



Stony Brook University

Learning Topological Representations for Deep Image Understanding

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Prof. Chao Chen (Advisor), Prof. Fuxin Li

Topology is everywhere

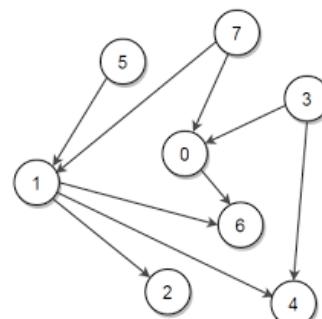
Image



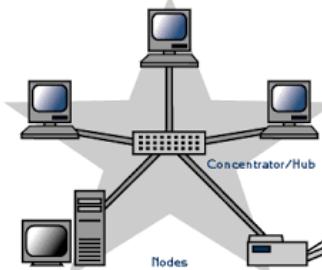
Point Cloud



Graph



Network



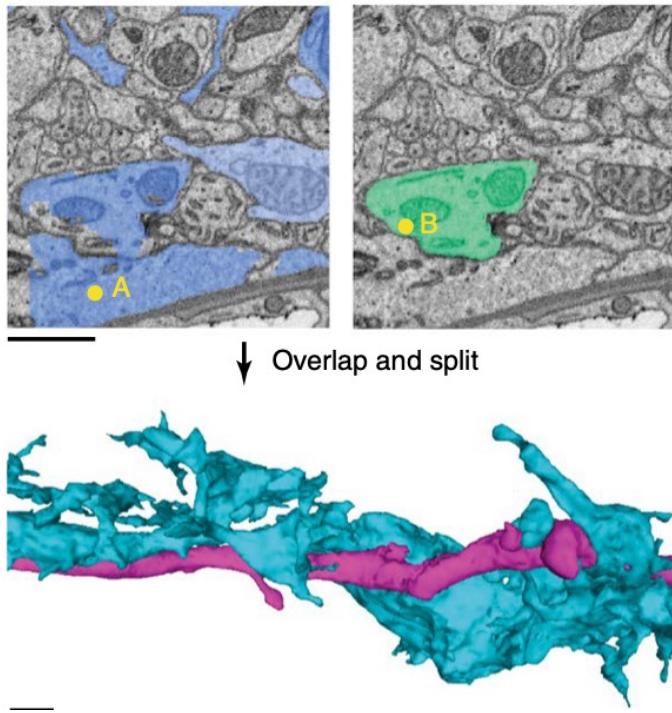
Road network reconstruction



*Topological correctness
is one of the main
challenges in road
network reconstruction!*

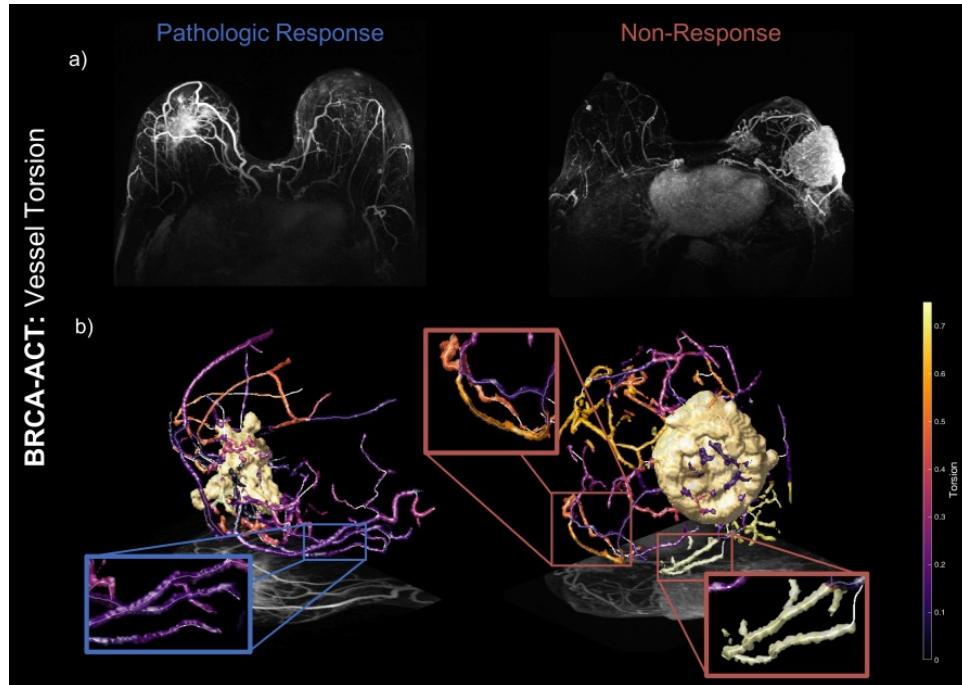
Zhu, Lingli, et al. "Automated 3D scene reconstruction from open geospatial data sources: Airborne laser scanning and a 2D topographic database." *Remote Sensing* (2015).

Neuron reconstruction



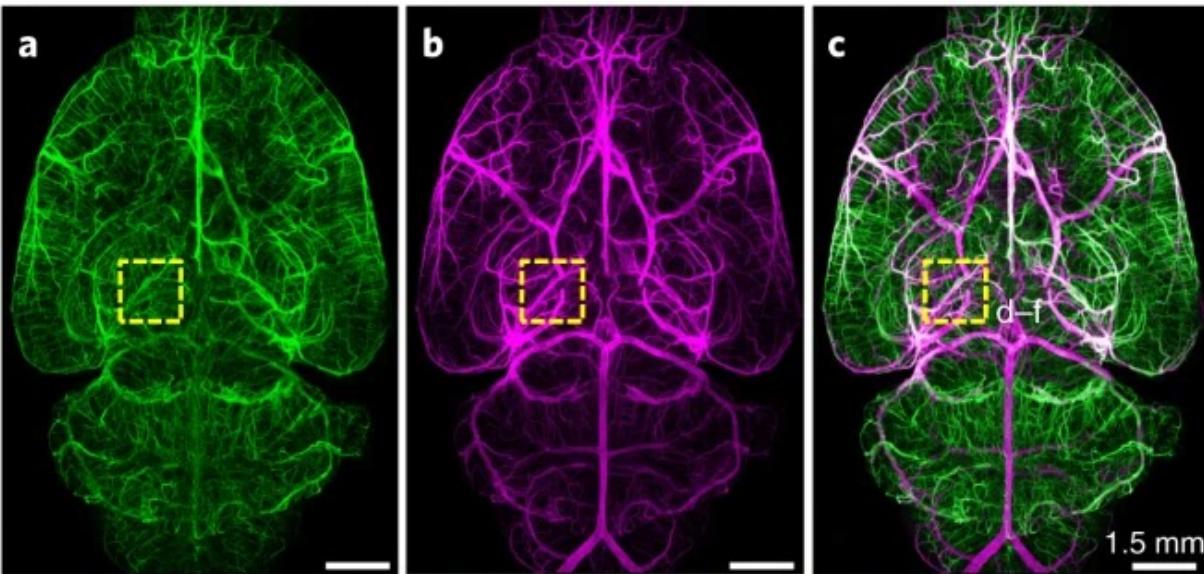
*Incorrect topology
results in incorrect
merge or split!*

Vasculation morphology measurement



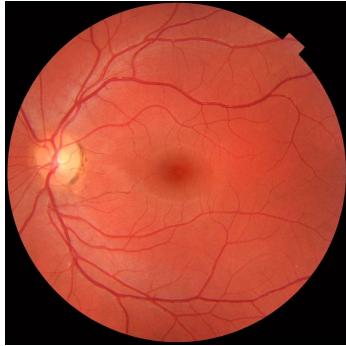
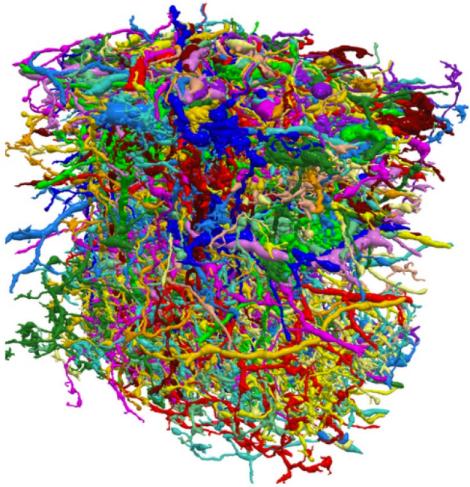
***Correct measurement
of topology leads to
powerful biomarkers!***

Quantification of mouse brain



*Structure yields
biological insights into
the vascular function
of the brain!*

Data with rich structural information



- Challenges

- Complex topology/structure
- Noisy data
- Limited labels

Difficult to analyze!

My research: Structure-informed image analysis

- **Problems**

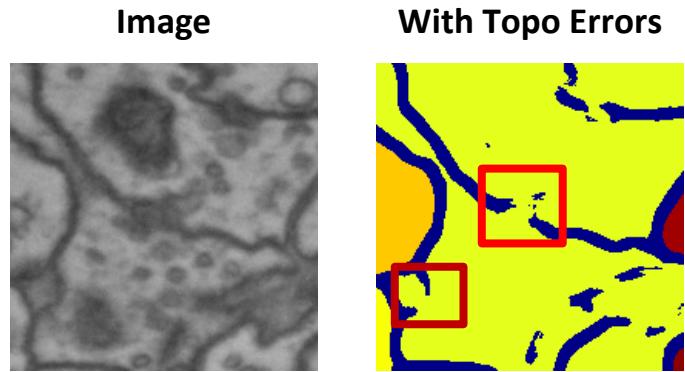
- Analyze structures with complex topology and geometry

- **Applications**

- Vessels, neurons, cells, etc.

- **Challenges**

- Incorrect topology (extraction)
- Purely data-driven methods are topology-agnostic
- Annotations are hard to obtain



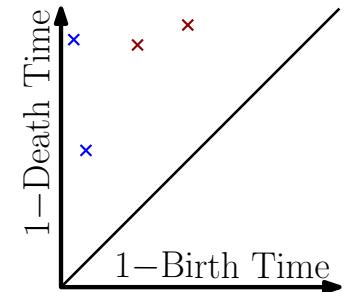
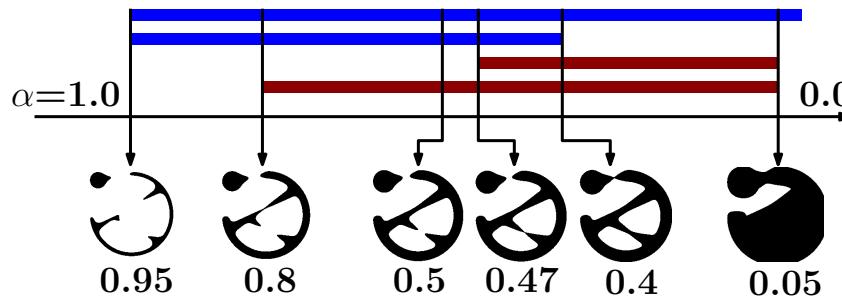
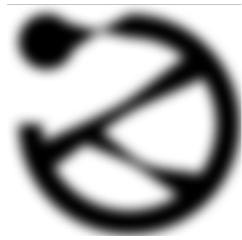
Hu et al. NeurIPS'19.

