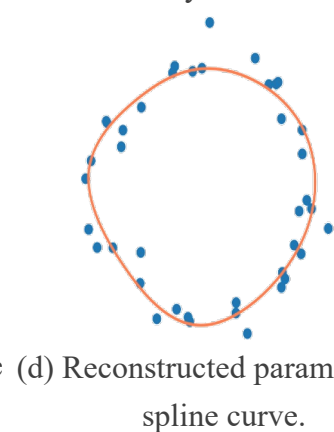
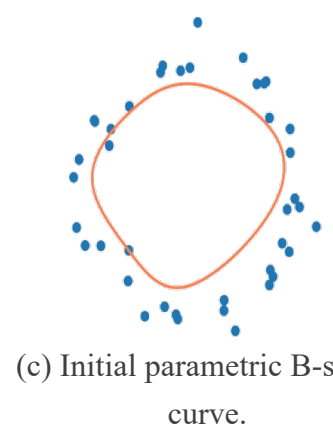
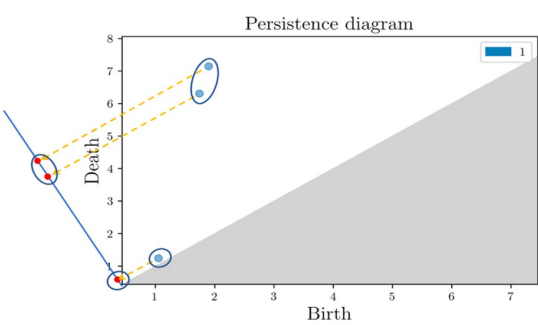
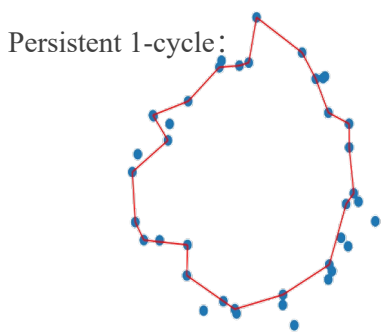
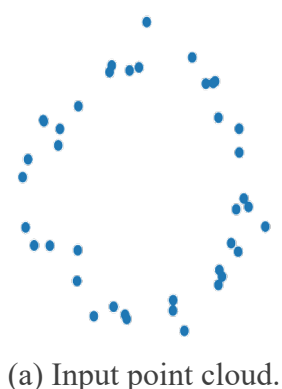
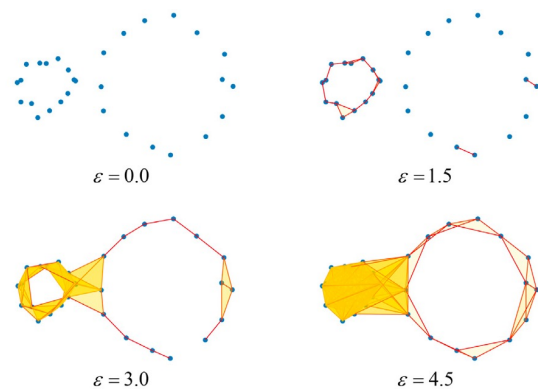
Application: Hole removal

Motivation: To remove the 1D holes (1D homology classes) on the shape

Topology-controllable optimization: To minimize $L^{(1)} = d_2 - b_2$, where (b_2, d_2) represents the persistence pair of the second most persistent feature

Result: The extracted surface was obtained with the removed small-scale handle loop

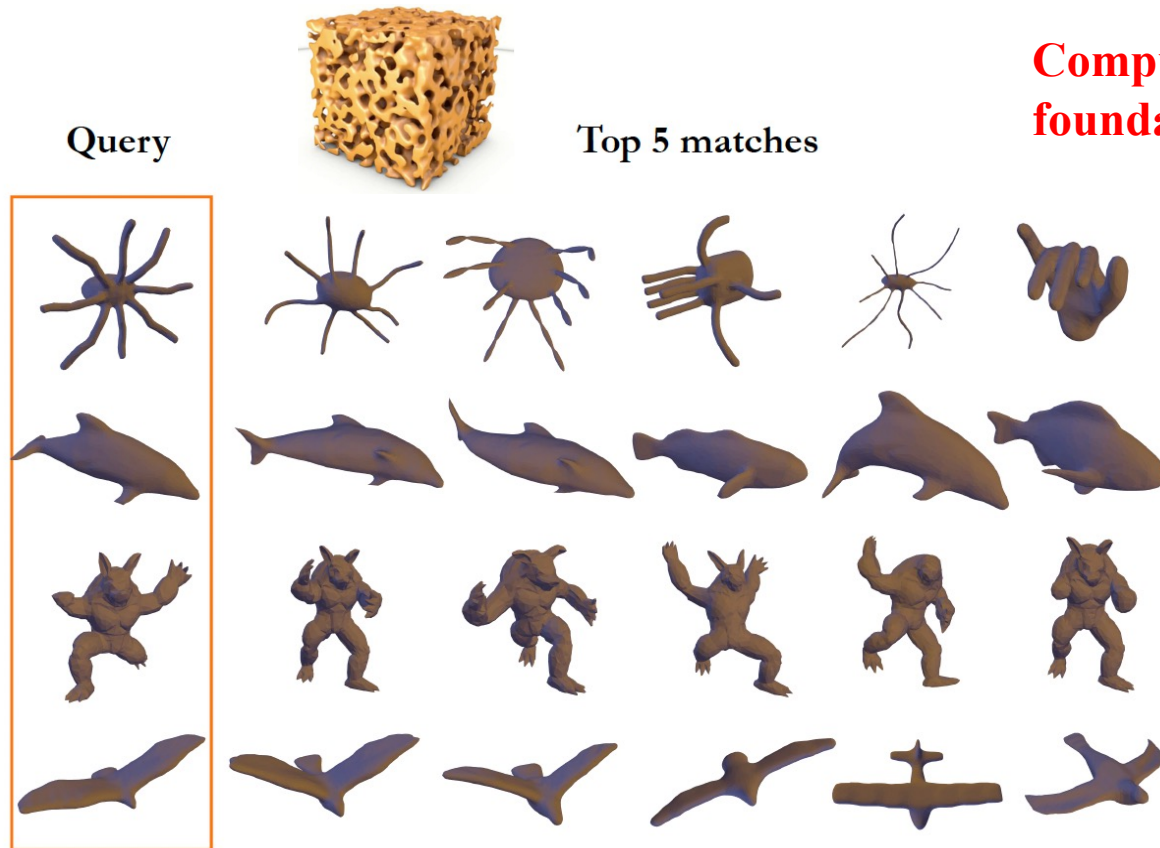
Topology understanding:





1. Introduction to computational topology
2. Applications in geometric design
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- **Porous Retrieval:** Given a query (3D model), retrieving models **most similar** to the query in a model base
- **Porous Design:** Keep **connectivity** of the designed porous
- **Porous Printing:** Guarantee **topology consistency** between design model and printing model

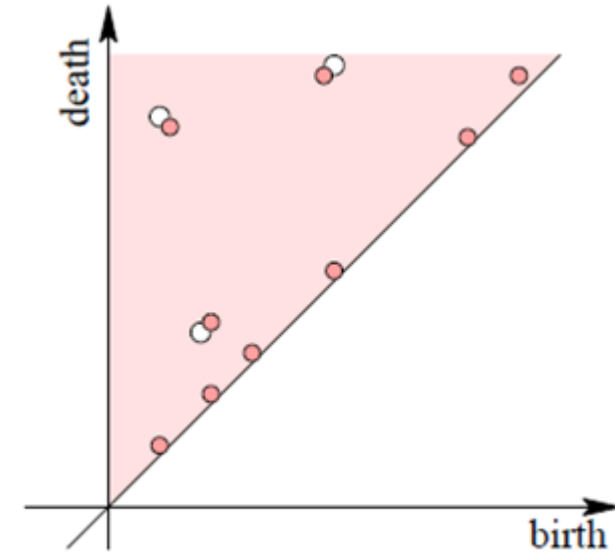


Computational topology is possible to be the theoretical foundation for the design and processing of porous structure



<https://youtu.be/dLTKNY1ZzAM?si=Fy4e6VWl6BYCplqY>

- **Analysis and applications of PDs**
 - To extract more statistical information from PDs
 - To learn from PDs via machine learning approaches
 - To design feature descriptors using PDs
- **Space of PD with metric W_p**
 - Irregular points on a PD
 - Inefficient to compute the W_p distance



PD should be transformed into a proper representation.

Vectorizing Representation of a PD:
to map a PD into a Hilbert space.

$$W_p(PD^{(1)}, PD^{(2)}) = \inf_b \left(\sum_{u \in PD^{(1)}} \|u - b(u)\|_\infty^p \right)^{1/p}$$

Representation: Persistence Images

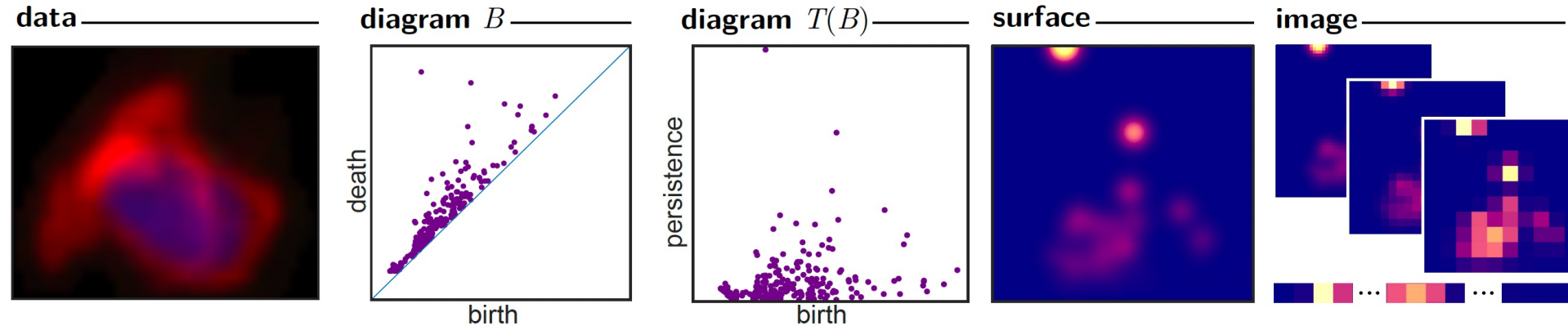
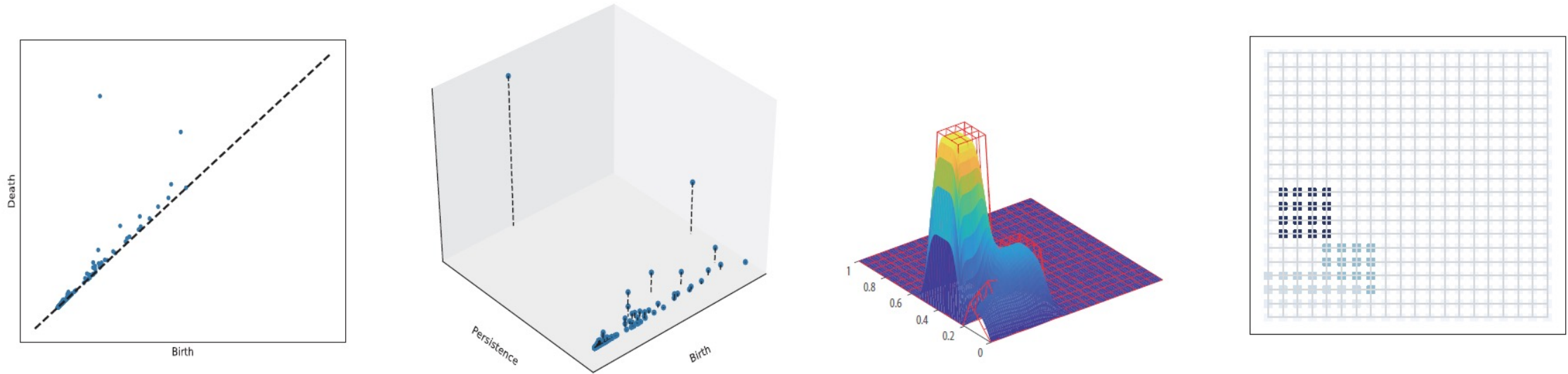


Figure 1: Algorithm pipeline to transform data into a persistence image.

- The **persistence image** (PI) provides a vector representation of the information in a persistence diagram
- The **Gaussian function** is chosen at each point in the transformed persistence diagram $T(B)$
- It makes the results of persistent homology **available in machine learning** algorithms such as linear SVM

Adams H, Emerson T, Kirby M, et al. Persistence images: A stable vector representation of persistent homology. *Journal of Machine Learning Research*, 2017, 18(8): 1-35.



- Transform a PD into the birth-persistence coordinates and assign a value to each point in a PD according to its importance
- Fit the data points in 3D by a **cubic uniform B-spline surface**
- The control grid is obtained to **generate a vector** by concatenating rows of z-coordinates of the control grid
- **Persistence B-spline Grid** is defined by the matrix formed by z-coordinates of the control points

PBSG performs better than PI in most cases

Zhetong Dong, Hongwei Lin, Chi Zhou, Ben Zhang, Gengchen Li. Persistence B-Spline Grids: Stable Vector Representation of Persistence Diagrams Based on Data Fitting. Machine Learning, 113(3): 1373-1420, 2024