Key methodology: Topology

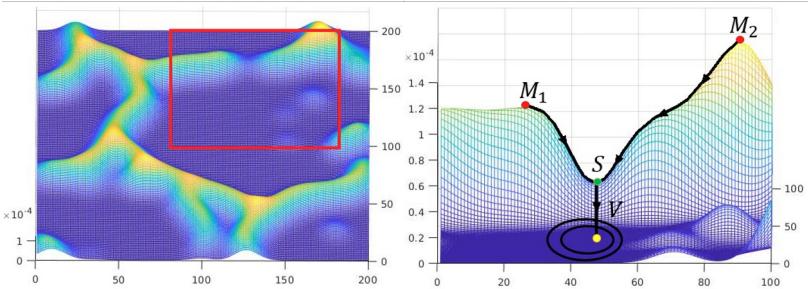
- **Explicit modeling of complex structures from data**
 - Math theory: algebraic topology
 - Persistent homology
 - Discrete Morse theory
 - Homotopy warping
- **Combine topology with deep learning organically**
 - Differentiability

DL methods incorporating classical topological theory

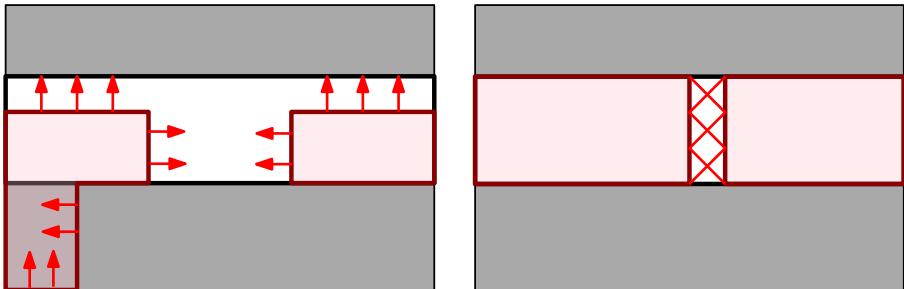
- Persistent homology



- Discrete Morse theory



- Homotopy warping



Research overview

Methodology

- Teach neural network to think in **topology/structure**
- Topological/structural **prior/regularization/feature**

Toolbox

- Persistent homology
- Discrete Morse theory
- Digital topology

Applications

- Image segmentation
- Uncertainty estimation
-

Future Directions

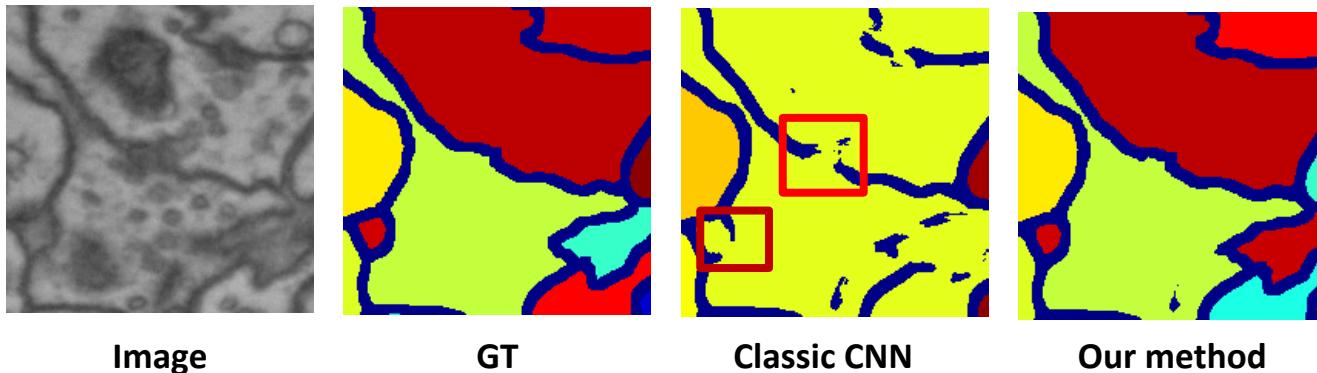
- Imperfect data
- Topological quantification
-

Outline

- **Topological loss for image segmentation**
 - Persistent homology based loss (NeurIPS'19, MICCAI'21)
 - Homotopy warping loss (NeurIPS'22)
- **Beyond pixel-wise representation**
 - Discrete Morse theory loss (ICLR'21, Spotlight)
 - Topological/Structural representation of images (ICLR'23, Spotlight)
- **Extensions**
 - Trojan detection with topological prior (ICLR'22)
- **Future work**

CNN are prone to topological errors

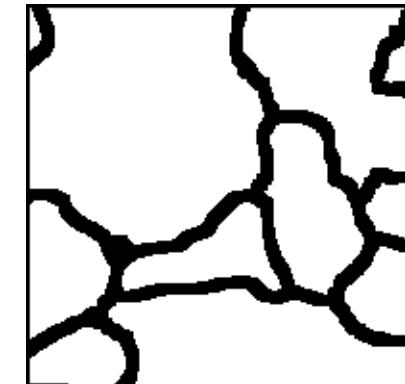
- Existing methods optimize w.r.t. per-pixel accuracy
- Topological errors
 - broken connection, missing components
- Broken membranes
 - small per-pixel error
 - topological error – large error in downstream analysis



Solution: Topological loss [NeurIPS'19]

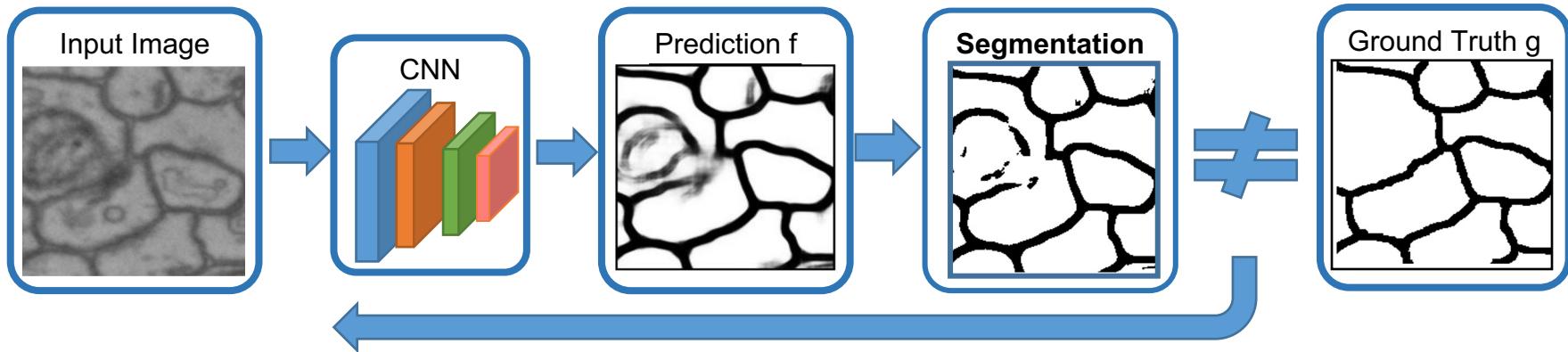
- Loss function – train the model to be topology-preserving
 - Repeatedly evaluate the accuracy in topology and force the model to correct mistakes
- Betti number
 - 0-dim betti number b_0 : number of connected components
 - 1-dim betti number b_1 : number of cycles
 - 2-dim betti number b_2 : number of voids
 -

$$b_0 = 1, b_1 = 11, b_{n \geq 2} = 0$$



Solution: Topological loss [NeurIPS'19]

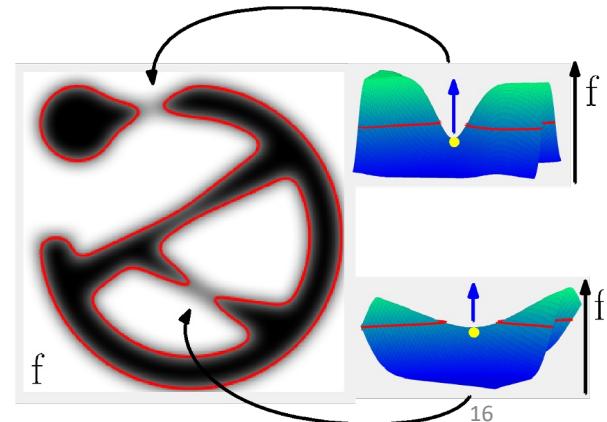
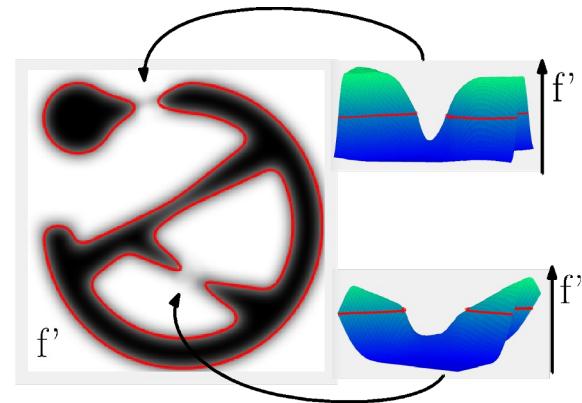
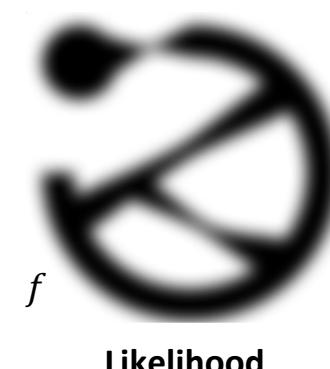
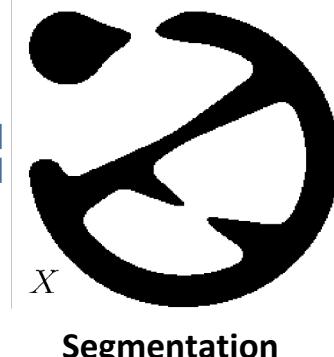
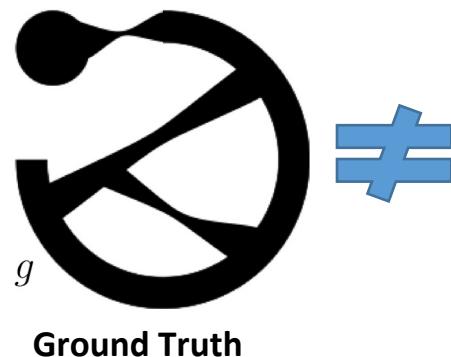
- Betti number error – **topological difference** between seg. and GT



- Challenge: **not differentiable**;
- Solution: persistent homology

Intuition: focus on likelihood f

- How far is f from generating a segmentation X with correct topology?
- What is the best way to fix X by changing f ?
- Compare with a worse likelihood f' (same segmentation X)

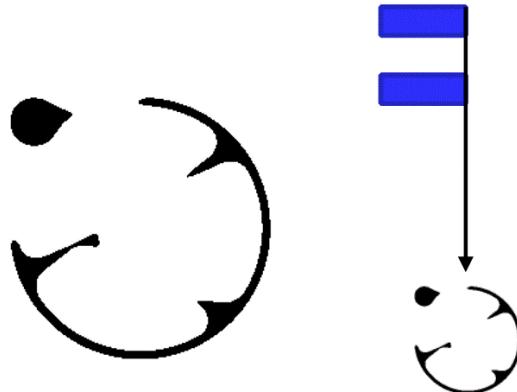


Persistent homology

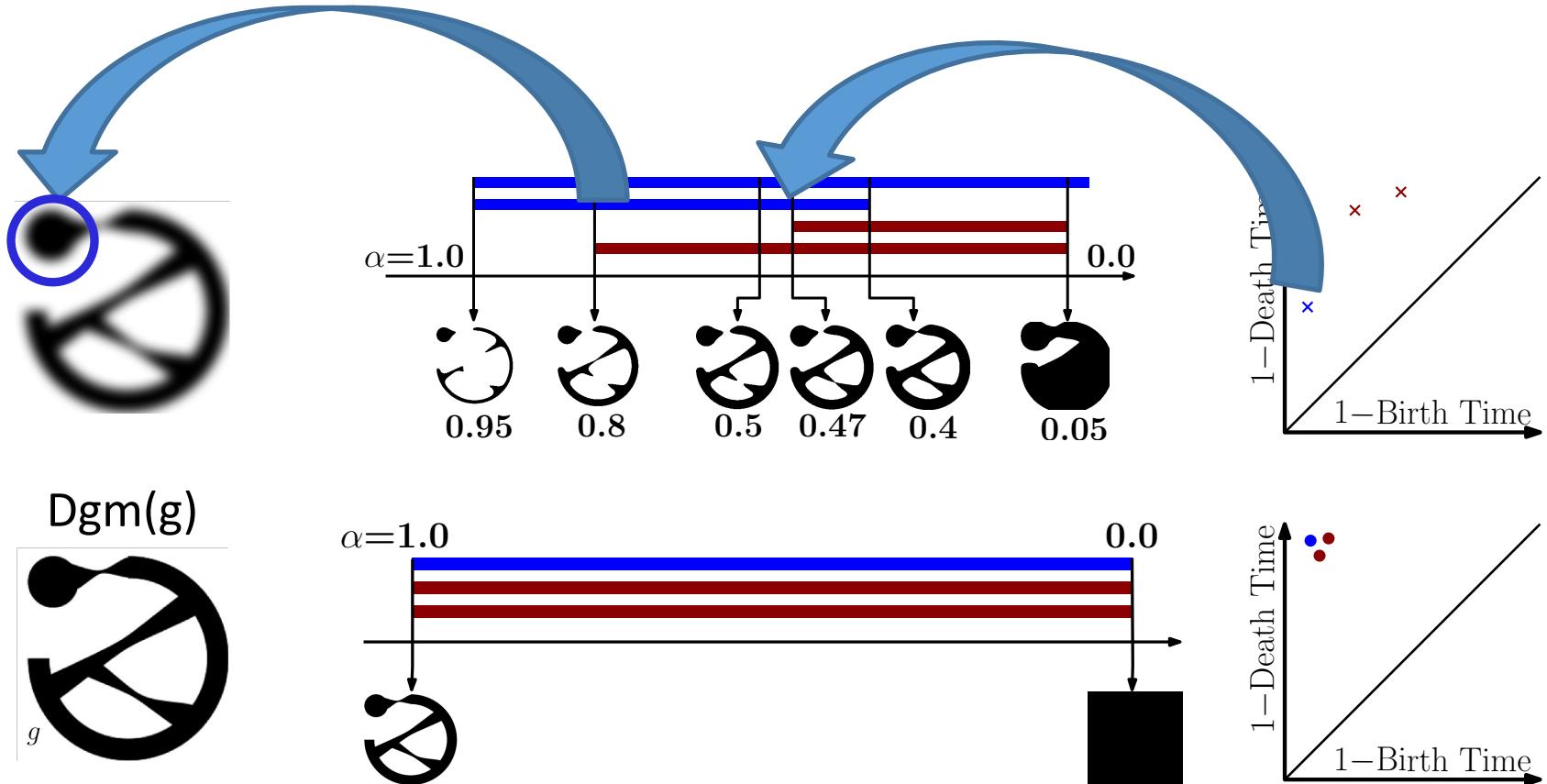
- Superlevel set: $f^\alpha = \{x \mid f(x) \geq \alpha\}$
- $\text{Dgm}(f) = \{\text{death}(p), \text{birth}(p)\}$, 0-dim (blue), 1-dim (burgundy)