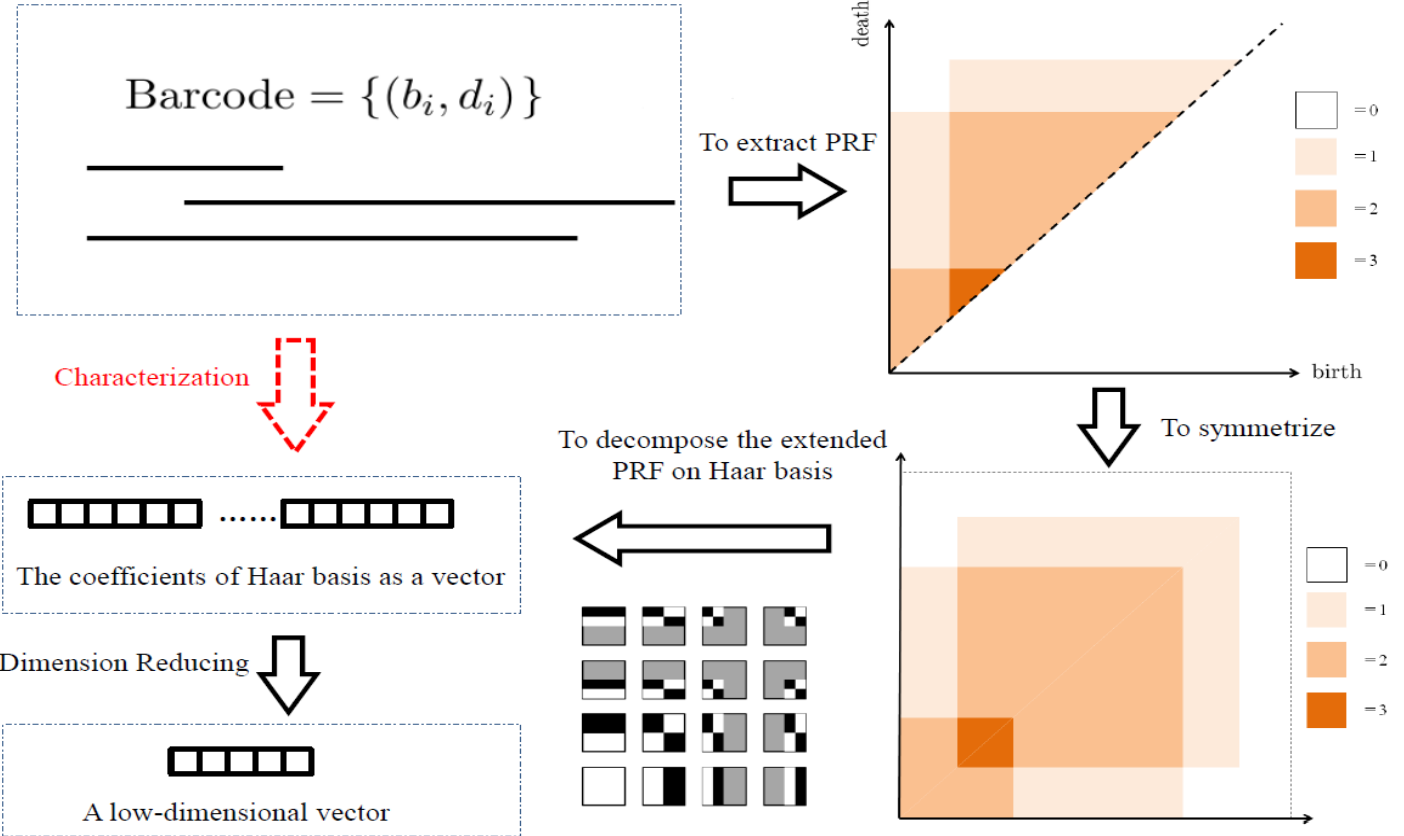
Characterization of Persistence Barcode by Haar Basis

- Transform Barcode to **extended PRF**
- Wavelet decomposition on extended PRF
- Generate **shape descriptor** by dimension reduction to the wavelet decomposition coefficients

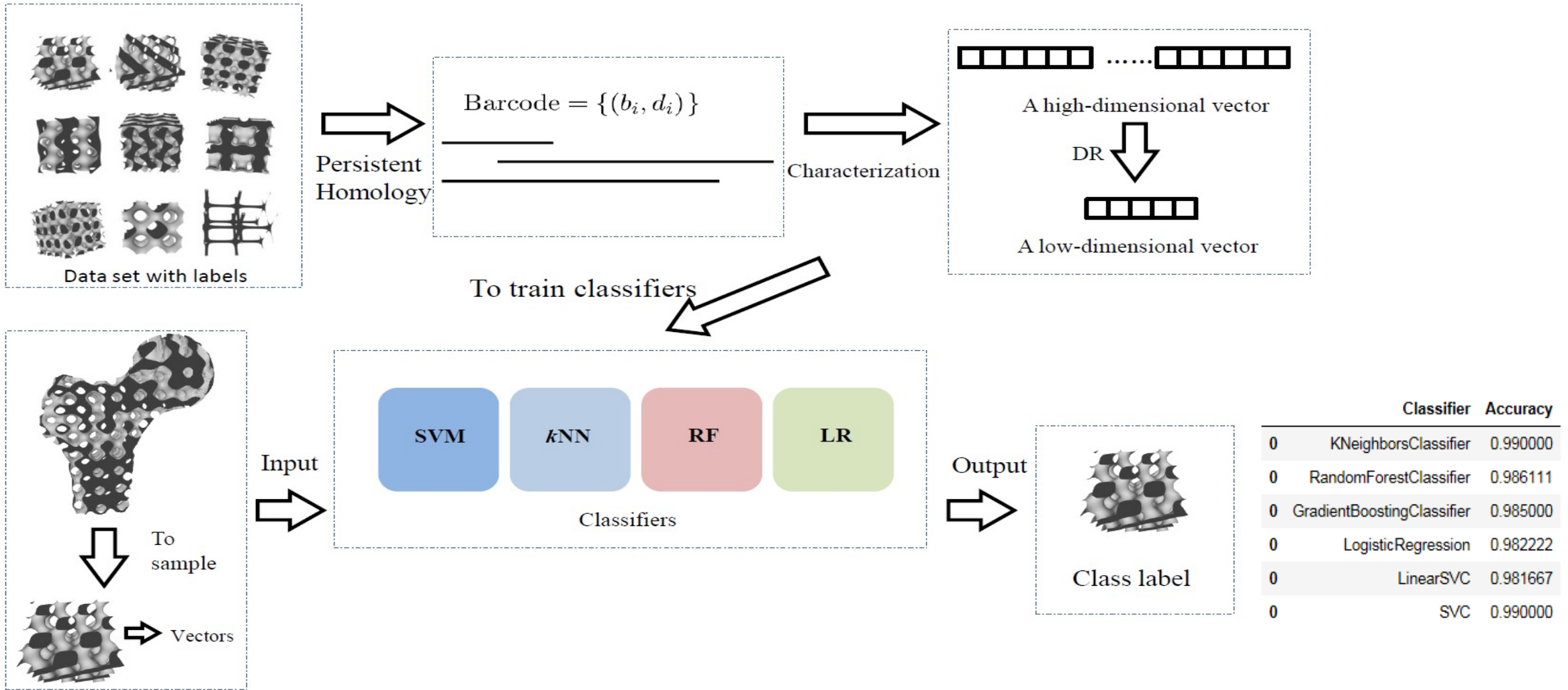
- Given Barcode $\{(b_i, d_i) | 0 \leq b_i \leq d_i, i \in I, |I| < \infty\}$

- **Extended persistent rank function** is defined as:

$$\tilde{r}_i(s, t) = \begin{cases} 1, & b_i \leq s, t \leq d_i \\ 0, & \text{otherwise} \end{cases}$$



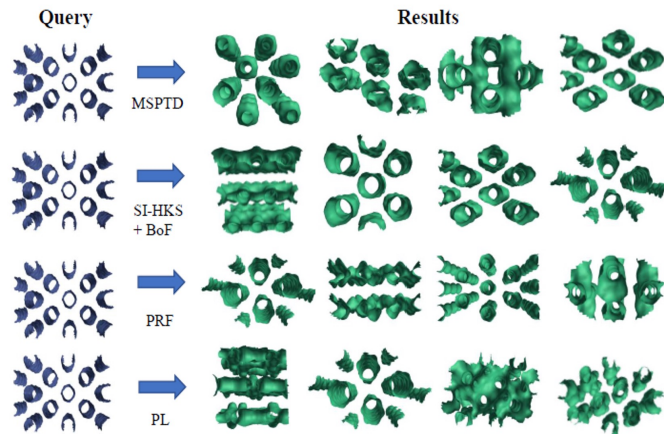
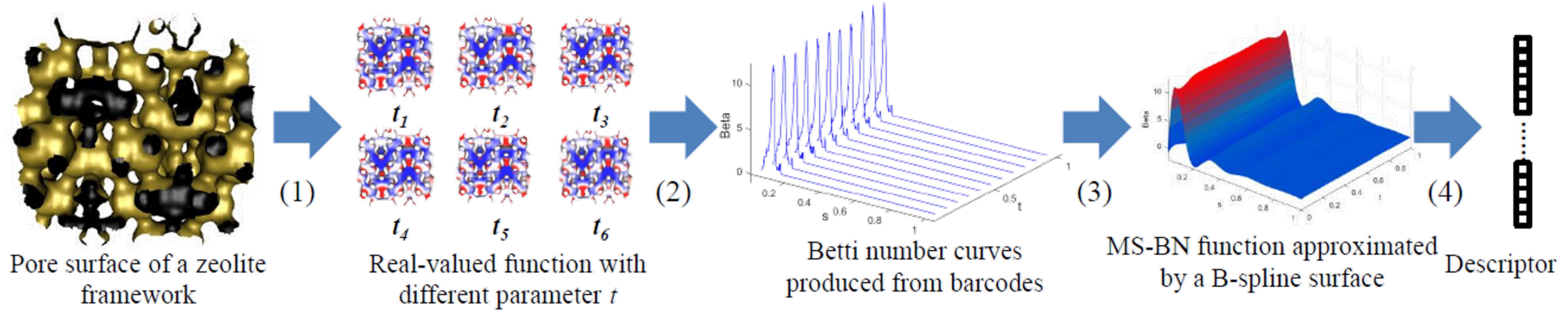
Characterization of Persistence Barcode by Haar Basis



Zhetong Dong, Chuanfeng Hu, Chi Zhou, Hongwei Lin, Vectorization of persistence barcode with applications in pattern classification of porous structures, Computers & Graphics, Volume 90, 2020, Pages 182-192

Multiscale Persistent Topological Descriptor

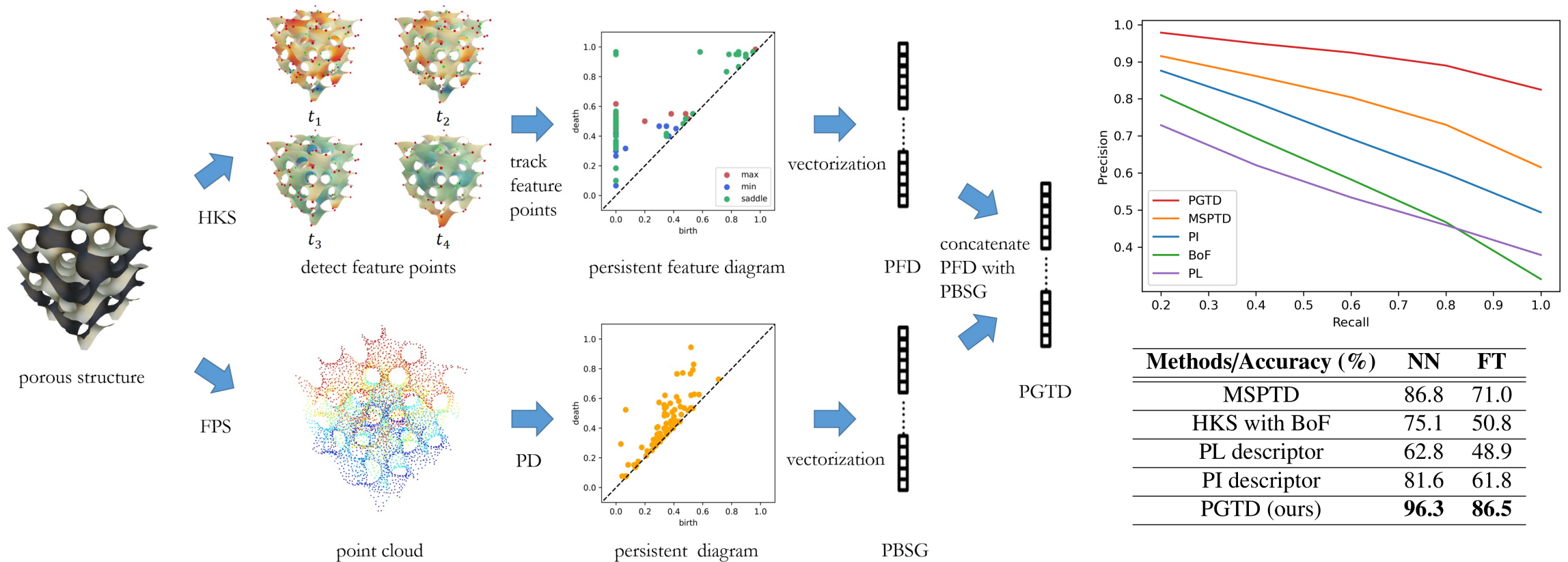
- Calculating a series of **Betti number curves** of the heat kernel on a porous surface at some times
- Generating the **B-spline surface** by lofting the Betti number curve sequence
- The **control grid of the B-surface surface** is taken as the **shape descriptor**



Methods/Accuracy (%)	NN	FT	ST	DCG
SI-HKS with histogram	90.1	73.3	91.6	92.7
SI-HKS with BoF	81.3	76.1	91.0	91.8
PL descriptor	68.1	59.3	75.0	83.4
PI descriptor	81.5	71.8	86.7	90.1
PRF descriptor	81.8	74.1	87.5	90.6
MSPTD (ours)	94.9	78.4	94.5	95.5

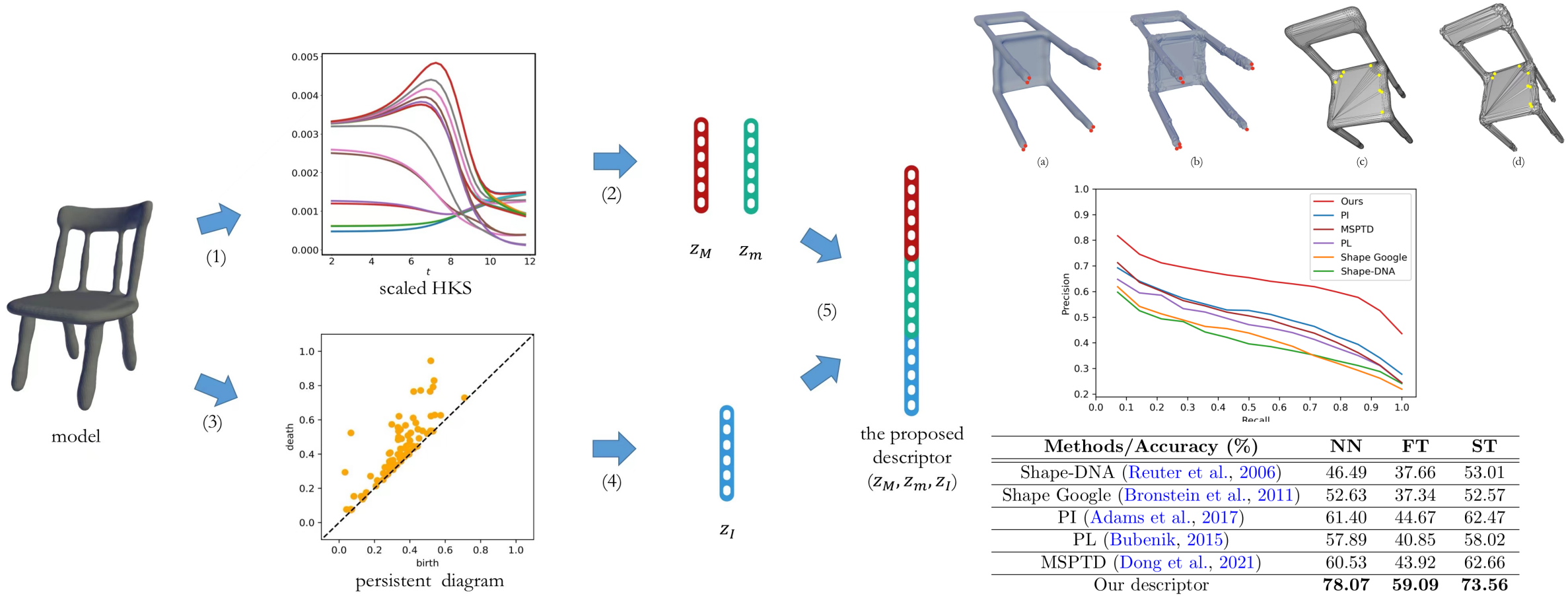
Persistent Geometry-Topology Descriptor

- Geometric information is represented by **persistent feature diagram (PFD)**, formed by tracing the emergence and disappear of the heat kernel feature points
- Topological information is represented by **persistent diagram (PD)**
- **Persistent Geometry-Topology Descriptor** is generated by concatenating the vectors of PFD and PD



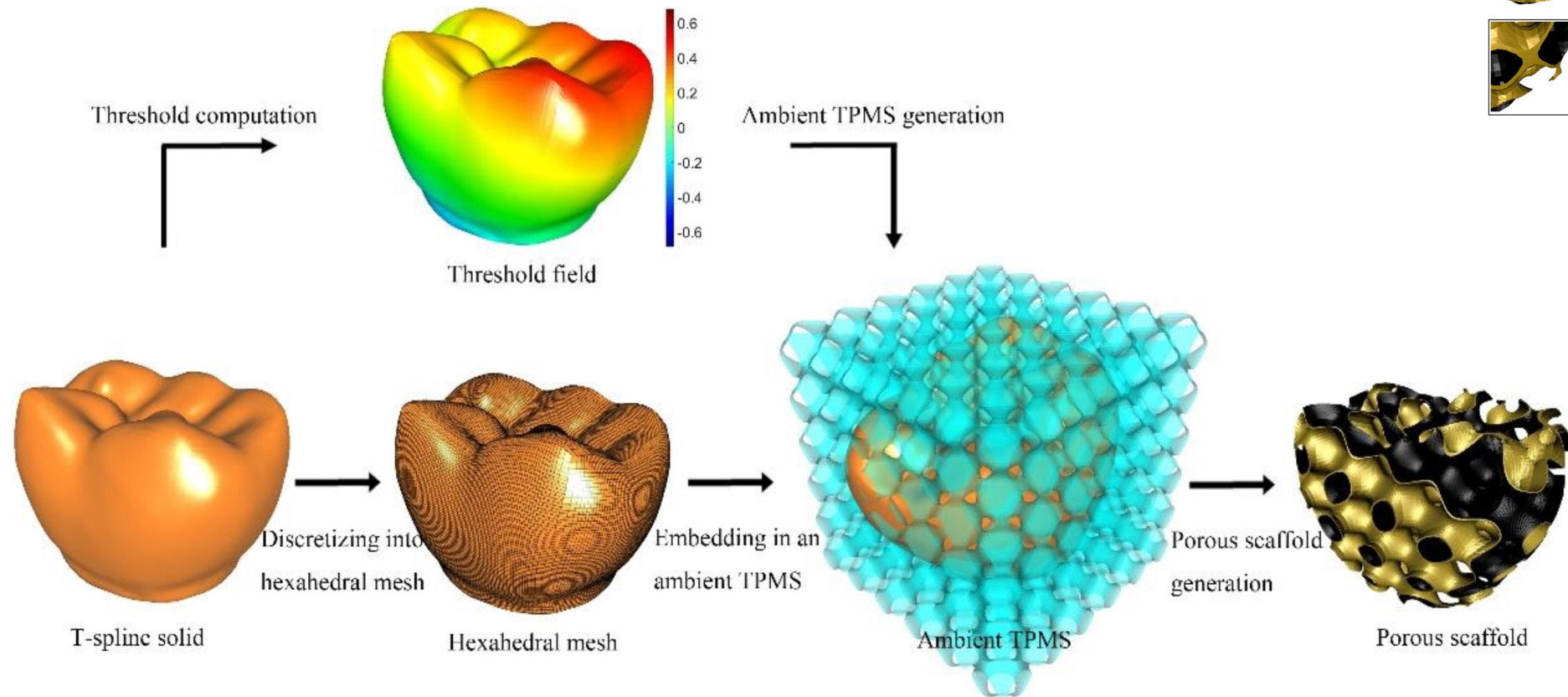
Persistent Heat Kernel Signature Descriptor

- Calculate the **heat kernel signature curve** at each mesh vertex, as well as the **maximums and minimums** on the curves
- **Shape descriptor** is formed by first sorting the maximums and minimums, and then concatenating them with the vector of PD

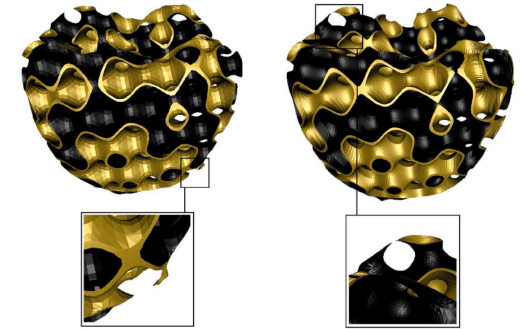


Zitong He, Peisheng Zhuo, Hongwei Lin, Junfei Dai. 3D shape descriptor design based on HKS and persistent homology with stability analysis. Computer Aided Geometric Design, 111 (2024) 102326

- Conventional porous generation methods

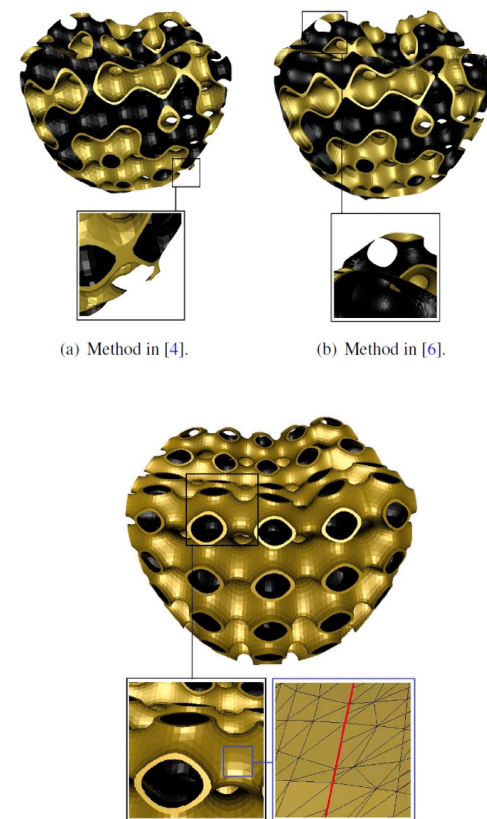
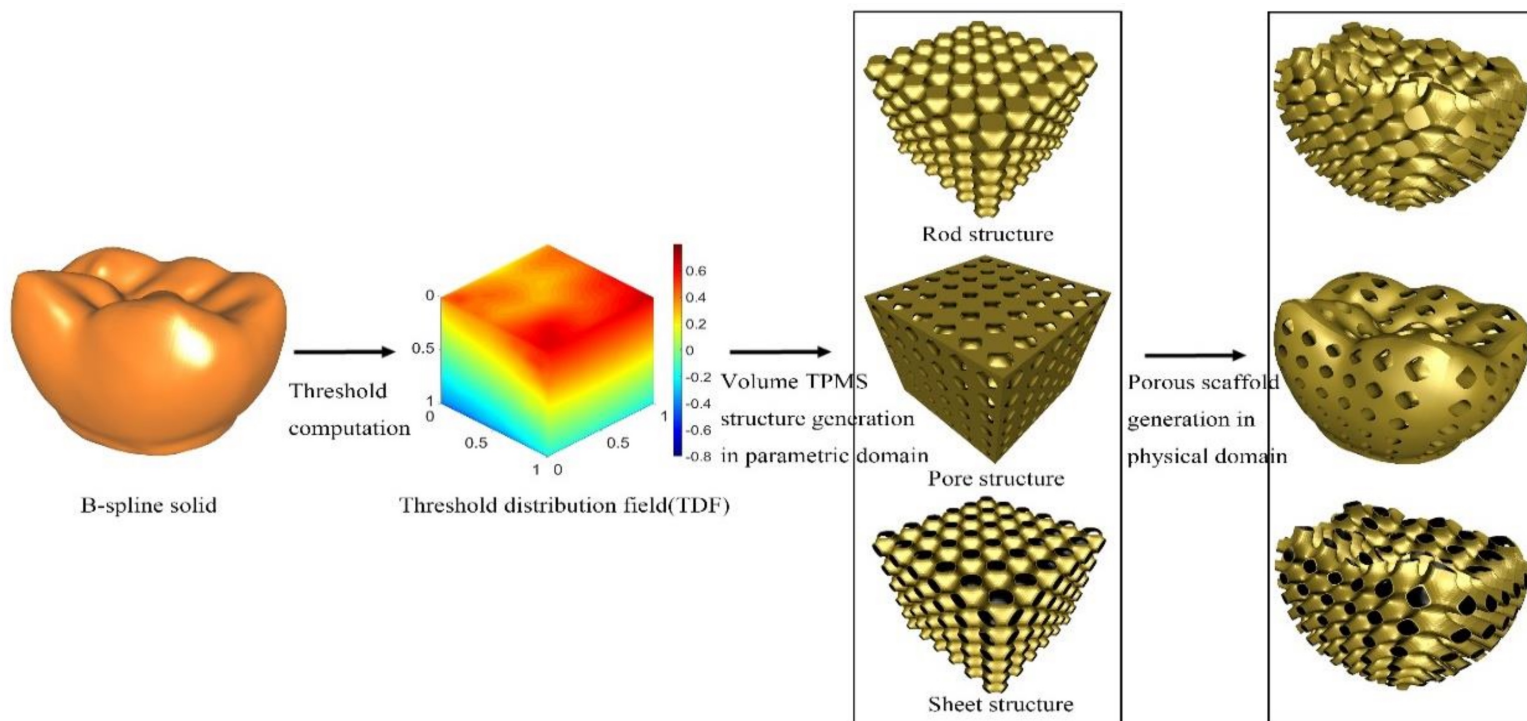


- **Huge storage**
- **Cracked surface**



Heterogeneous porous : Our Methods

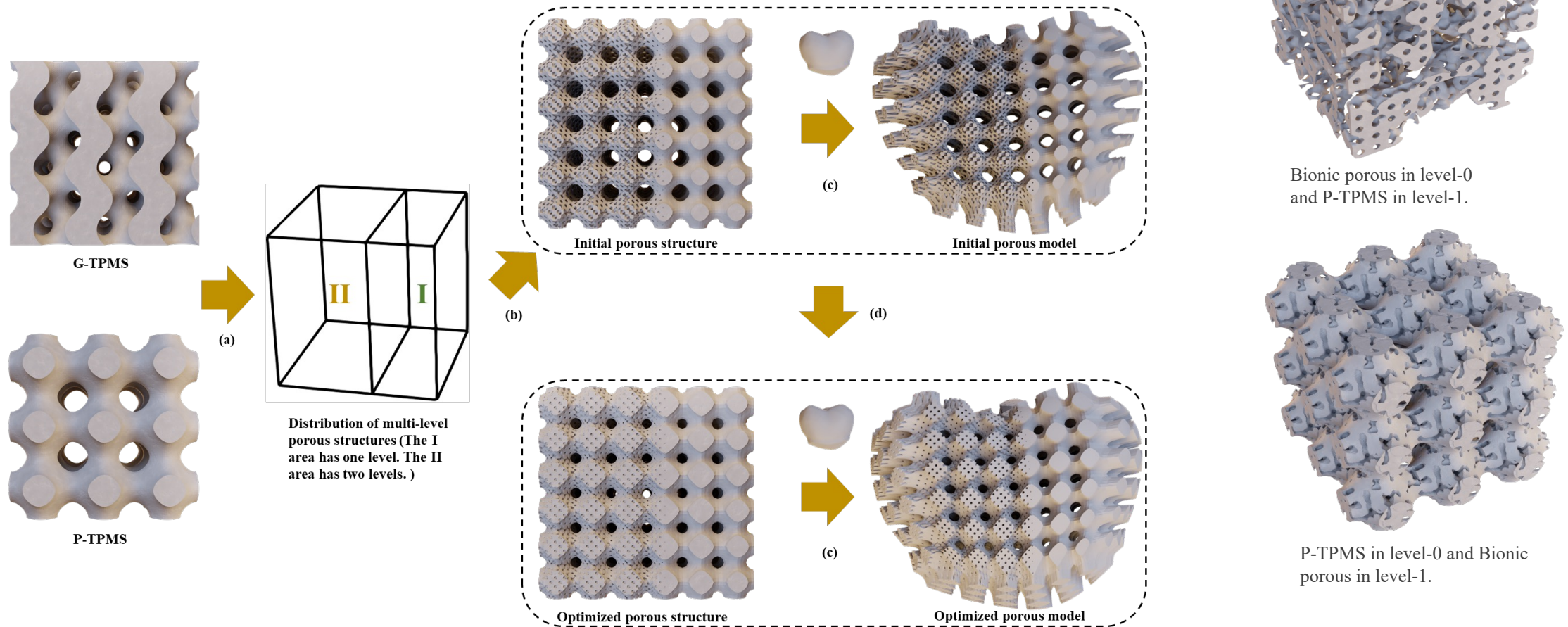
- Our method: The **composition** of the free form shape represented by **tri-variate B-spline** and the **implicit B-spline** in the parametric domain
- Save at least 99% storage
- Surface integrity



Chuanfeng Hu, Hongwei Lin. Heterogeneous porous scaffold generation using trivariate B-spline solids and triply periodic minimal surfaces. Graphical Model. 115: 101105, 2021

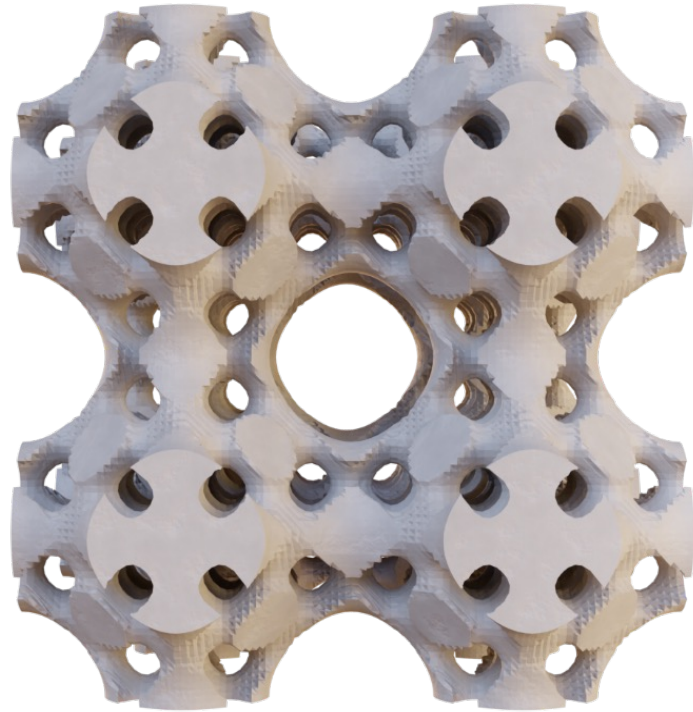
Multilevel porous structure: Algorithm flow

- Represent multilevel porous structure by **hierarchical B-spline**
- **Implicit B-spline** is employed to represent porous at each level parametric domain