Likelihood f

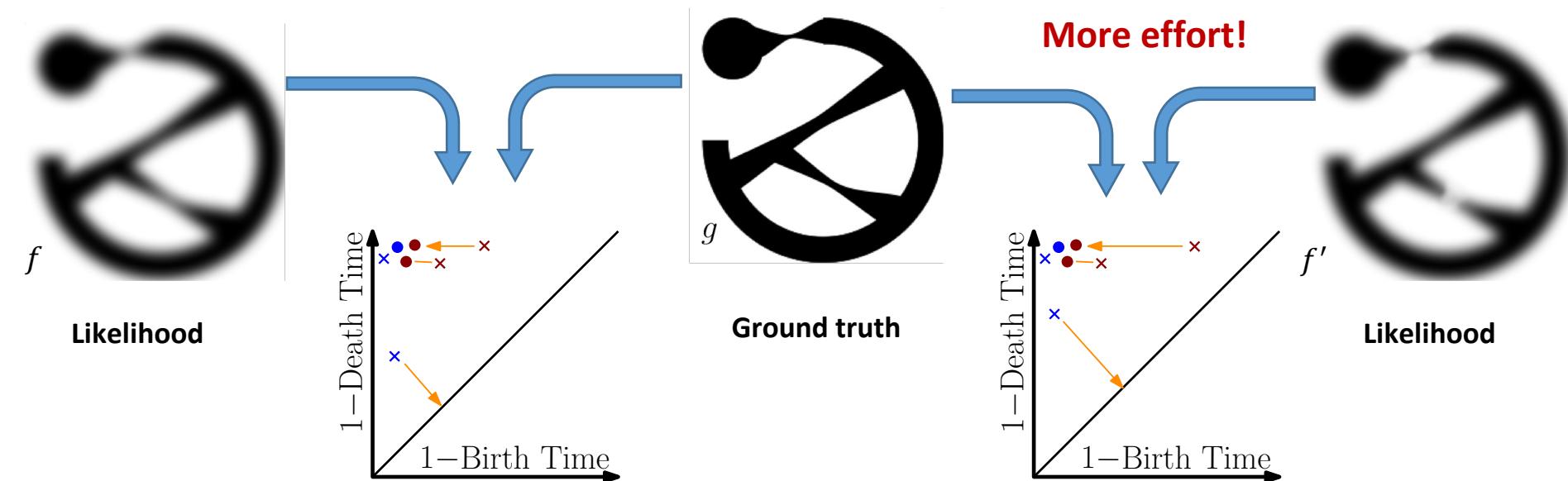


Persistence barcodes/diagrams



Topological loss (L_{topo}) = Distance between diagrams

$$\min_{\gamma \in \Gamma} \sum_{p \in \text{Dgm}(f)} \|p - \gamma(p)\|^2 = \sum_{p \in \text{Dgm}(f)} [\text{birth}(p) - \text{birth}(\gamma^*(p))]^2 + [\text{death}(p) - \text{death}(\gamma^*(p))]^2$$

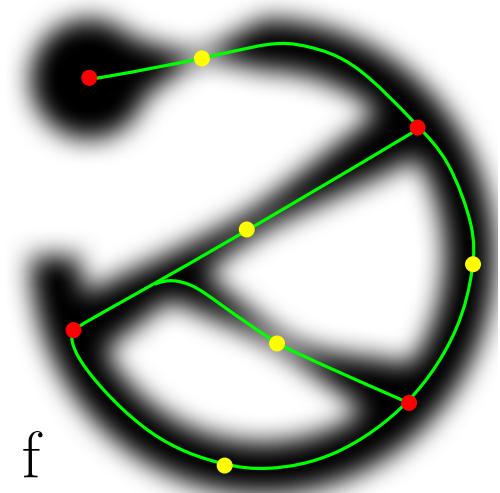


Differentiable?

$$\min_{\gamma \in \Gamma} \sum_{p \in \text{Dgm}(f)} \|p - \gamma(p)\|^2 = \sum_{p \in \text{Dgm}(f)} [\text{birth}(p) - \text{birth}(\gamma^*(p))]^2 + [\text{death}(p) - \text{death}(\gamma^*(p))]^2$$

- Depending on **critical thresholds**: topological changes happen, e.g., birth/death times
- Uniquely determined by the critical locations/pixels (including maxima, minima and saddle points)

Topological loss is actually defined on specific pixels!



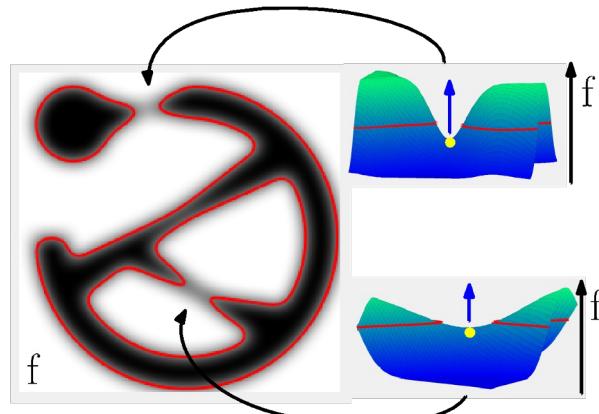
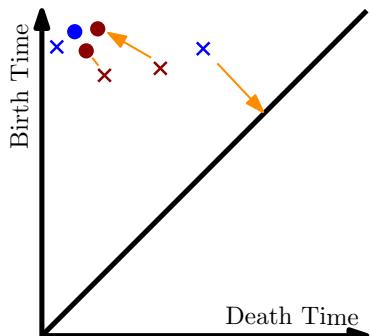
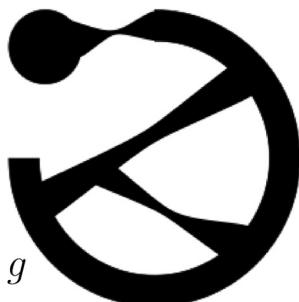
Gradient

- $c_b(p)$ – birth critical point of p ; $c_d(p)$ – death critical point of p
- Assume γ^* fixed, $c_b(p)$ and $c_d(p)$ are fixed

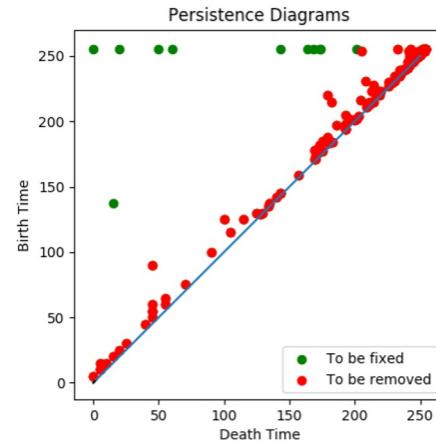
$$\sum_{p \in \text{Dgm}(f)}$$

$$2[f(c_b(p)) - \text{birth}(\gamma^*(p))] \frac{\partial f(c_b(p))}{\partial \omega}$$

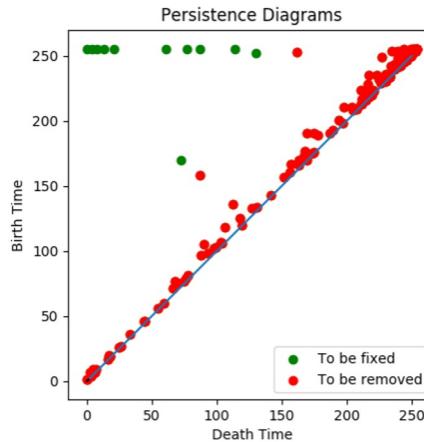
$$+ 2[f(c_d(p)) - \text{death}(\gamma^*(p))] \frac{\partial f(c_d(p))}{\partial \omega}$$



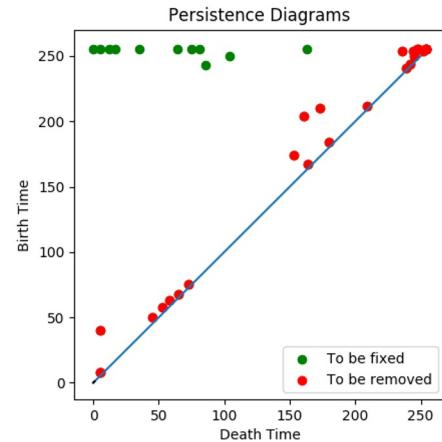
How it looks like in training?



Epoch 10



Epoch 30

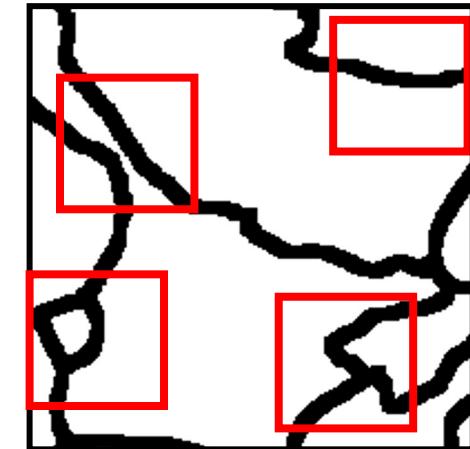
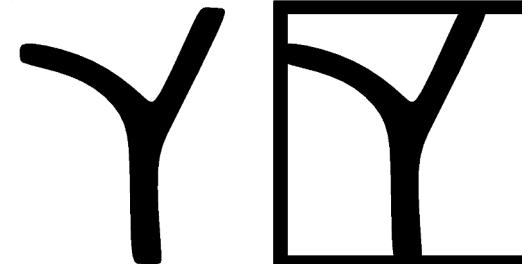
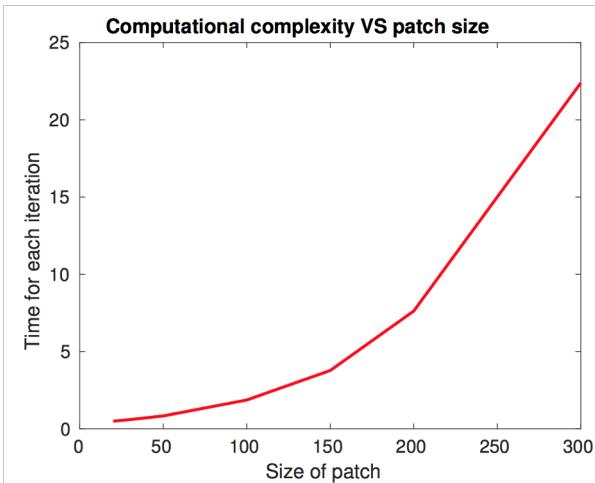


Epoch 50

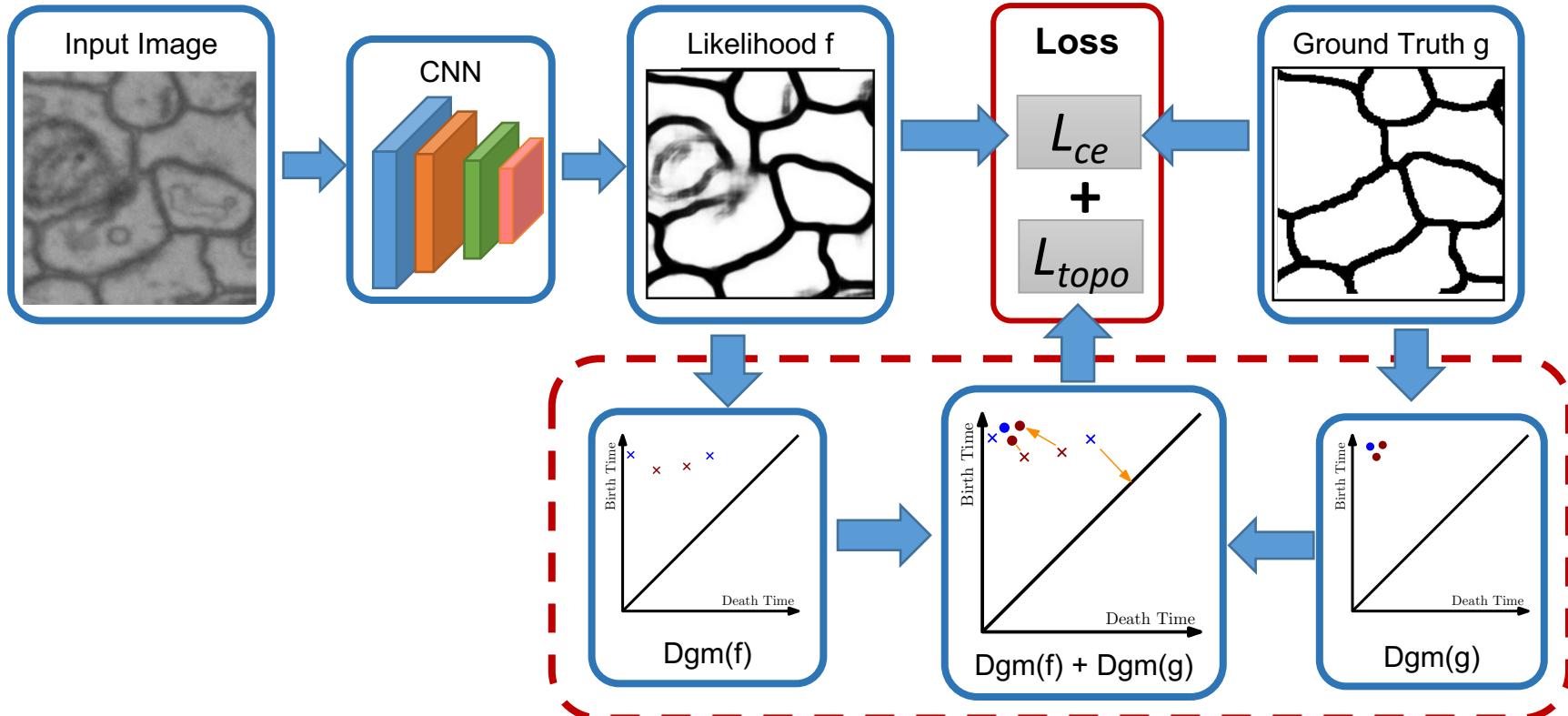
- Green dots: to be fixed; Red dots: to be removed
- As training continues
 - fewer red dots as noises are removed
 - green dots move closer to upper left corner (getting fixed)

Localized topological loss

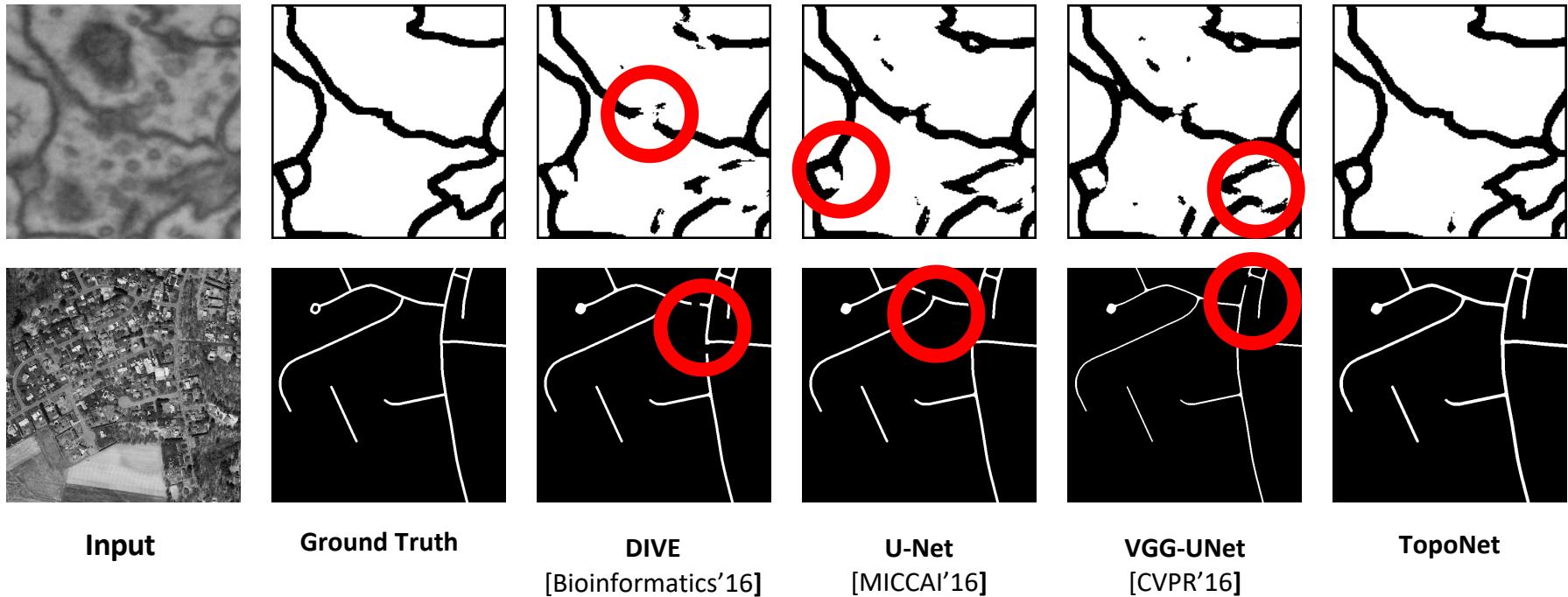
- Evaluate topology in whole image
 - Expensive
 - Too many dots: matching is difficult
- Localized topological measure: relative homology
- Sample patches over images and evaluate topology loss



Overview



Qualitative results

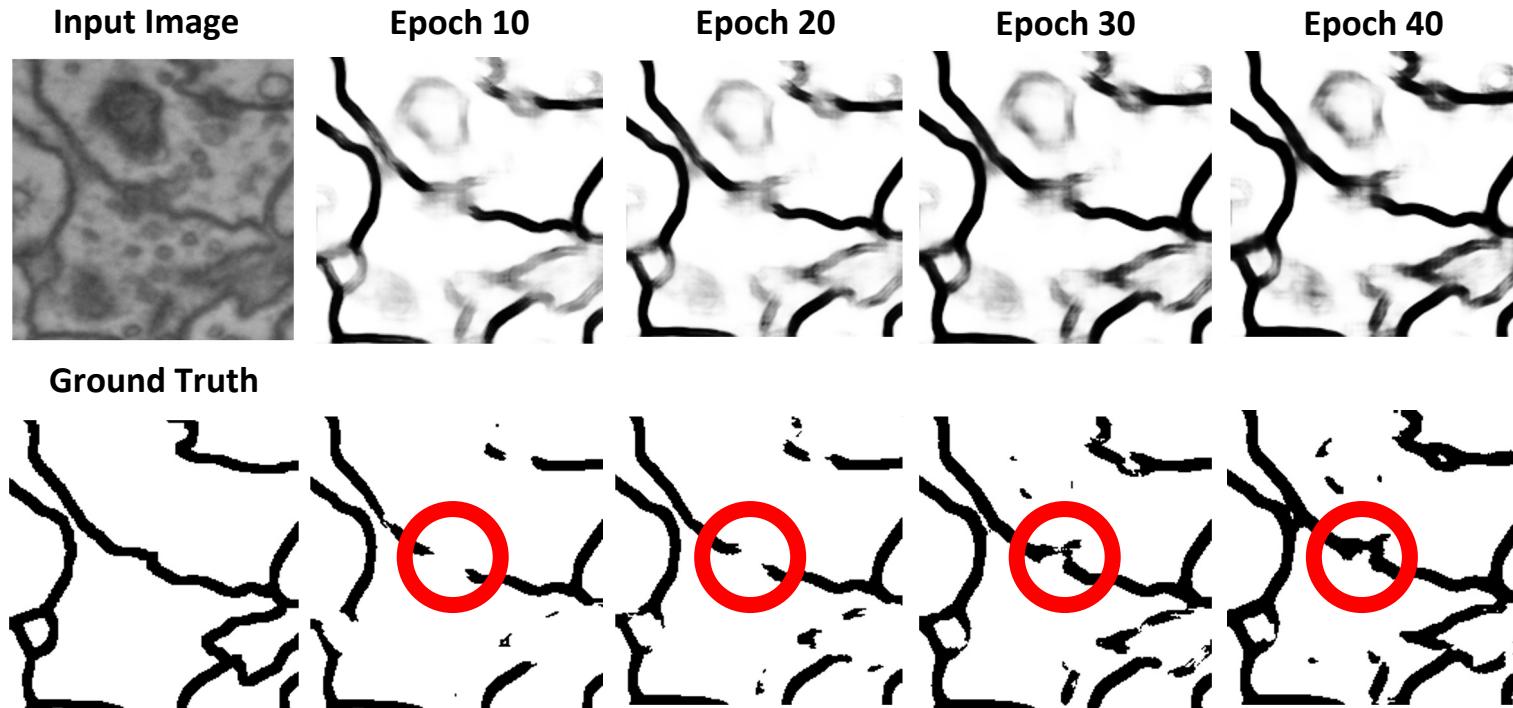


Quantitative results

- Per-pixel accuracy, Adapted Rand Index, Variation of Information
- Betti number error
 - Measures topological differences/errors directly
- EM (neuron) image segmentation datasets

Dataset	Method	Accuracy	ARI	VOI	Betti Error
ISBI12	DIVE	0.9640 ± 0.0042	0.9434 ± 0.0087	1.235 ± 0.025	3.187 ± 0.307
	U-Net	0.9678 ± 0.0021	0.9338 ± 0.0072	1.367 ± 0.031	2.785 ± 0.269
	Mosin.	0.9532 ± 0.0063	0.9312 ± 0.0052	0.983 ± 0.035	1.238 ± 0.251
	TopoLoss	0.9626 ± 0.0038	0.9444 ± 0.0076	0.782 ± 0.019	0.429 ± 0.104
ISBI13	DIVE	0.9642 ± 0.0018	0.6923 ± 0.0134	2.790 ± 0.025	3.875 ± 0.326
	U-Net	0.9631 ± 0.0024	0.7031 ± 0.0256	2.583 ± 0.078	3.463 ± 0.435
	Mosin.	0.9578 ± 0.0029	0.7483 ± 0.0367	1.534 ± 0.063	2.952 ± 0.379
	TopoLoss	0.9569 ± 0.0031	0.8064 ± 0.0112	1.436 ± 0.008	1.253 ± 0.172
CREMI	DIVE	0.9498 ± 0.0029	0.6532 ± 0.0247	2.513 ± 0.047	4.378 ± 0.152
	U-Net	0.9468 ± 0.0048	0.6723 ± 0.0312	2.346 ± 0.105	3.016 ± 0.253
	Mosin.	0.9467 ± 0.0058	0.7853 ± 0.0281	1.623 ± 0.083	1.973 ± 0.310
	TopoLoss	0.9456 ± 0.0053	0.8083 ± 0.0104	1.462 ± 0.028	1.113 ± 0.224