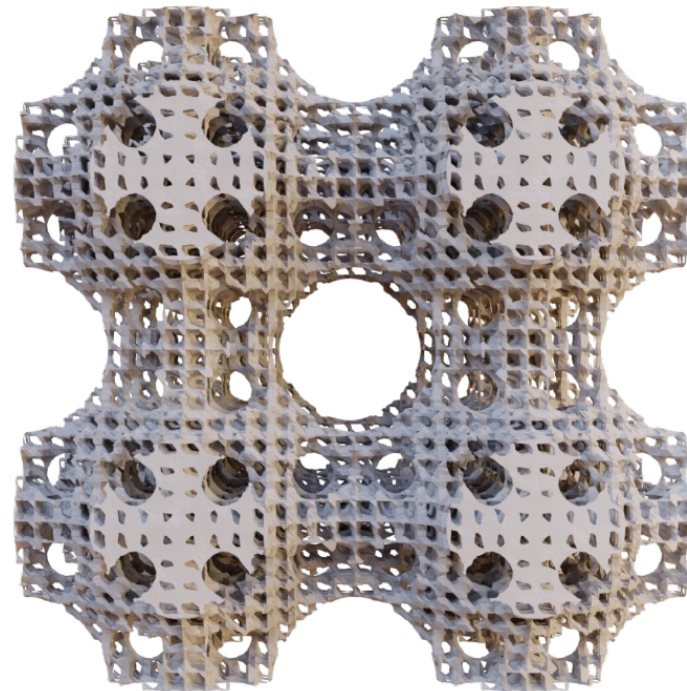


Depeng Gao, Hongwei Lin, Zibin Li. Free-form multi-level porous model design based on truncated hierarchical B-spline functions. Computer-Aided Design, 2023, 162: 103549

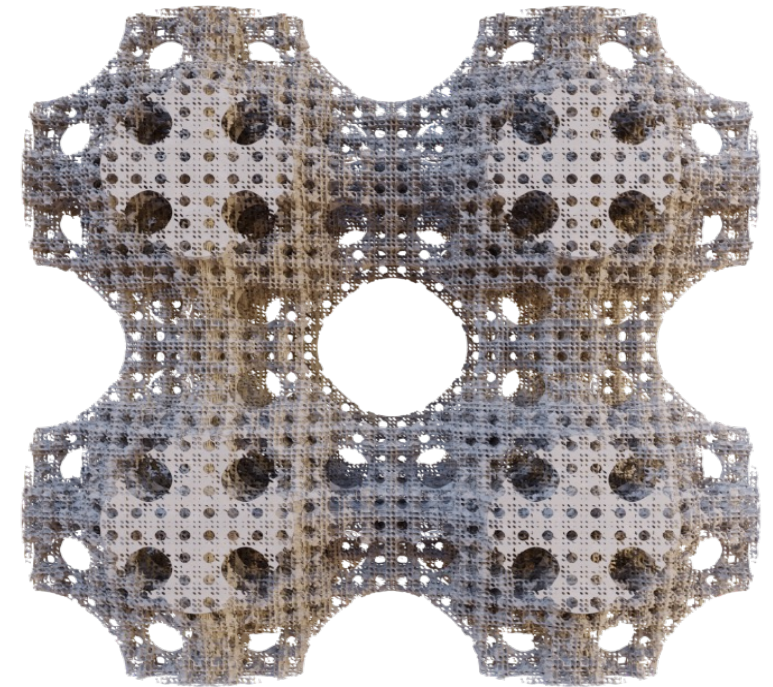
Multilevel porous structure: Examples



Two level



Three level

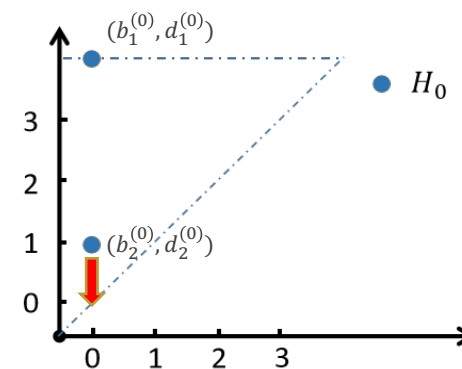
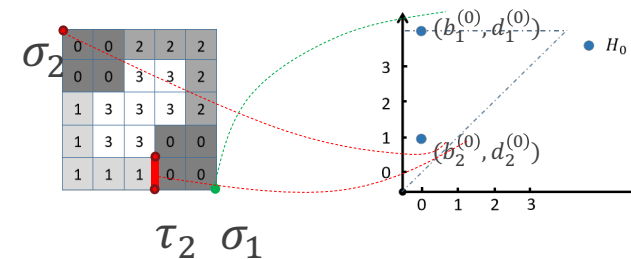
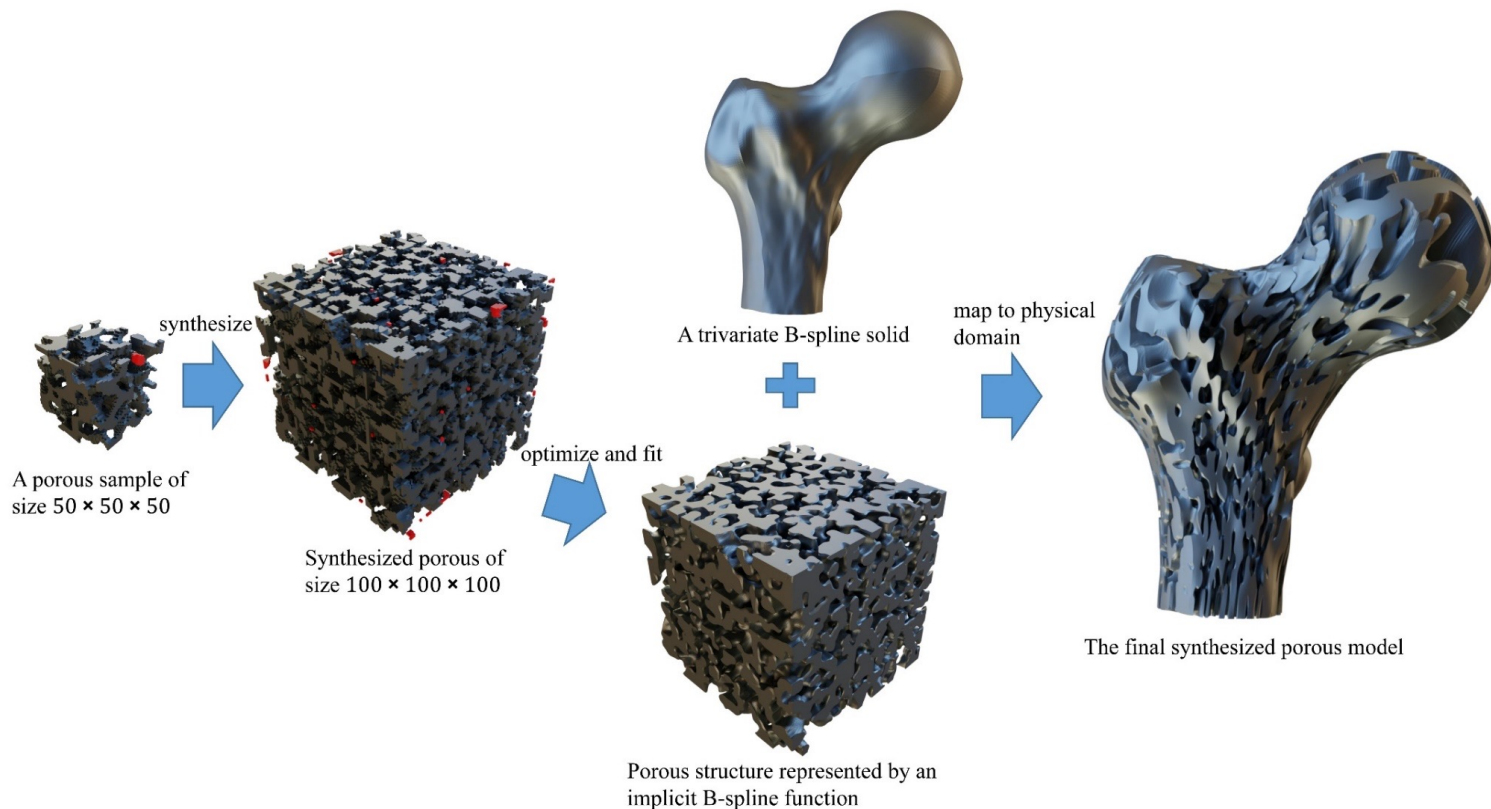


Four level

Depeng Gao, Hongwei Lin, Zibin Li. Free-form multi-level porous model design based on truncated hierarchical B-spline functions. *Computer-Aided Design*, 2023, 162: 103549

Connectivity-guaranteed porous synthesis

- Synthesize the porous in a large region from a small region porous sample using texture synthesis method
- **Guarantee the connectivity** of the synthesized porous by **optimizing the PD**

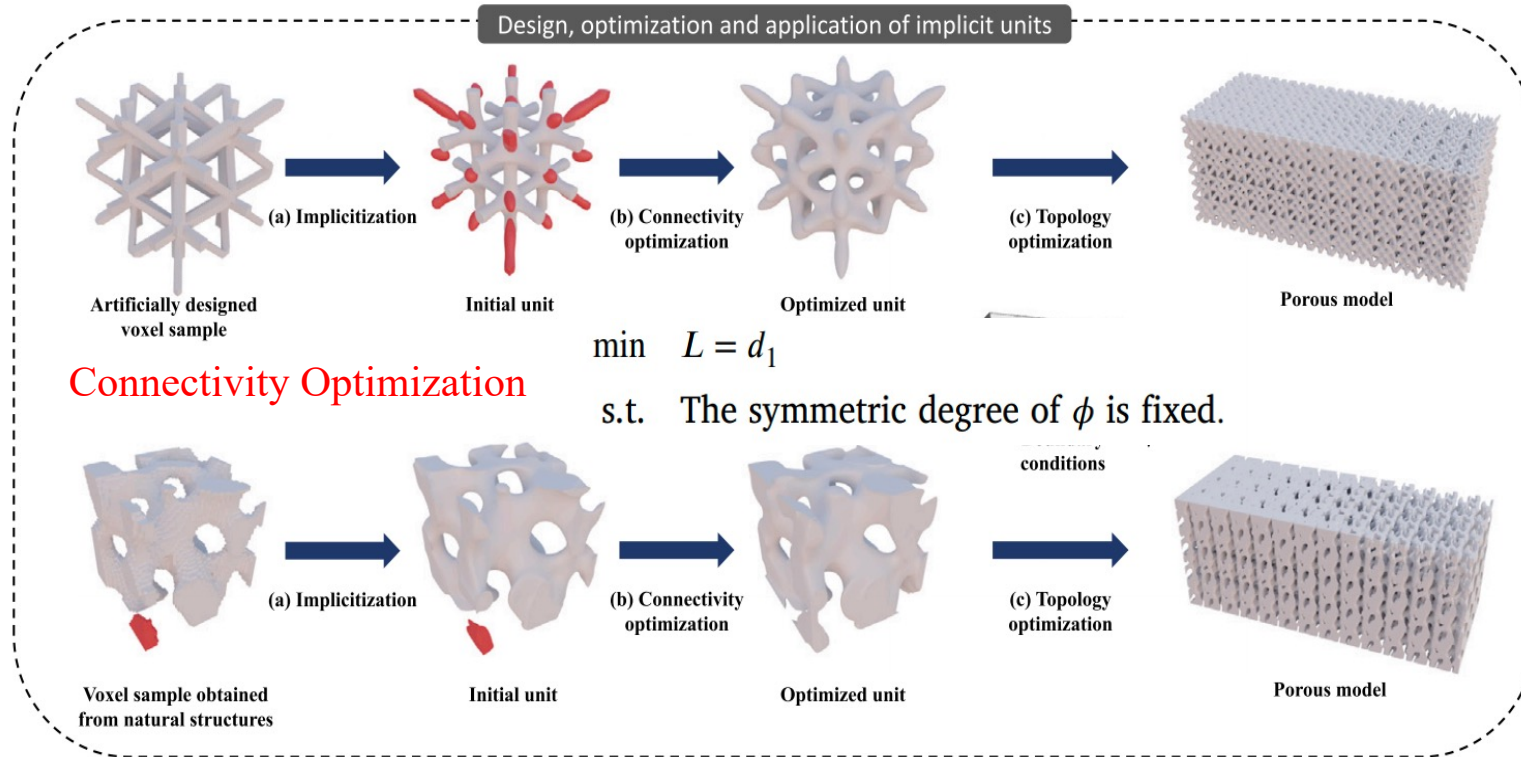


- DTM based filtration
- PD optimization

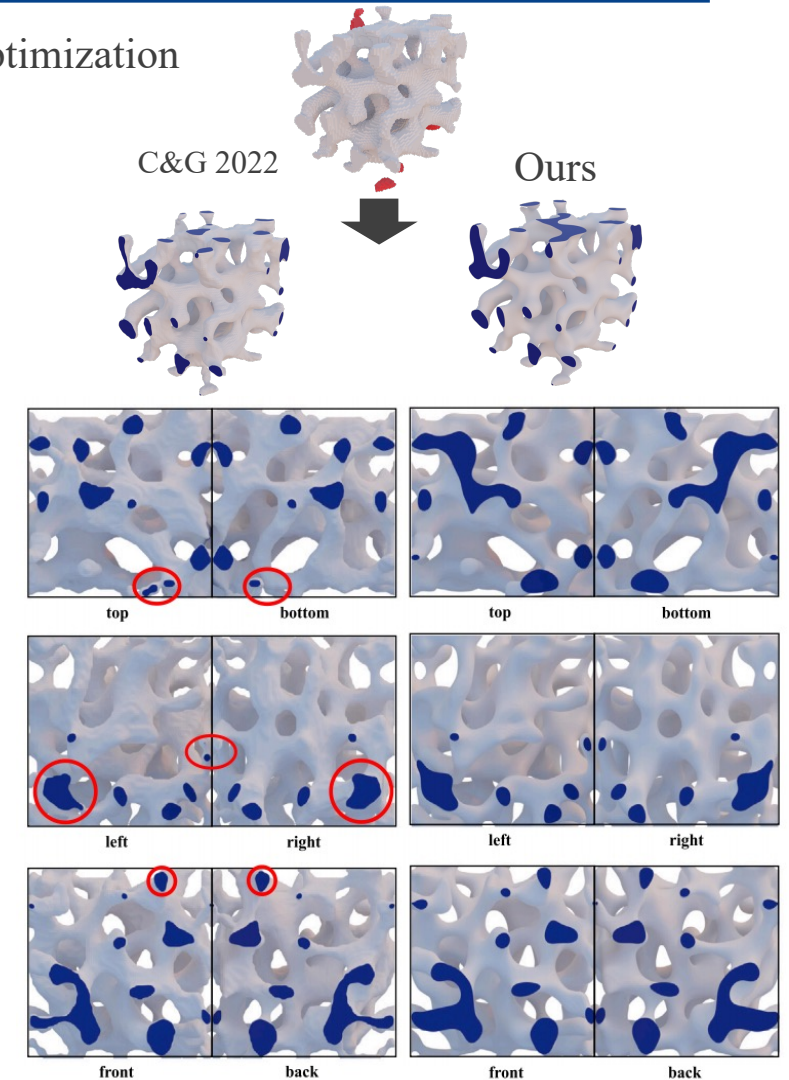
Depeng Gao, Jinhao Chen, Zhetong Dong, Hongwei Lin. Connectivity-guaranteed porous synthesis in free form model by persistent homology. Computers & Graphics, 106: 33-44 (2022)