Segmentation during training



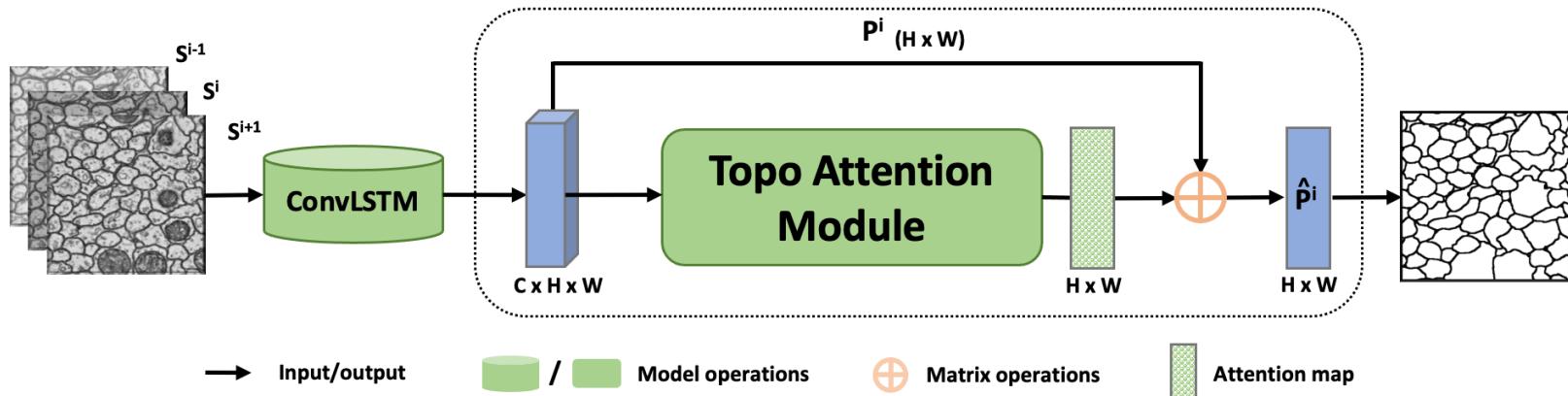
Rationale of topological loss

- Likelihood map/segmentation are stabilized globally
 - Mostly because of cross-entropy loss
- Topological errors are gradually fixed by the topological loss
 - Likelihood map only change at topology-relevant locations
- Topological loss complements cross-entropy
 - **Combating sampling bias**
 - Identifying difficult locations and increase their weights in training
- Without cross-entropy loss, inferring topology from a completely random likelihood map is meaningless



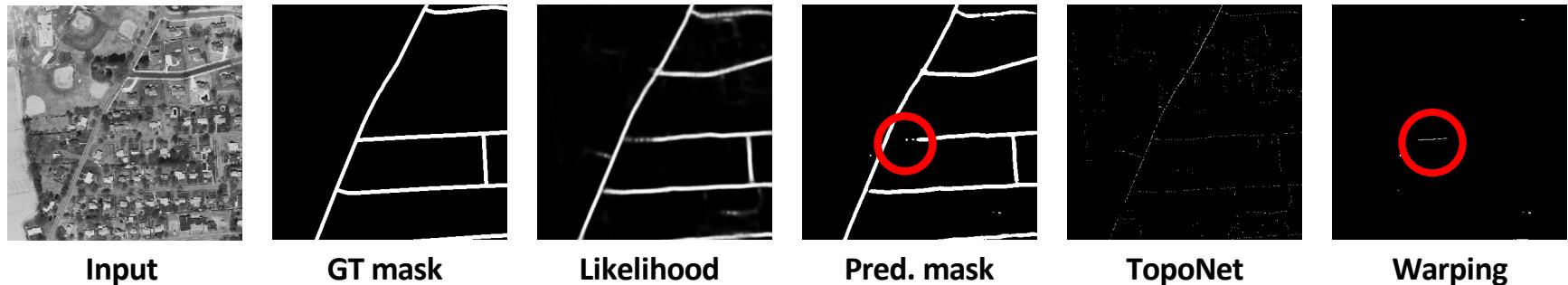
3D topology-preserving segmentation (MICCAI'21)

- Topological loss for 3D anisotropic cases
 - *Spatial topological-attention*: Spatial topological information across adjacent slices
 - *Iterative topological-attention*: Improve the stability of the topologically critical maps



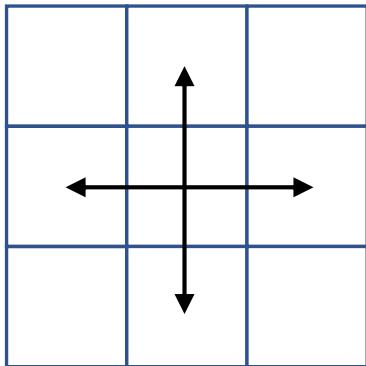
Homotopy warping loss (NeurIPS'22)

- Efficiently identify topological critical points
 - [Hu et al. NeurIPS'19] – Topological loss by matching persistence diagram

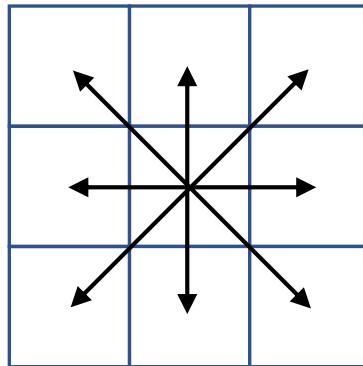


Simple points

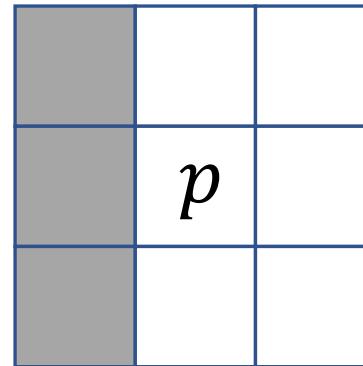
- Flipping the label of p will not change the topology



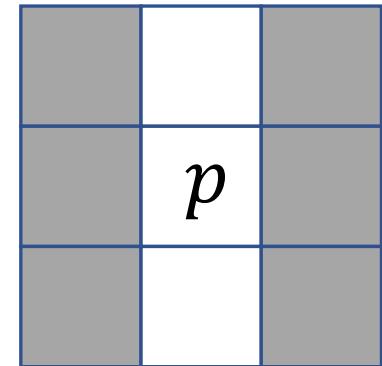
4-adjacent



8-adjacent



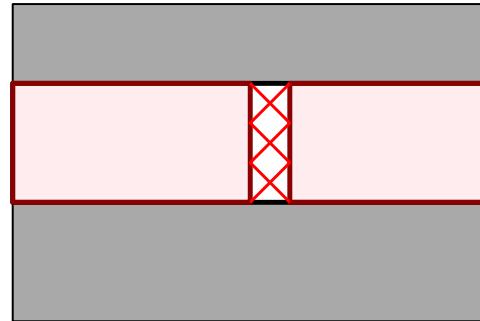
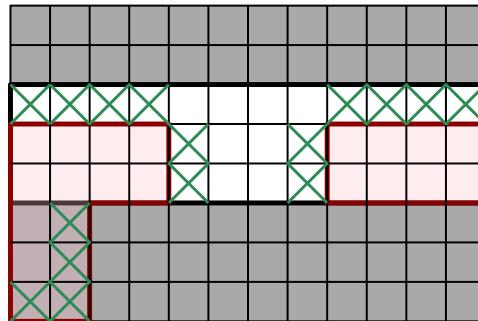
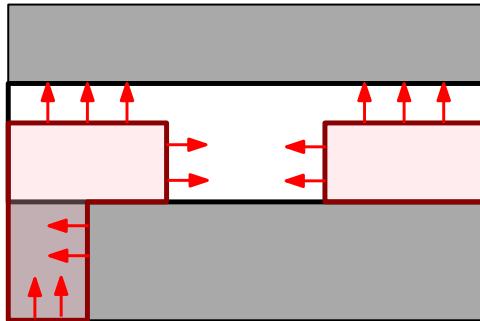
Simple Point



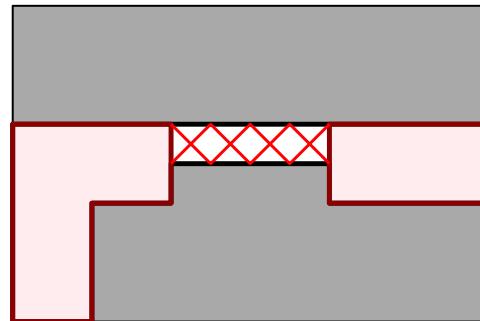
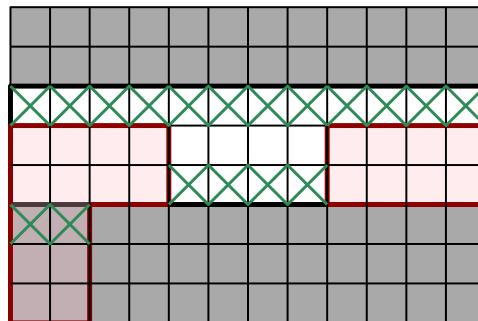
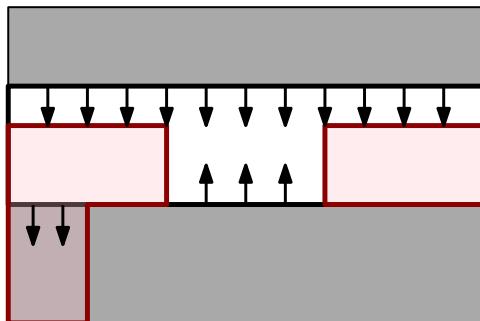
Non-simple Point

Homotopy warping: flip simple points

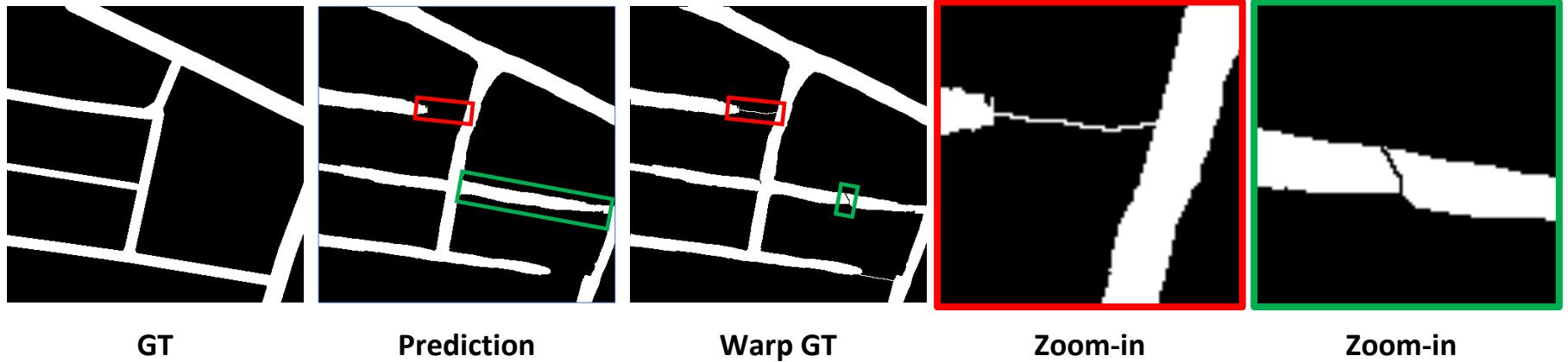
- Warping red mask towards the white



- Warping white mask towards the red



Warping example

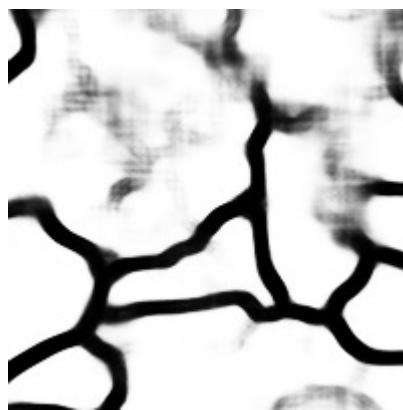


Question: Pixel VS structure representations?

- Models make pixel level predictions



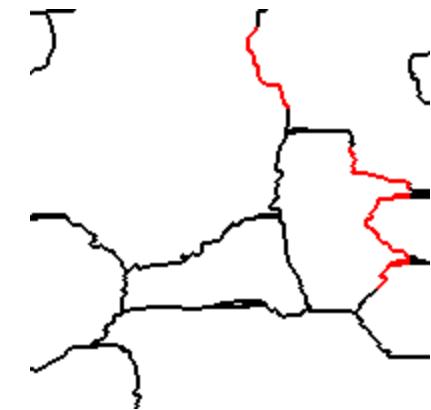
Ground Truth



Likelihood Map



Segmentation



Structure Inference

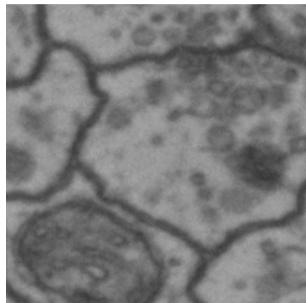
Structure-level reasoning/prediction/inference!