Periodic Implicit Representation: Flowchart

- Represent the porous unit by **periodic implicit B-spline**
- The porous units can be stitched watertight and smoothly
- Enrich the representation forms and design methods of porous structures

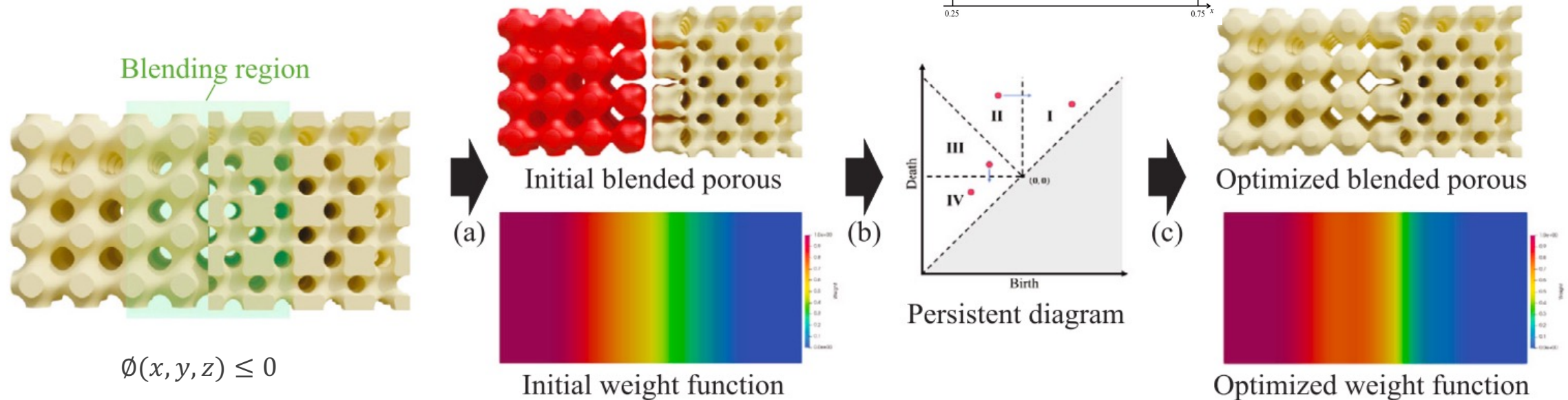


Optimization



Topology-aware blending method

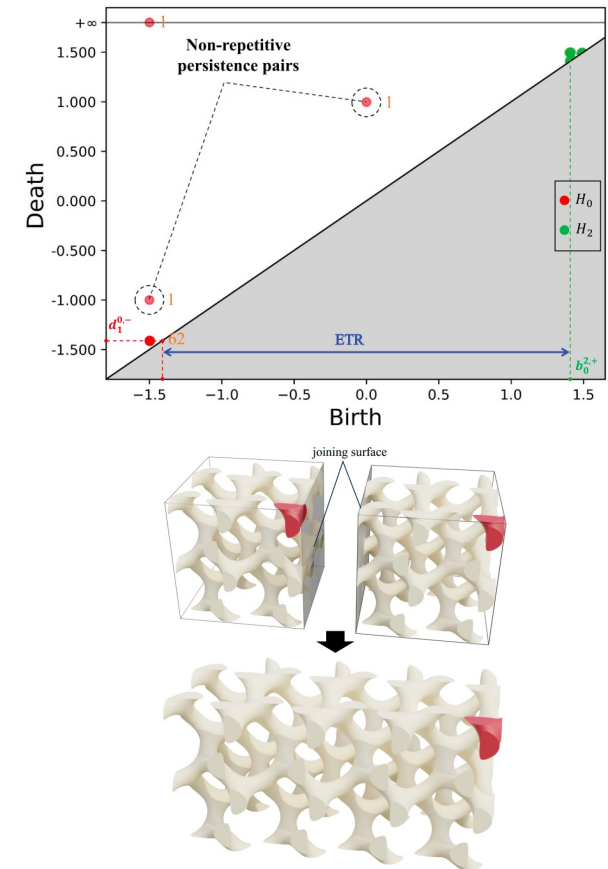
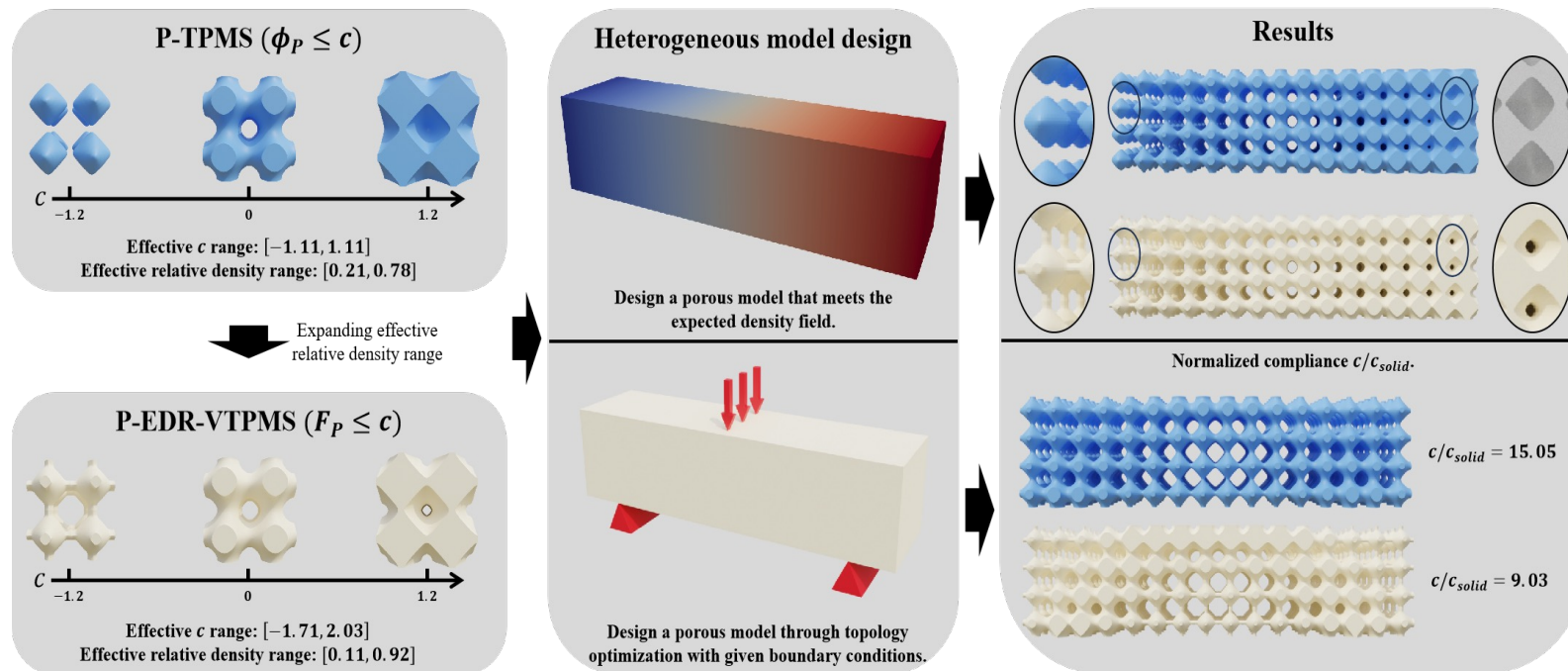
- Blend two implicitly represented porous structures smoothly
- **Eliminate the topological errors** in the blending region by **PD optimization**
- Keep the porous outside the blending region unchanged



Depeng Gao, Yang Gao, Yuanzhi Zhang, Hongwei Lin. Topology-aware blending method for implicit heterogeneous porous model design. Computer Aided design, 177:103782 (2024)

Persistent Homology-Driven Optimization of Effective Relative Density Range

- Traditional porous representation is TPMS $\Phi(x) < C$
- $\Phi(x)$ is a trigonometric function, with a little adjustable parameters, and limited valid range of C
- Replace $\Phi(x)$ with B-spline, and enlarge the valid range of C by **PD optimization**

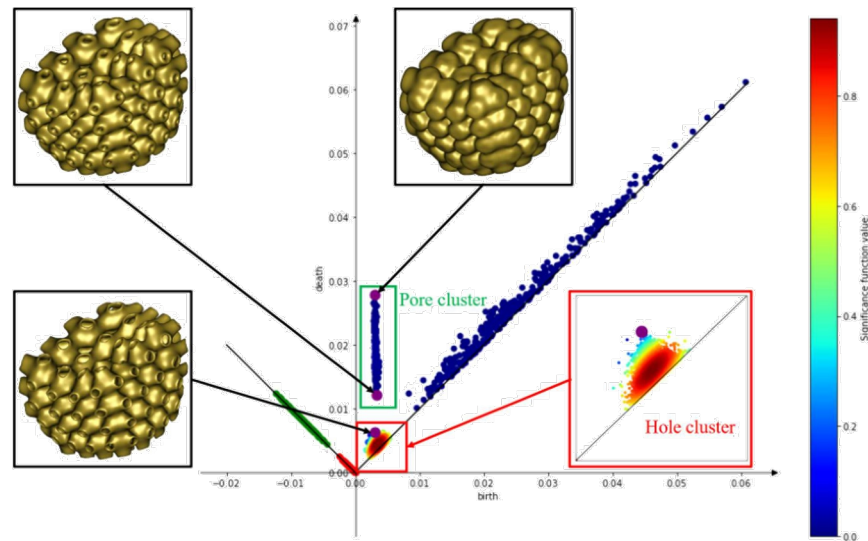


EDR-VTPMS: Effective relative density range-Variant TPMA

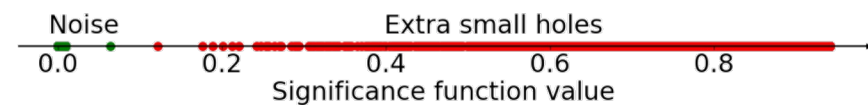
Depeng Gao, Yuanzhi Zhang, Hongwei Lin. Persistent Homology-Driven Optimization of Effective Relative Density Range for Triply Periodic Minimal Surface. Computer-Aided Design, in revision.

Reasonable thickness determination for sheet structure

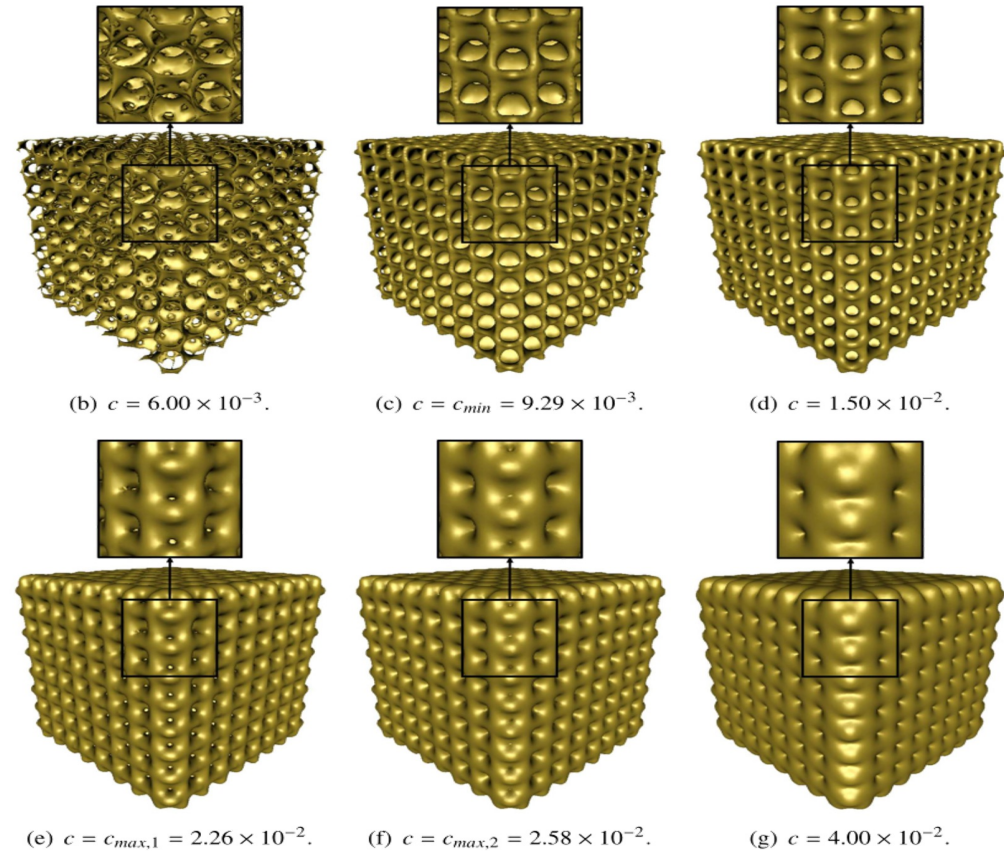
- TPMS surface represented porous should have thickness for 3D
- With too small thickness, there will be **extra small holes**; with too large thickness, porous will be **closed**
- By **clustering the points in a PD**, determine the reasonable thickness range



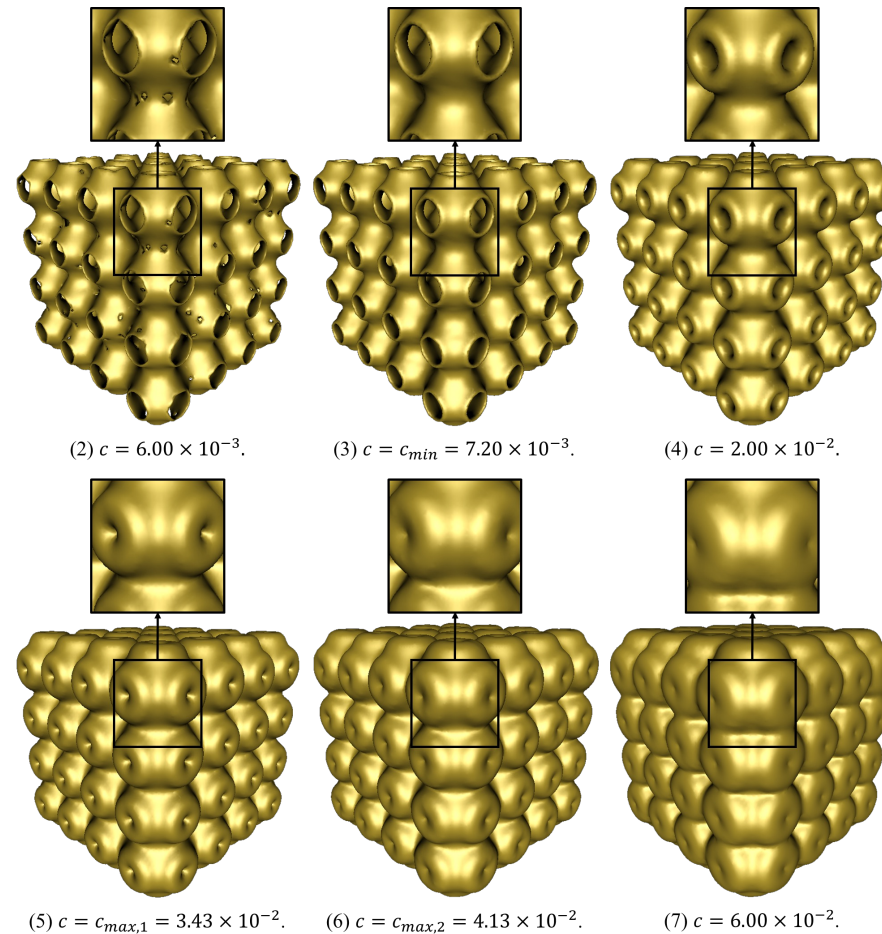
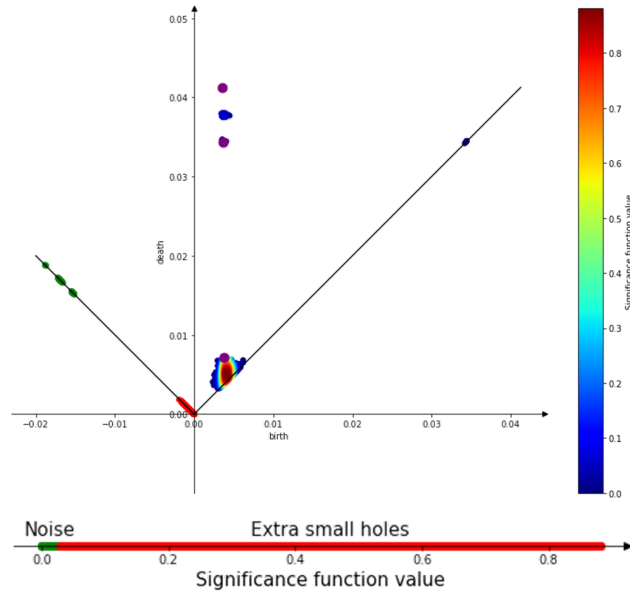
(a) 1-PD of the scalar field $|f(x, y, z)|$.



(b) Significance function values of the points in the short persistence cluster.



Experimental Results:



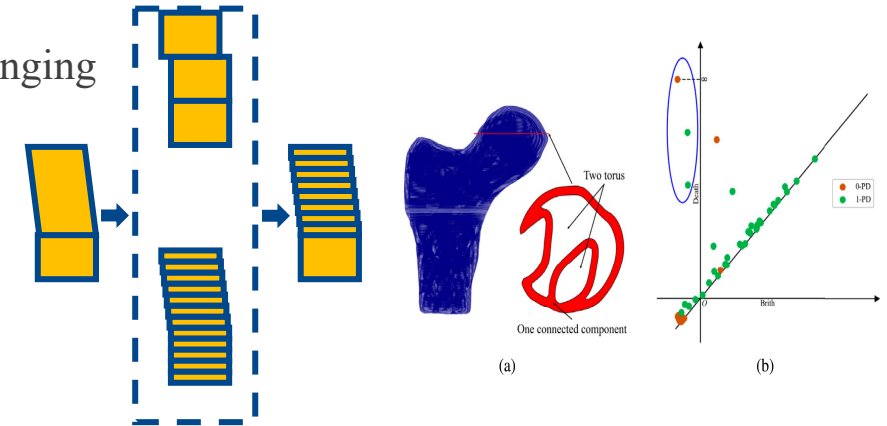
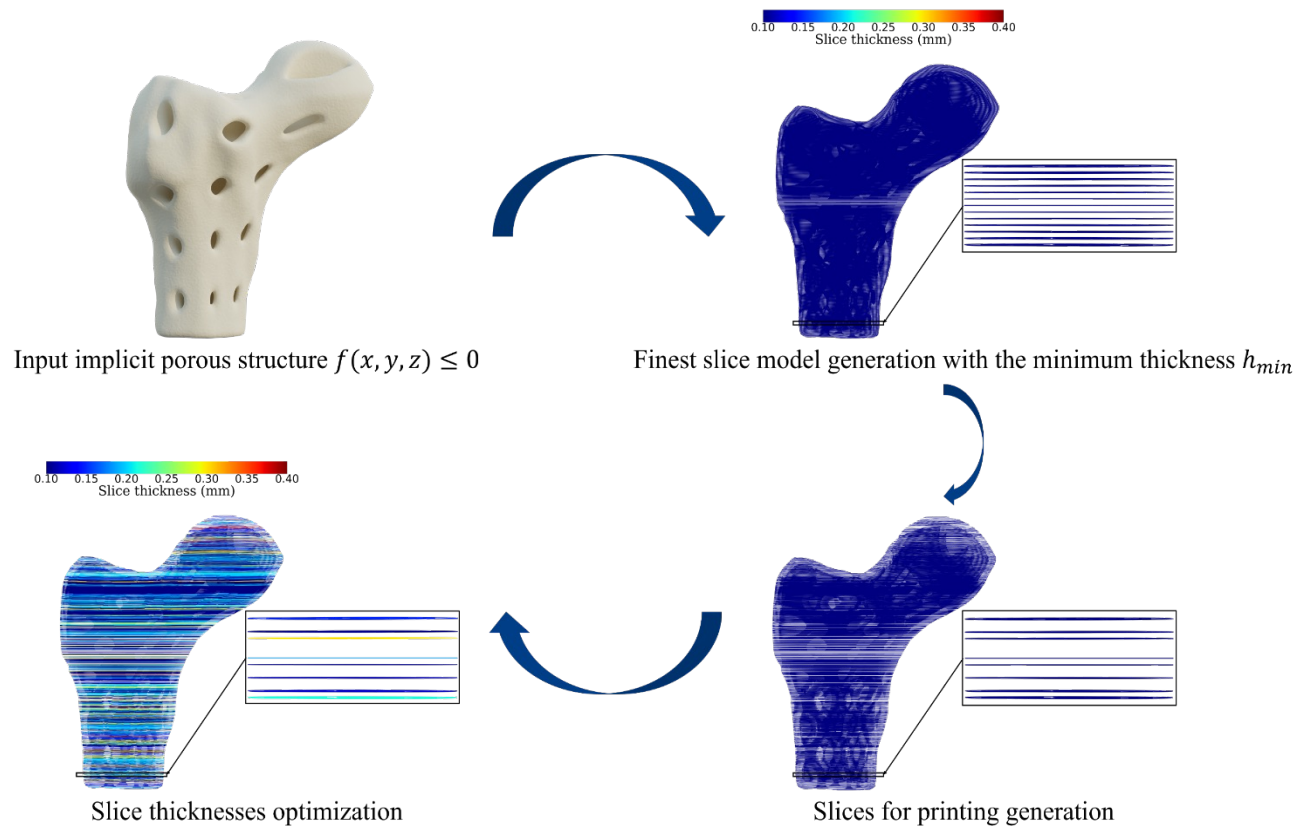
The variation of the number of pores and holes in these sheet structures

Parameter c	Topological measurement $\bar{\beta}$
$c < c_{min}$	5.661
$c = c_{min}$	1.000
$c_{min} < c < c_{max,1}$	1.000
$c = c_{max,1}$	0.998
$c = c_{max,2}$	0.000
$c > c_{max,2}$	0.000

Jiacong Yan, Hongwei Lin. Reasonable thickness determination for implicit porous sheet structure using persistent homology. Computers & Graphics, 115, 236-245, 2023

Adaptive slicing with topology guarantee

- The 2D slice of a porous has **complicated topological structure**
- By **comparing the PDs of adjacent slices**, find the critical slice with topology changing
- **Guarantee the topology consistency** between design model and printed model



Model	Method	Slice number	Topology detection error	Cusp height sum (mm)	Volume deviation
Balljoint	Our method	502	0	44.34	0.31%
	Cusp height based method	502	192	47.52	0.39%
	Boolean operations based method	502	197	46.34	0.40%
Moai	Our method	580	0	35.56	0.40%
	Cusp height based method	580	192	37.45	0.41%
	Boolean operations based method	580	148	37.02	0.41%
Tooth	Our method	652	0	54.63	0.58%
	Cusp height based method	652	274	56.84	0.62%
	Boolean operations based method	652	233	55.93	0.62%
Venus	Our method	569	0	51.31	0.55%
	Cusp height based method	569	227	54.23	0.60%
	Boolean operations based method	569	264	53.20	0.61%

Jiacong Yan, Hongwei Lin. Adaptive Slicing of Implicit Porous Structure with Topology Guarantee. Computer-Aided Design, 162, 103557, 2023 (SPM 2023).



1. Introduction to computational topology
2. Applications in geometric design
3. Porous retrieval, design, and printing
- 4. Interpretability of DNN**
5. Applications in computational psychology
6. Conclusion

- Neural networks have a close relationship between their **structures and functions**
- We propose the concept of the **functional network** of neural networks
- By **exploring the topological structure** of these functional networks, we can **gain a better understanding of the connection between their structures and functions**

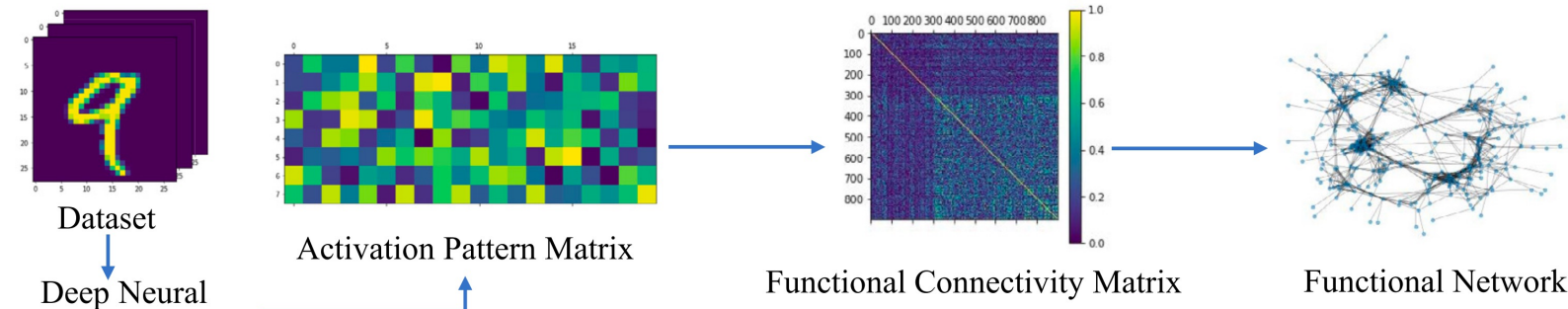
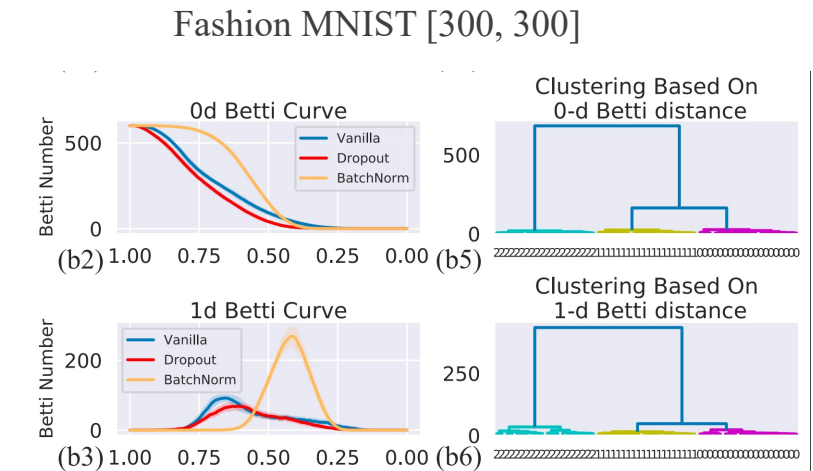
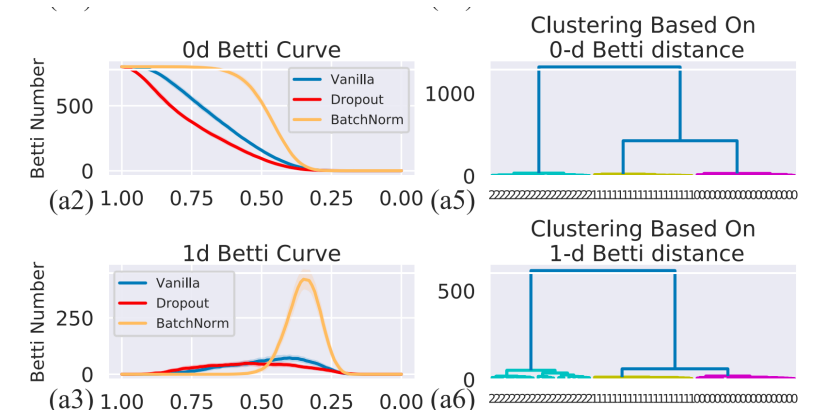
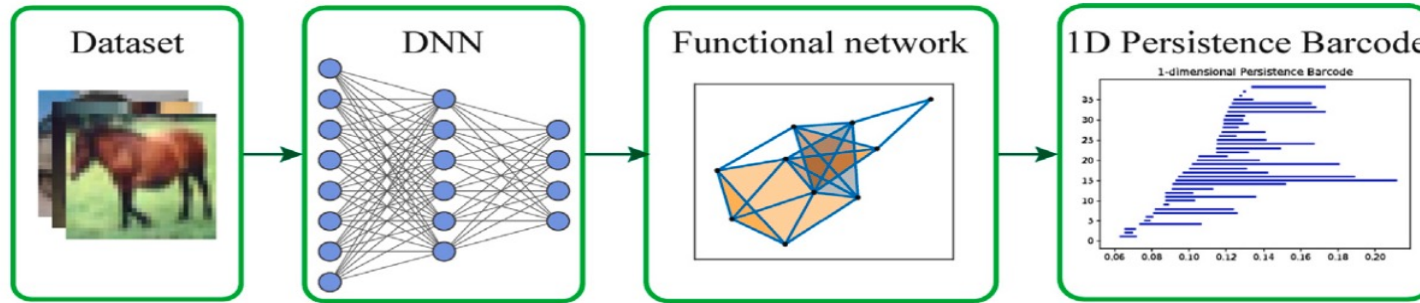


Fig. 1. Flow chart of constructing the functional network for a given deep neural network.