Outline

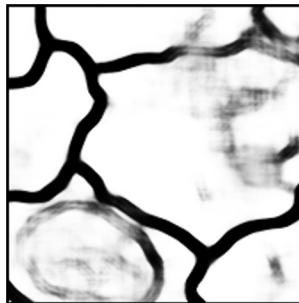
- **Topological loss for image segmentation**
 - Persistent homology based loss (NeurIPS'19, MICCAI'21)
 - Homotopy warping loss (NeurIPS'22)
- **Beyond pixel-wise representation**
 - Discrete Morse theory loss (ICLR'21, Spotlight)
 - Topological/Structural representation of images (ICLR'23, Spotlight)
- **Extensions**
 - Trojan detection with topological prior (ICLR'22)
- **Future work**

Structural loss

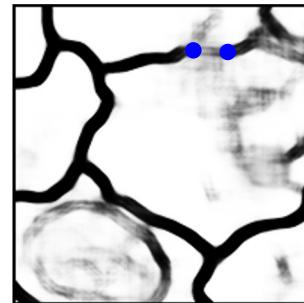
- Fix topological errors by identifying **critical pixels**
 - [Hu et al. NeurIPS'19] – Topological loss by matching persistence diagram



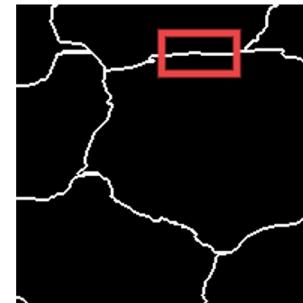
Input Image



Likelihood Map



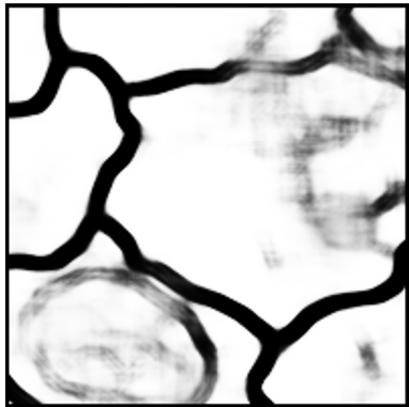
Critical Points



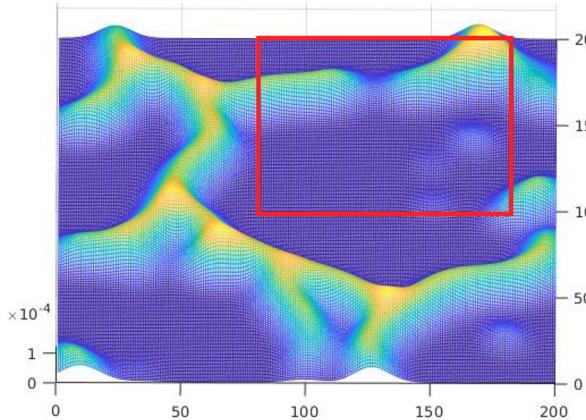
DMT Structures

Not efficient enough!

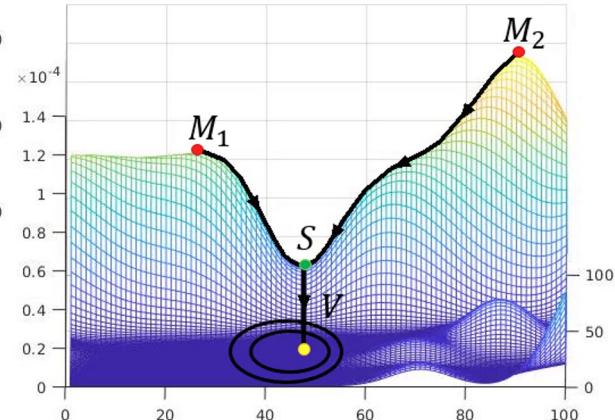
Discrete Morse theory



Likelihood Map



Density Map

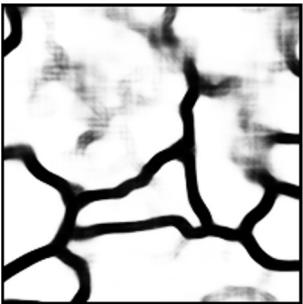


Density Map for highlighted region

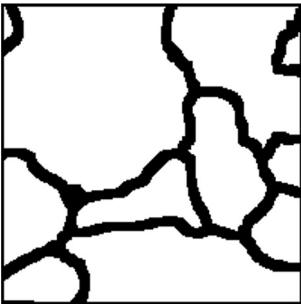
Gradient: $\nabla f(x) = \left[\frac{\partial f}{\partial x_1}, \frac{\partial f}{\partial x_2}, \dots, \frac{\partial f}{\partial x_d} \right]^T$

Critical Points (minimum, maximum, saddle) $\nabla f(x) = 0$

Persistence-based structure pruning



Likelihood Map



Ground Truth



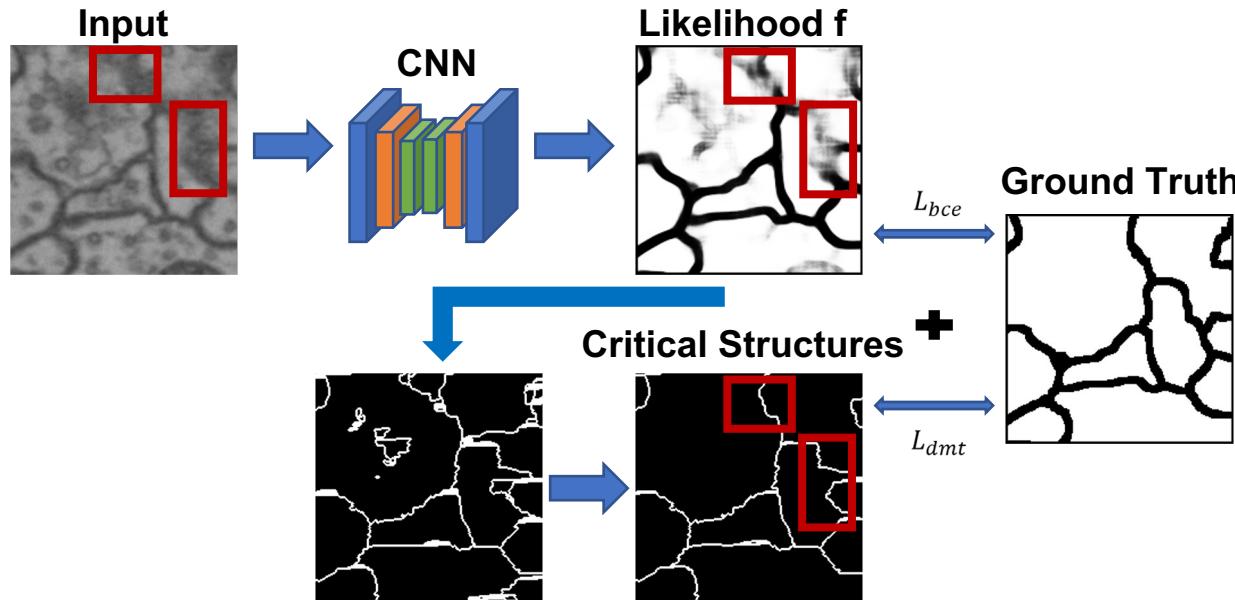
Improperly pruned
structures



Properly pruned
structures

DMT loss [ICLR'21, Spotlight]

- Loss function – train the model to be topology-aware
 - Identity the critical structures instead of critical points



New problem

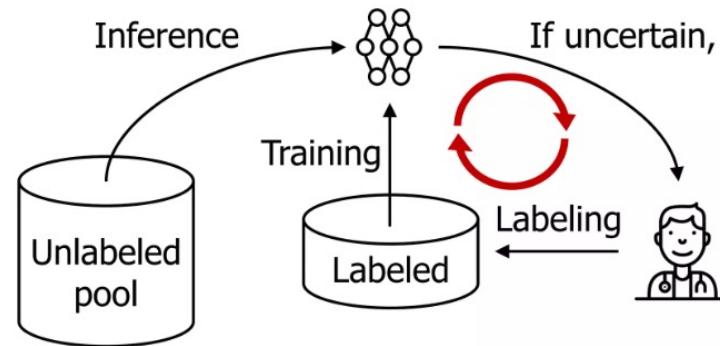
- Limited annotated samples

- Annotations are expensive
- Annotations can be noisy

- Solution

- Active learning

Active Learning

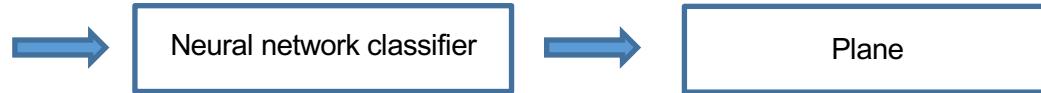


Yoo et al. CVPR'19.

The key of active learning is how to measure the uncertainty.

Uncertainty estimation

- What is uncertainty estimation?
 - How models are confident of their predictions



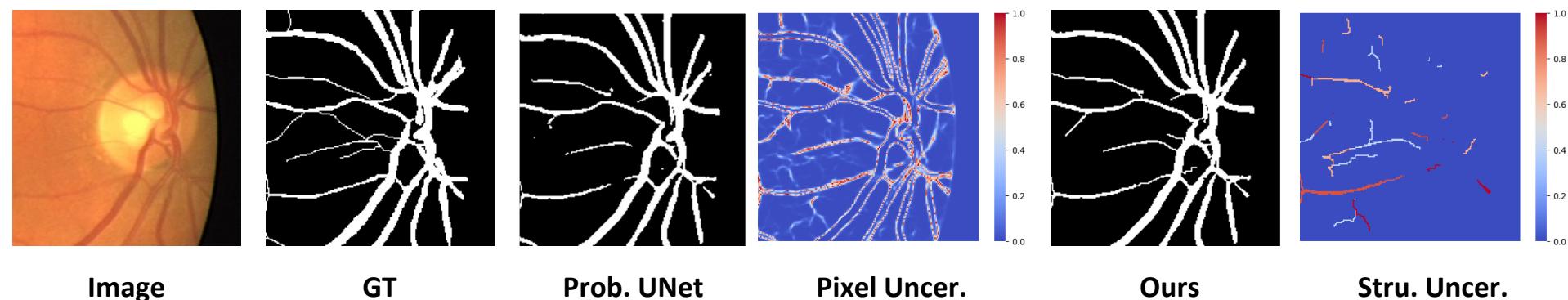
Question: How certain is classifier of this prediction? Can we quantify it?

- Importance of uncertainty?

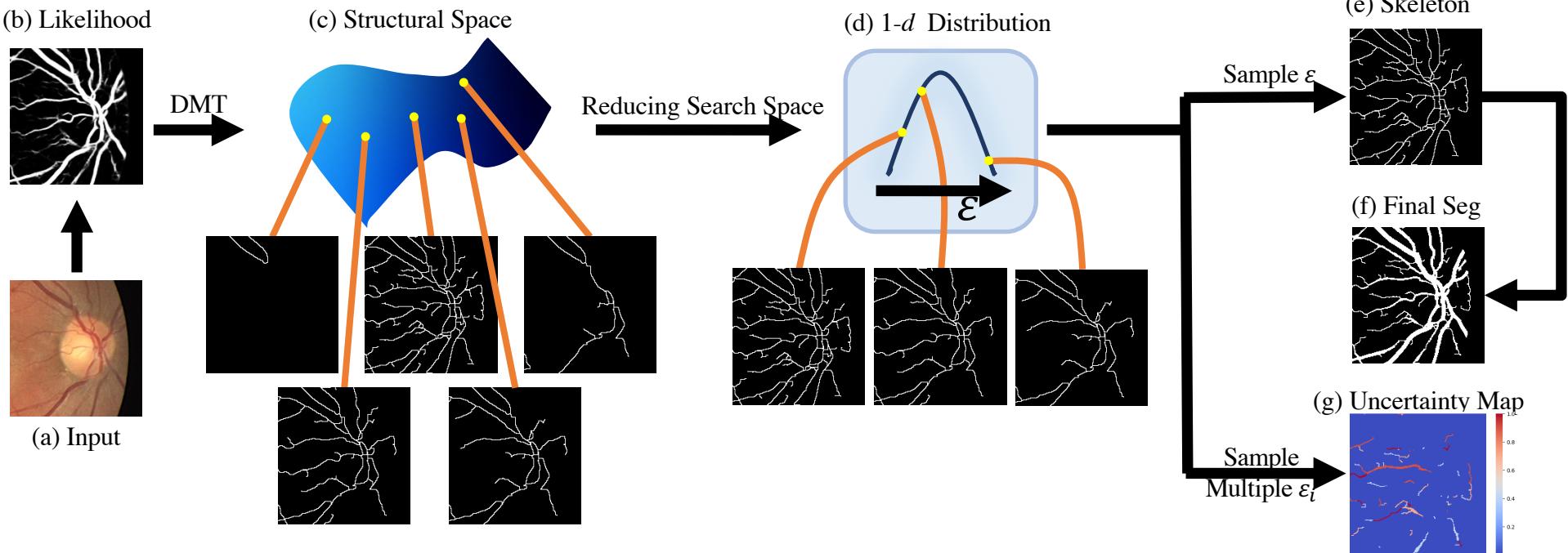
- Interpretability
- Active learning

Probabilistic structural representation [ICLR'23, Spotlight]