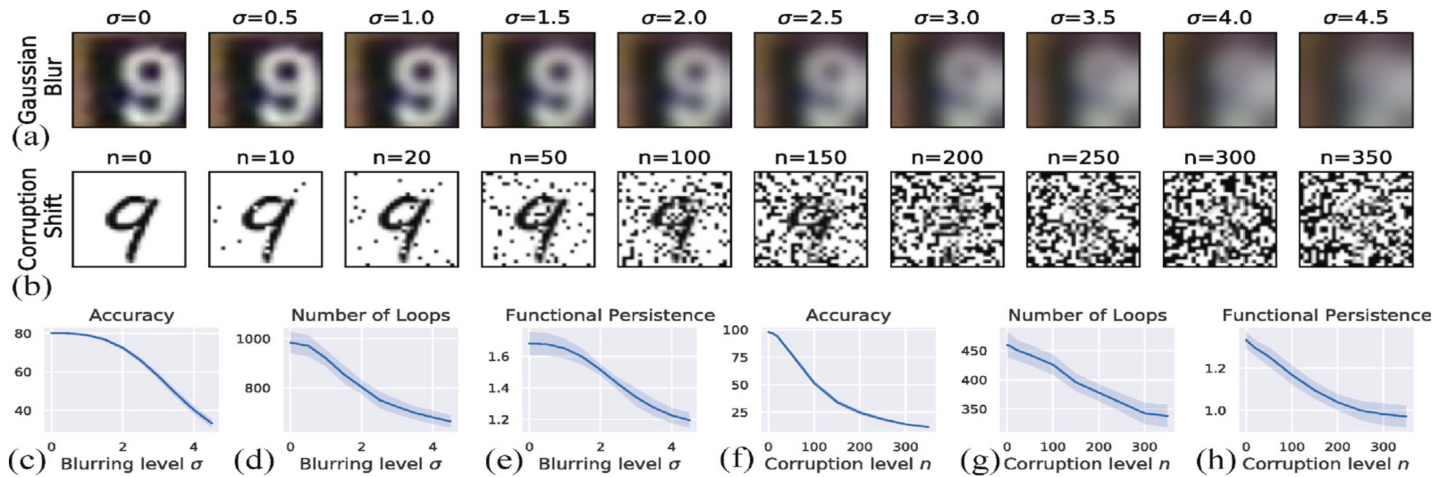


MNIST [300, 300]
Influence of different regularizations

- The relationship between functional organizations and network performance is explored using algebraic topology
- The **functional loops** reveal **functional interaction patterns** of multiple neurons in DNNs.



- The functional network is constructed as a simplicial complex $K(M, S)$ by computing the functional similarities between neurons
- The **1-dimensional persistent barcode** is calculated to measure the functional complexity of the DNN



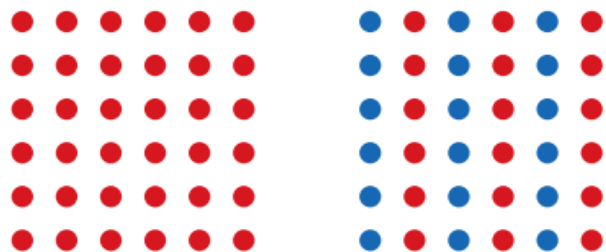
- The number of loops, functional persistence, and accuracy decrease as the dataset shifts
- Therefore, the **number of loops may reflect the number of features extracted by models** from unseen samples

Ben Zhang, Hongwei Lin. Functional loops: Monitoring functional organization of deep neural networks using algebraic topology. Neural Networks 174: 106239 (2024)

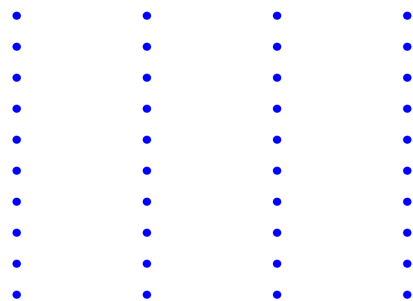


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- **Computational psychology** studies computational models of psychological rules
- The **Gestalt theory** is a classic theory in cognitive psychology used to explain the role of visual perception
- We established the **Gestalt computational model** using persistent homology theory in computational topology
- Gestalt theory includes five core principles: similarity, proximity, closure, good continuation, and pragnanz



Similarity



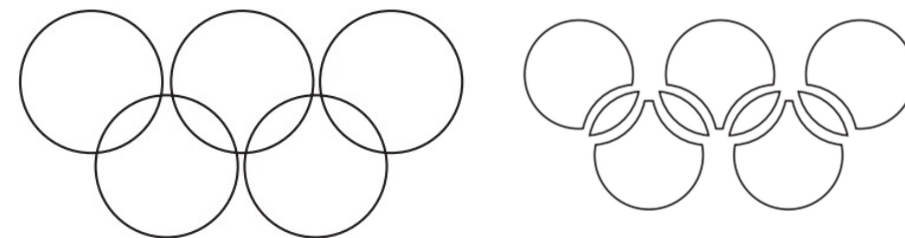
Proximity



Closure



Good continuation



Pragnanz

Gestalt Computational Model-Step 1,2,3

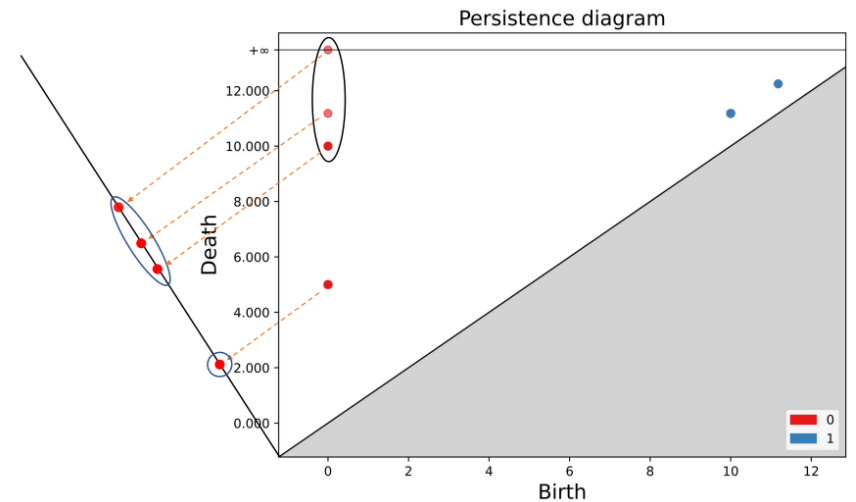
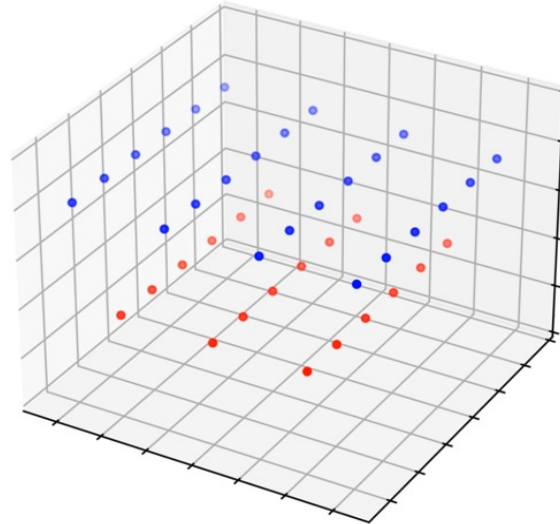
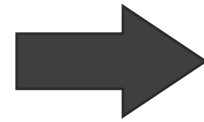
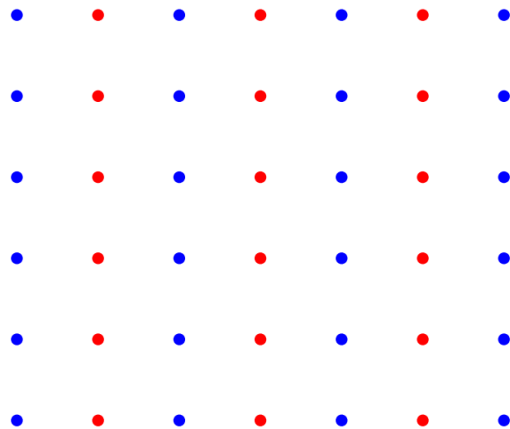
1. **Set additional coordinates:** According to the attributes of points set that affect the visual perception, assign an additional z-coordinate,

$$\{Q_i = (x_i, y_i, z_{i,1}, z_{i,2}, \dots, z_{i,m}), i = 1, 2, \dots, n\}$$

2. **Calculate PD:** Construct VR filtration and calculate the corresponding PD

3. **Cluster the points on the PD:**

- Project the points in the PD onto the line $y = -x$ and cluster them into two categories
- The category far from the origin is the important feature points



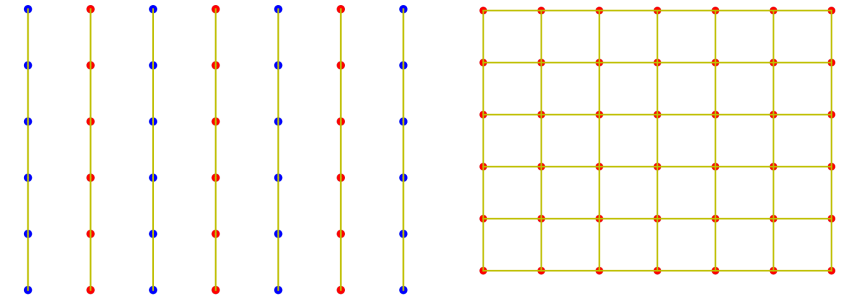
Gestalt Computational Model-Step 4, 5

4. **Determine the threshold:** Determine a suitable threshold ε_g so that important topological features have appeared and not disappeared

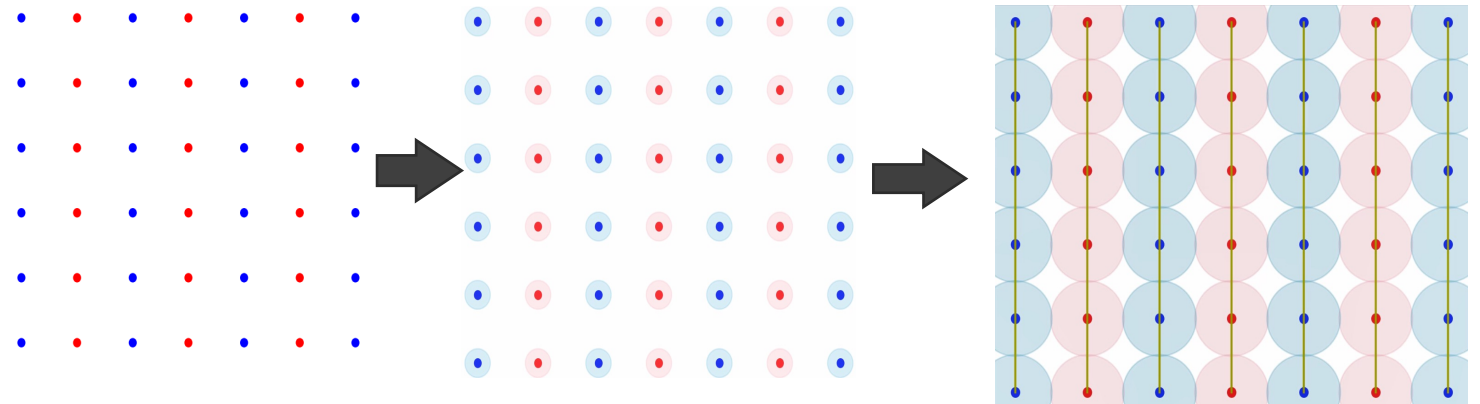
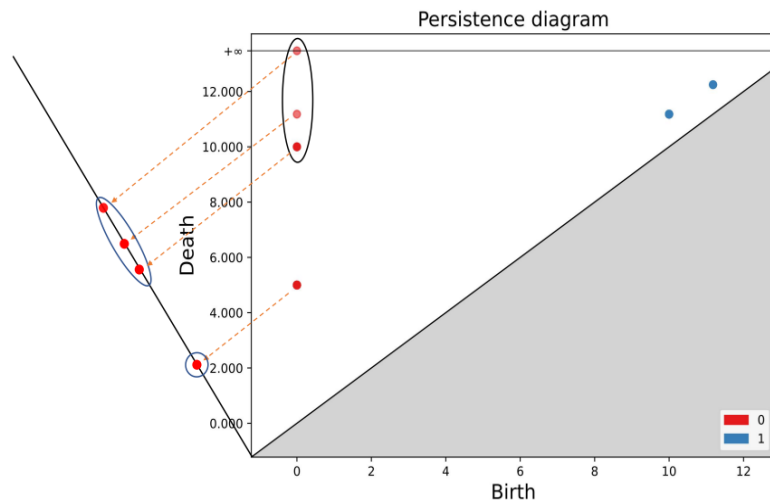
- For 0-PD, select ε_g as the maximum value of the extinction values of all noise points
- For 1-PD, select ε_g as the maximum value of the birth values of all important points

5. **Reconstruction of visual perception results:**

- Reconstruct the results of visual perception from $VR(X, \varepsilon_g)$

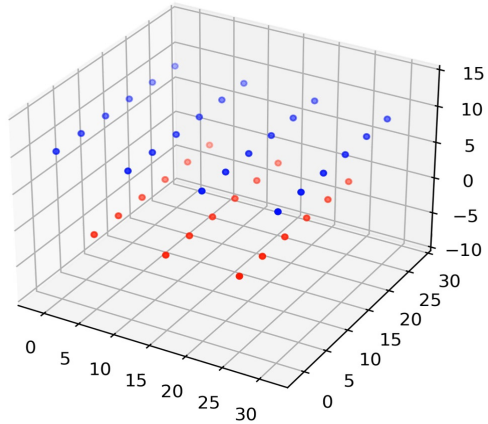


The visual perception results reconstructed by the above method are in line with Gestalt principles



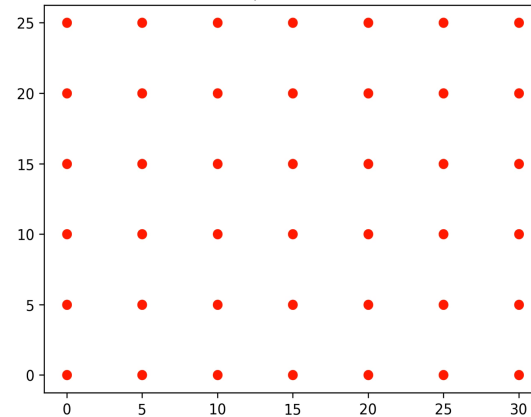
Gestalt Computational Model: Results

epsilon=0.0



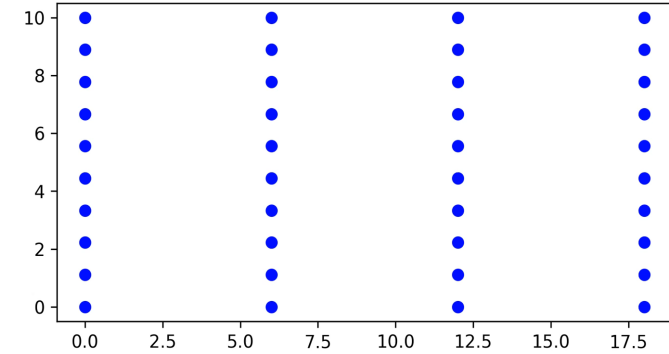
Similarity: 3D

epsilon=0.0



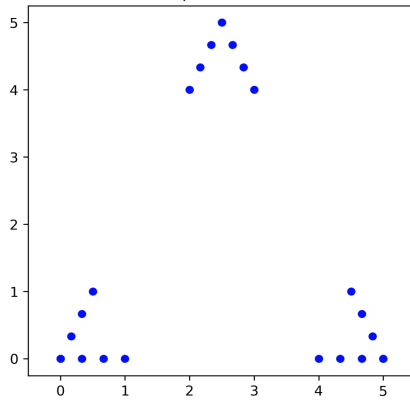
Similarity: 2D

epsilon=0.0



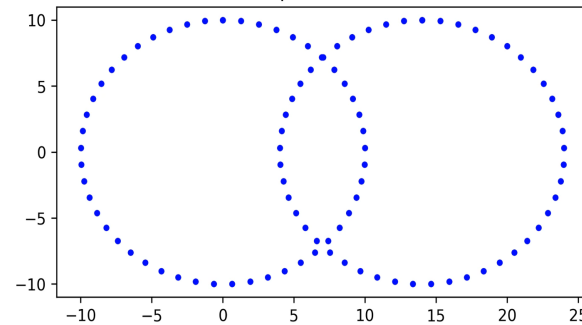
Proximity

epsilon=0.0



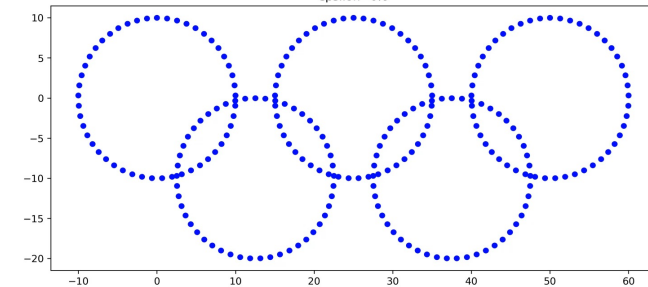
Closure

epsilon=0.0



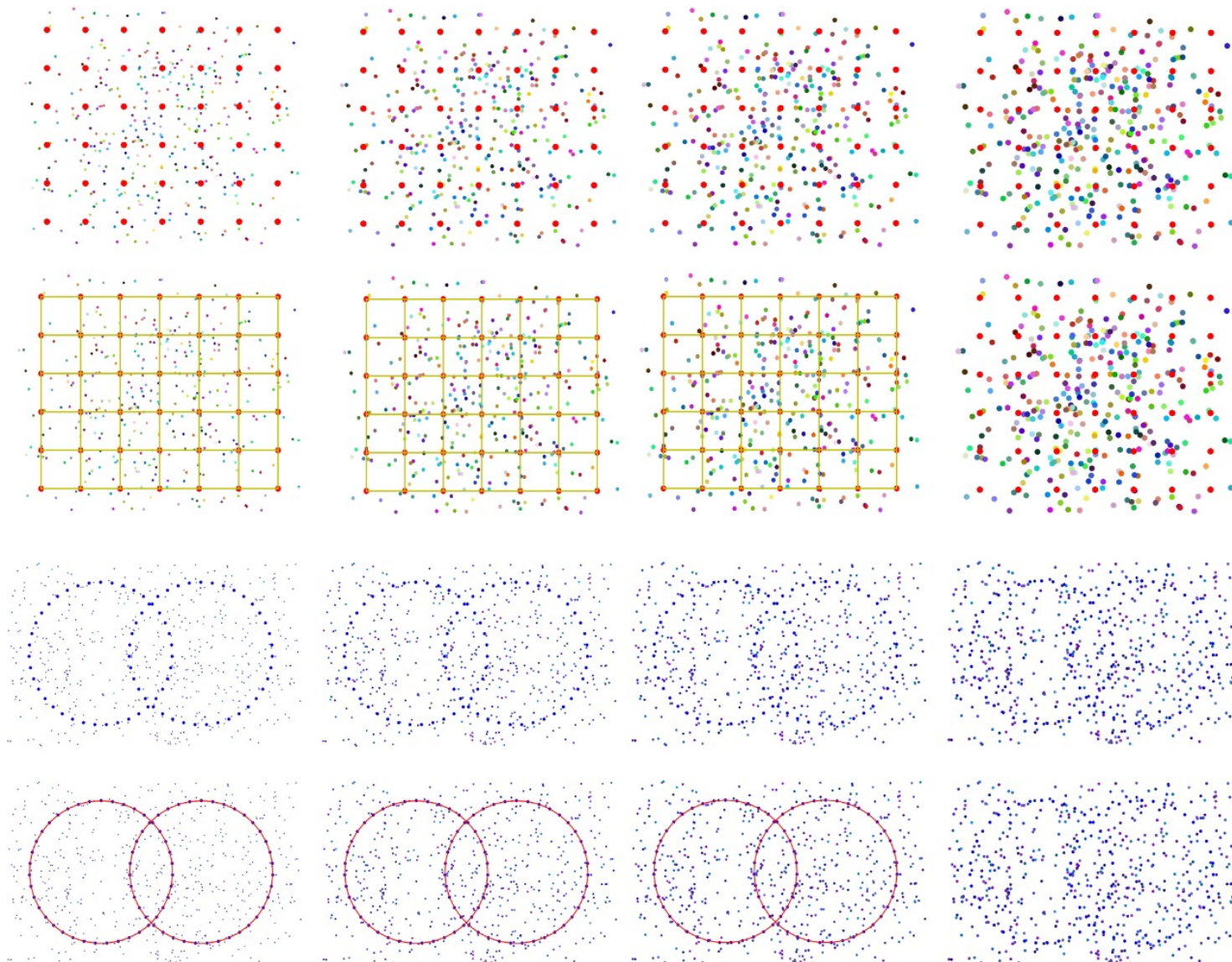
Good continuation

epsilon=0.0

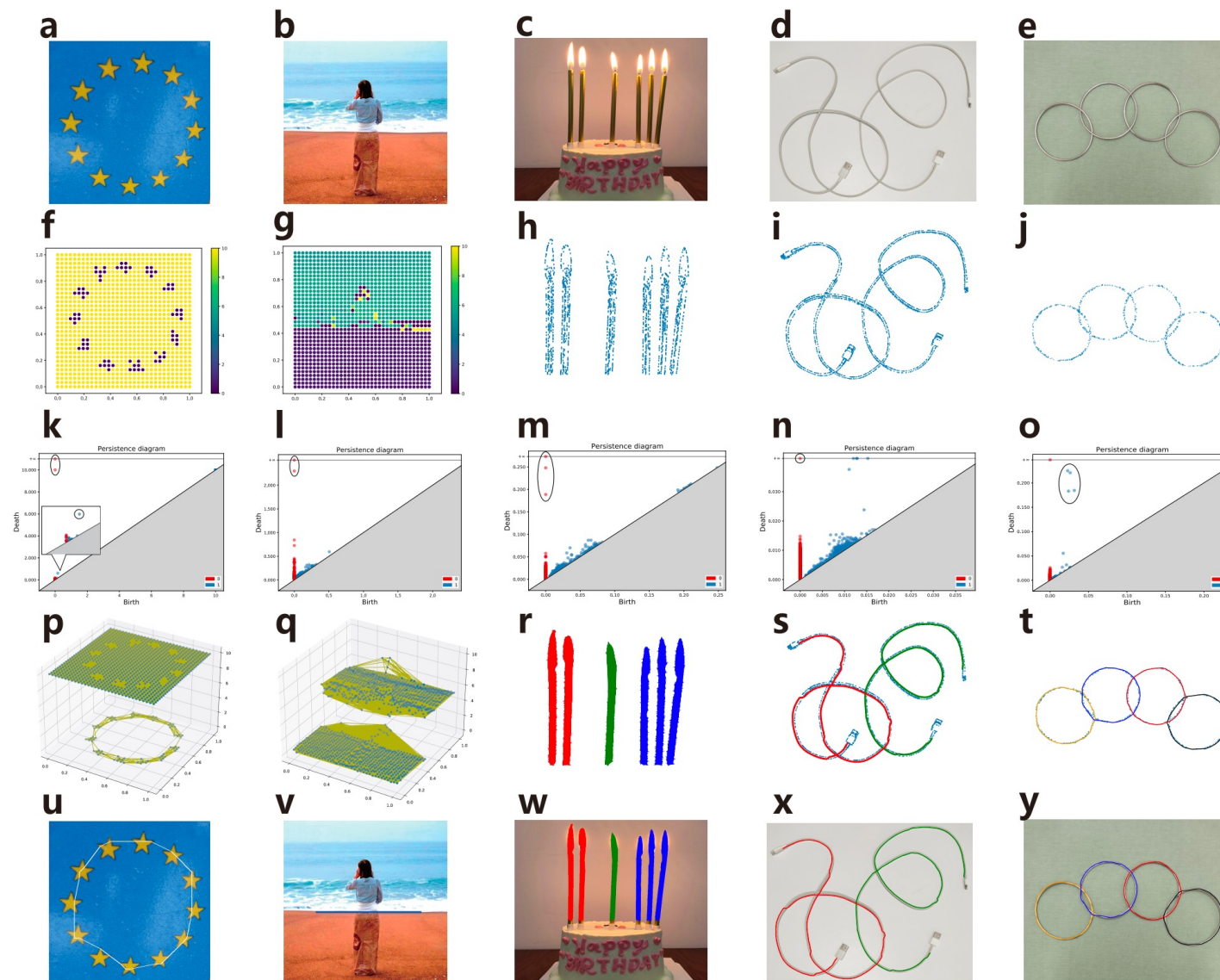


Pragnanz

Influence of noise



Computational Results on Real Images





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- Computational Geometry → Computational Topology
- Computer Aided Geometric Design → **Computer Aided Topological Design**
- **计算机辅助拓扑设计：以持续同调为主要理论工具，系统解决几何设计和几何处理中的拓扑问题**

2022年 12月
第43卷 第6期

图学学报
JOURNAL OF GRAPHICS

December 2022
Vol.43 No.6

计算机辅助拓扑设计

——持续同调在几何设计和处理中的应用

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2. 浙江大学CAD&CG国家重点实验室, 浙江 杭州 310058)

摘要: 持续同调是一种计算不同尺度拓扑特征的有效方法。其从一簇向后包含的单纯复形序列中提取出拓扑特征的出现和消失时刻, 并使用拓扑特征的“生命周期”来量化地衡量该特征的几何尺度和重要程度。拓扑特征的提取与应用在几何设计中扮演着重要角色, 催生出了一些基于持续同调的几何设计研究。从持续同调特征的提取与基于持续同调的建模和优化两方面进行综述, 在持续同调特征的提取方面, 介绍了从点云和三角网格数据中提取拓扑特征的不同方法, 总结了拓扑特征在部分几何设计问题中的应用路径。在建模和优化方面, 综述了基于拓扑变换的单纯复形重建方法、拓扑可感知的曲面重建方法与基于持续同调的拓扑去噪和优化方法。

关键词: 持续同调; 拓扑特征提取; 形状重建; 去噪与优化; 几何设计; 拓扑设计

中图分类号: TP 391

DOI: 10.11996/JGj.2095-302X.2022060957

文献标识码: A

文章编号: 2095-302X(2022)06-0957-10

Computer aided topological design

——survey on geometric design and processing based on persistent homology

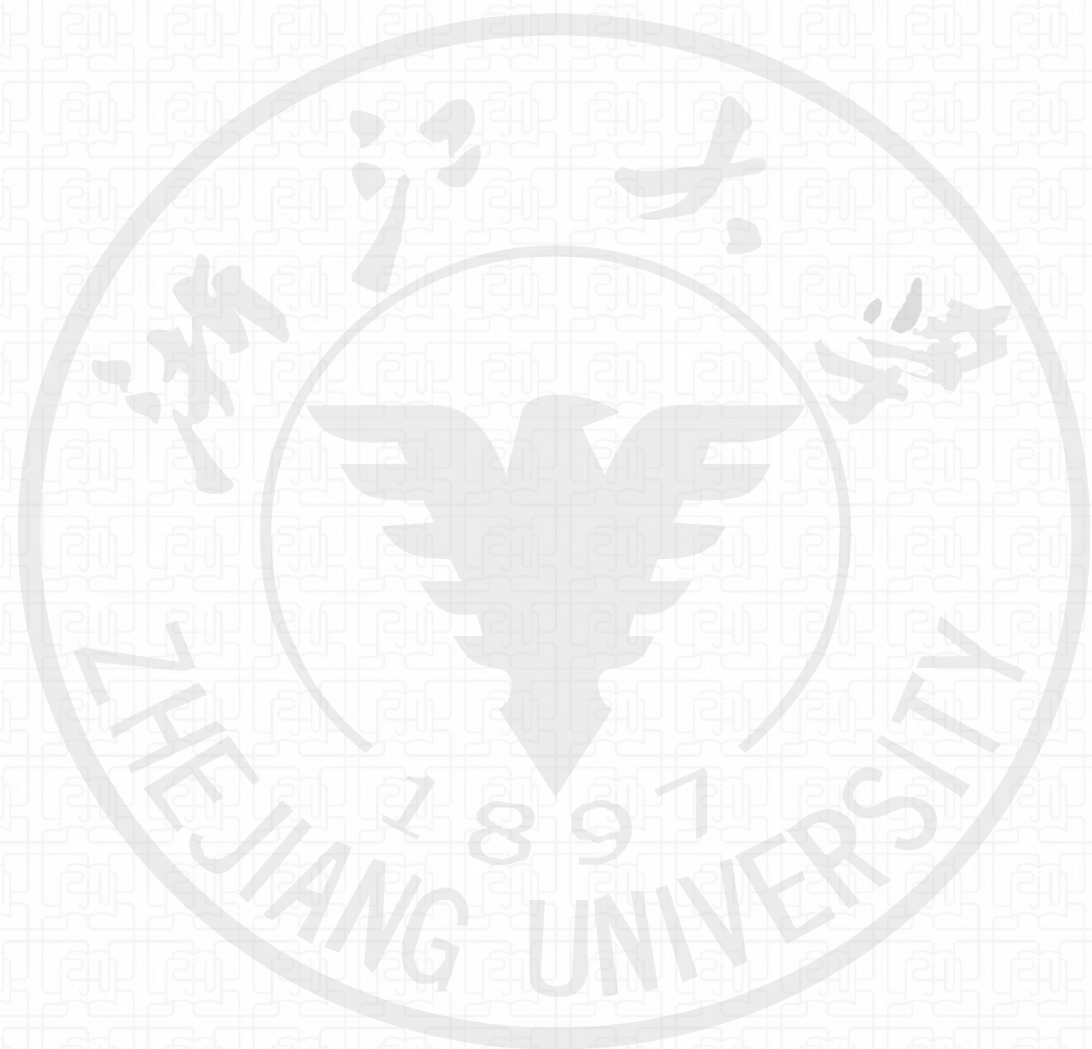
DONG Zhe-tong^{1,2}, LIN Hong-wei^{1,2}

(1. School of Mathematical Sciences, Zhejiang University, Hangzhou Zhejiang 310027, China;
2. State Key Laboratory of CAD&CG, Zhejiang University, Hangzhou Zhejiang 310058, China)

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- 点云拓扑理解及曲线曲面重建
- 深度神经网络的可解释性
- 股票数据处理

谢 谢!



浙江大学-几何与拓扑计算