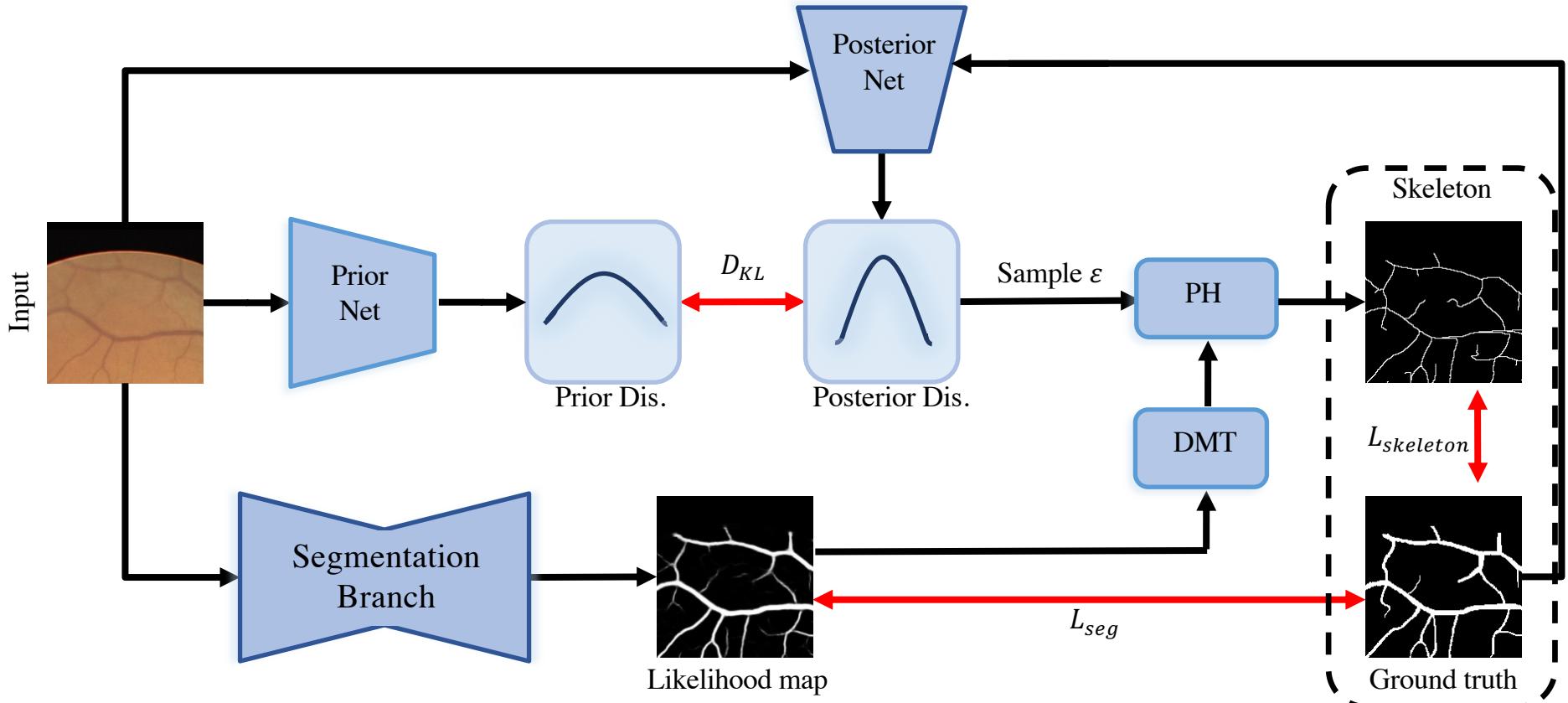
- Structure-level uncertainty estimation
 - Focus on structure instead of pixel level
 - Easy to correct



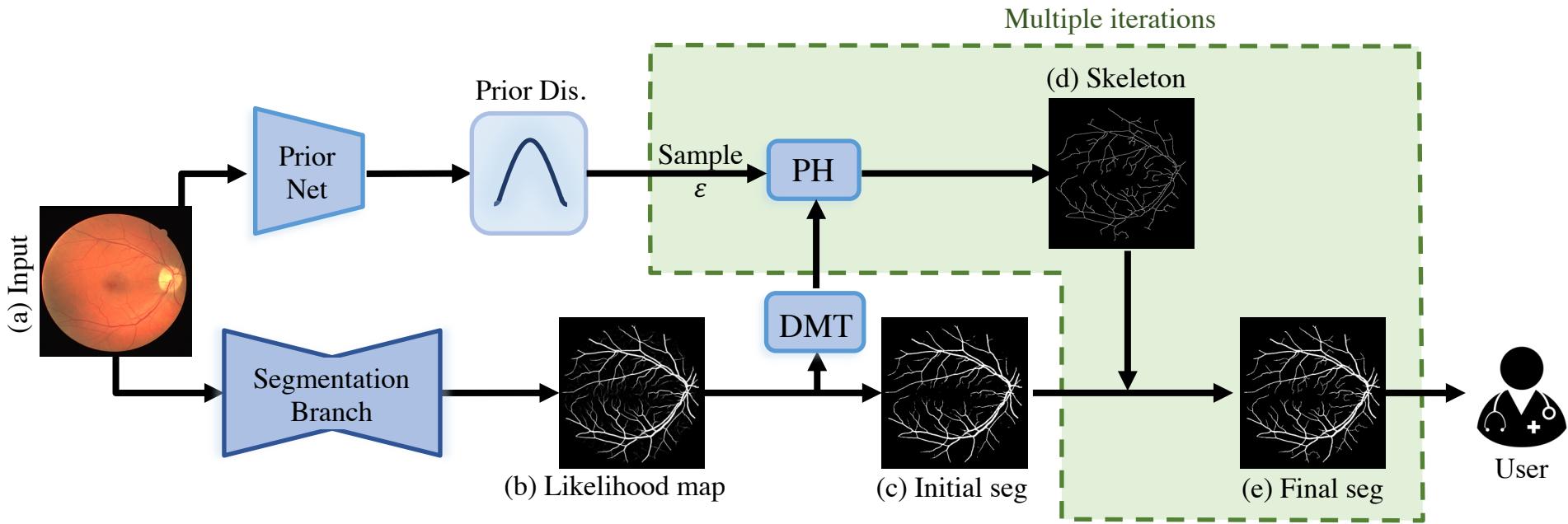
Overview



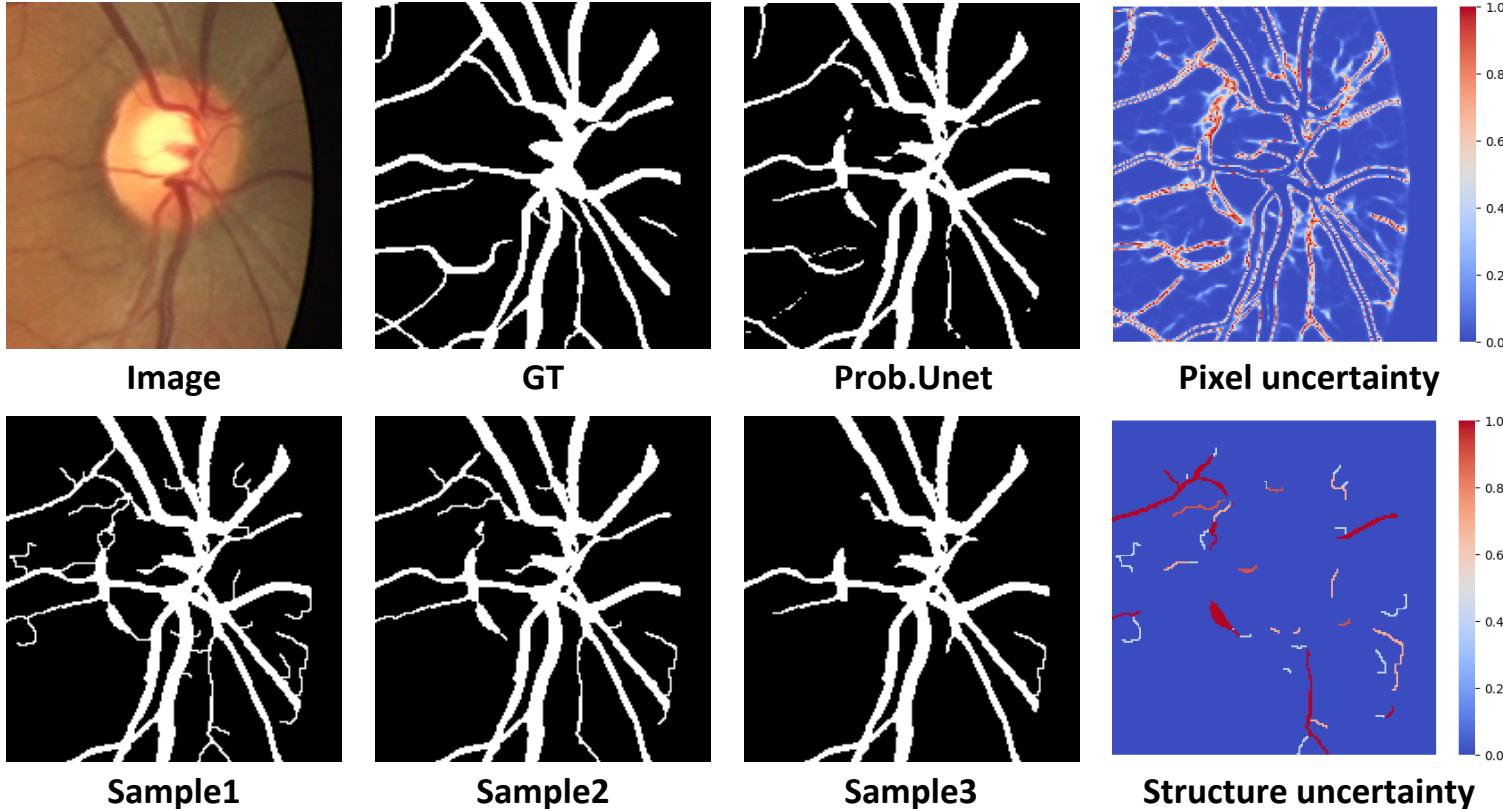
Probabilistic model



Inference and efficient annotation pipeline



Uncertainty illustration



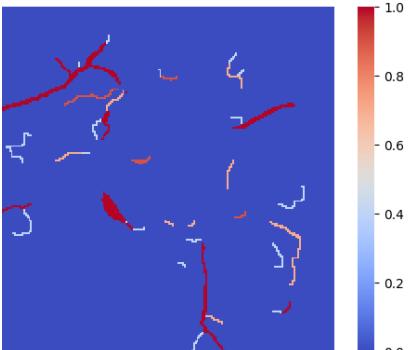
Semi-automatic efficient annotation/proofreading



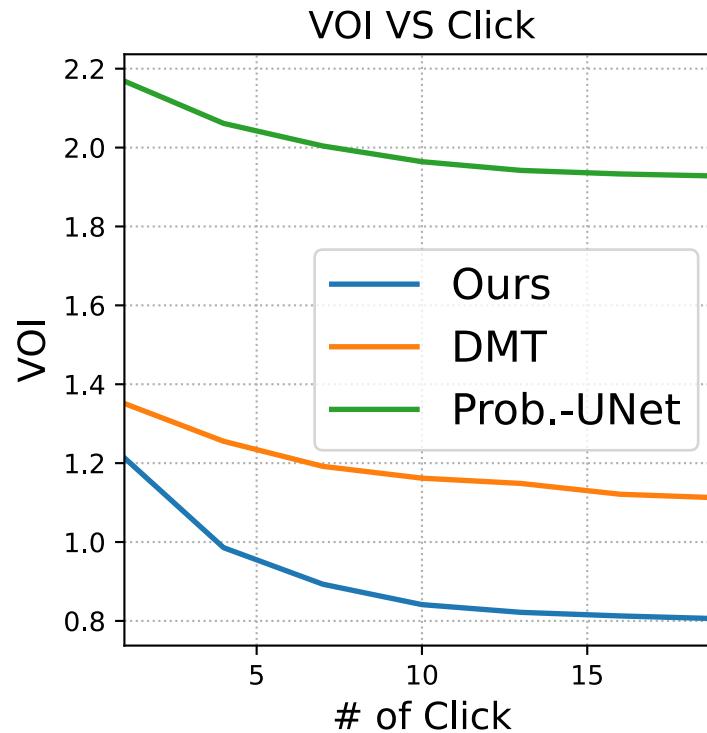
Image



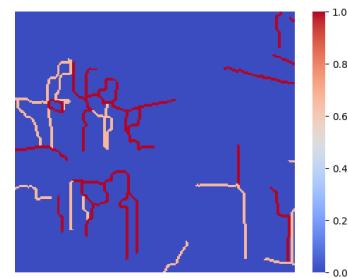
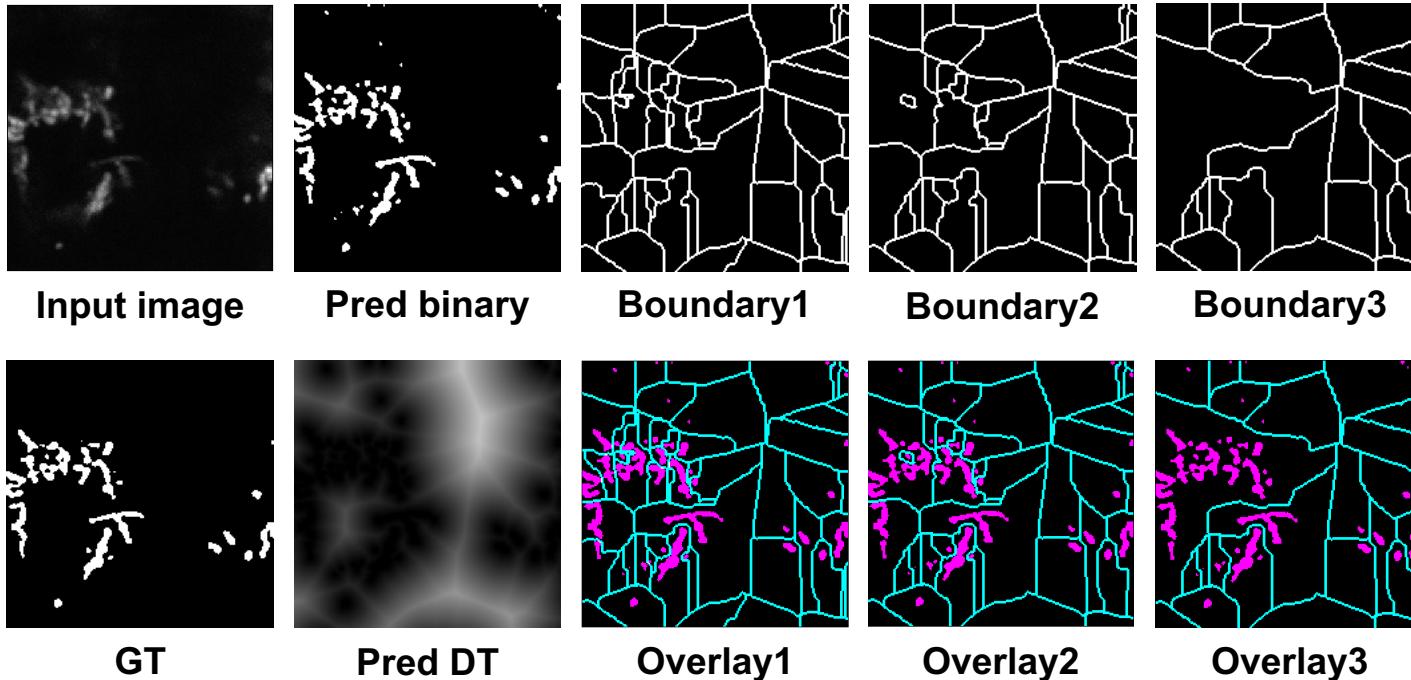
Segmentation



Structure uncertainty



Application on mitochondria segmentation



Uncertainty map

Outline

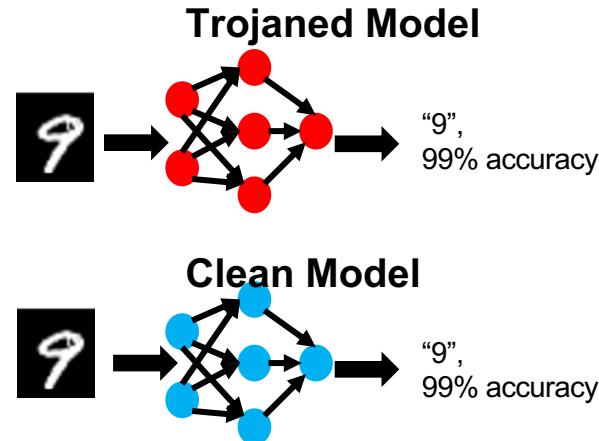
- **Topological loss for image segmentation**
 - Persistent homology based loss (NeurIPS'19, MICCAI'21)
 - Homotopy warping loss (NeurIPS'22)
- **Beyond pixel-wise representation**
 - Discrete Morse theory loss (ICLR'21, Spotlight)
 - Topological/Structural representation of images (ICLR'23, Spotlight)
- **Extensions**
 - Trojan detection with topological prior (ICLR'22)
- **Future work**

Trojan detection (ICLR'22)

- Goal: Find a classifier to distinguish clean models and Trojaned models
- Challenges
 - Limited-data setting: only a few clean samples per class; Clean and Trojaned models perform the same on them
 - If Trojaned, trigger (location, shape, color) is unknown



(a) Trojaned examples



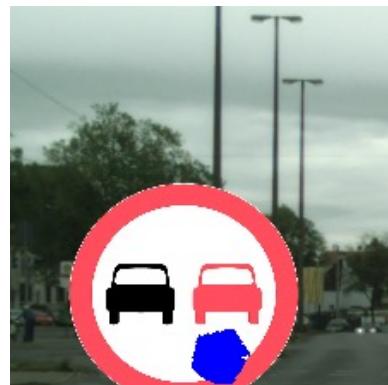
(b) Perform the same on clean images

Trigger reconstruction

- Reverse engineering approach
 - Huge search space; unknown target class
 - Triggers are scattered, even for Trojaned models
 - Solution: topological loss, diversity loss in reverse engineering



Clean sample

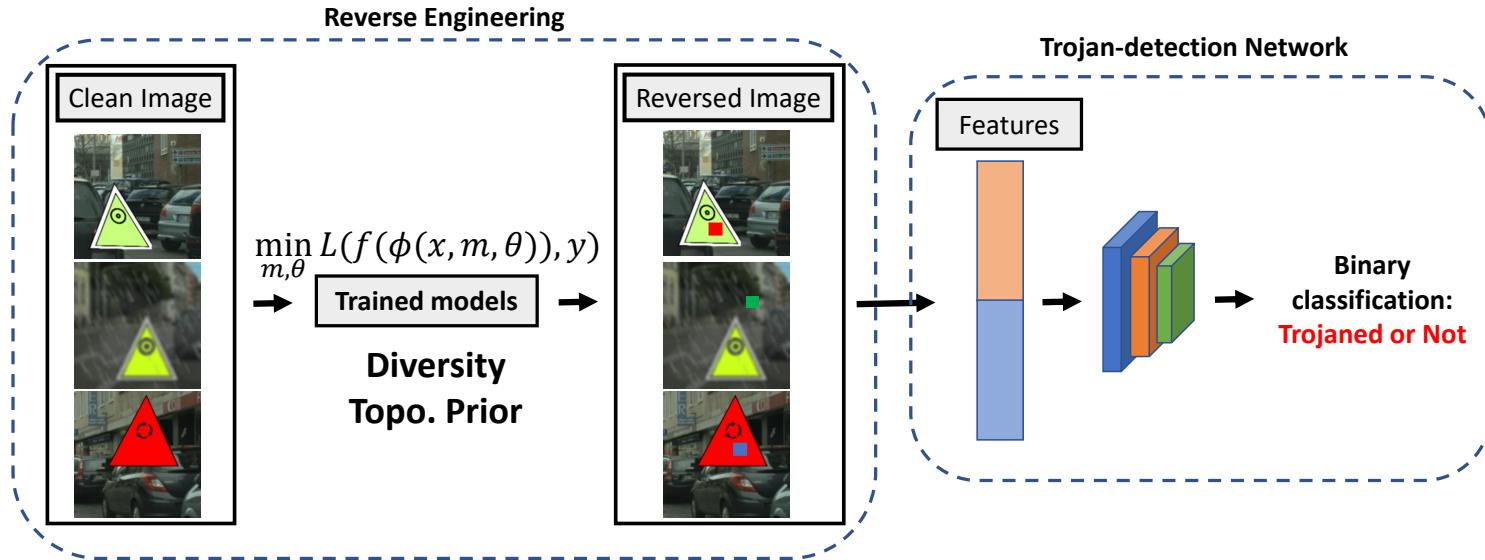


True trigger



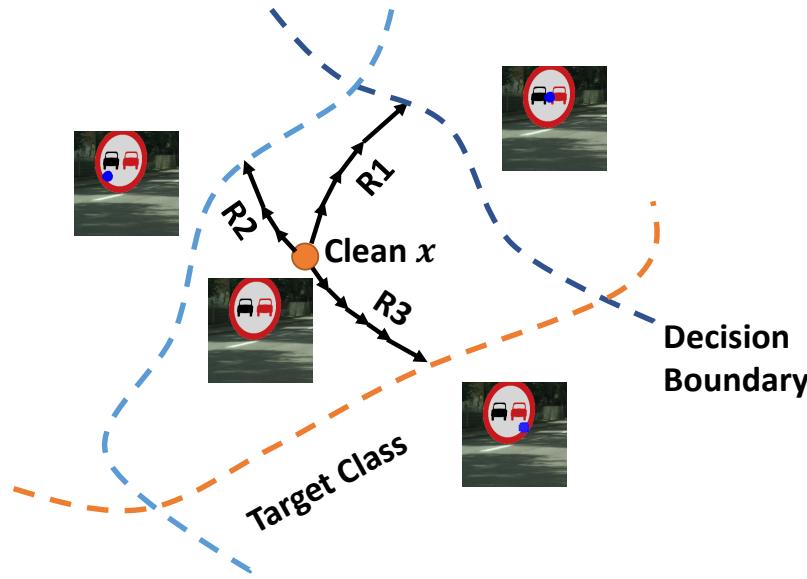
Reconstructed

Reverse-engineering pipeline



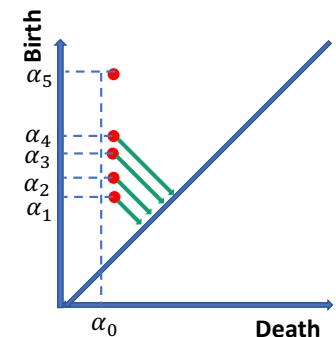
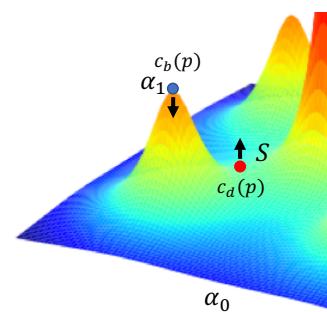
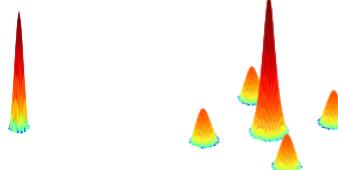
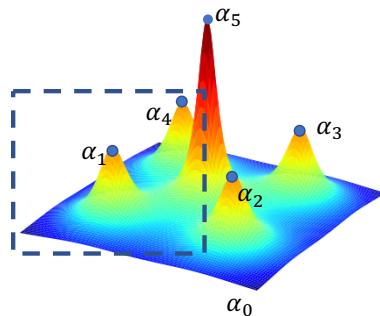
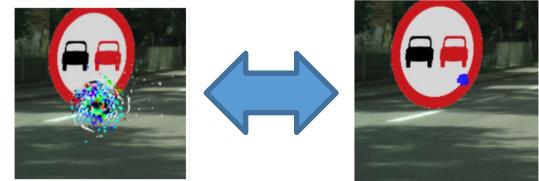
Diversity loss

- Trigger candidates different from each other



Topological loss

- Topological constraint: the trigger is a single component
 - Localized trigger
 - No strong assumption on shape/size
 - Can be written as a **topological loss**



Final loss

- **Total loss**

$$L(\mathbf{m}, \boldsymbol{\theta}; \mathbf{x}, f, c^*) = L_{flip}(\dots) + \lambda_1 L_{div}(\dots) + \lambda_2 L_{topo}(\dots) + R(\mathbf{m})$$

- **Flip loss**

$$L_{flip}(\mathbf{m}, \boldsymbol{\theta}; \mathbf{x}, f, c^*) = f_{c^*}(\phi(\mathbf{x}, \mathbf{m}, \boldsymbol{\theta}))$$

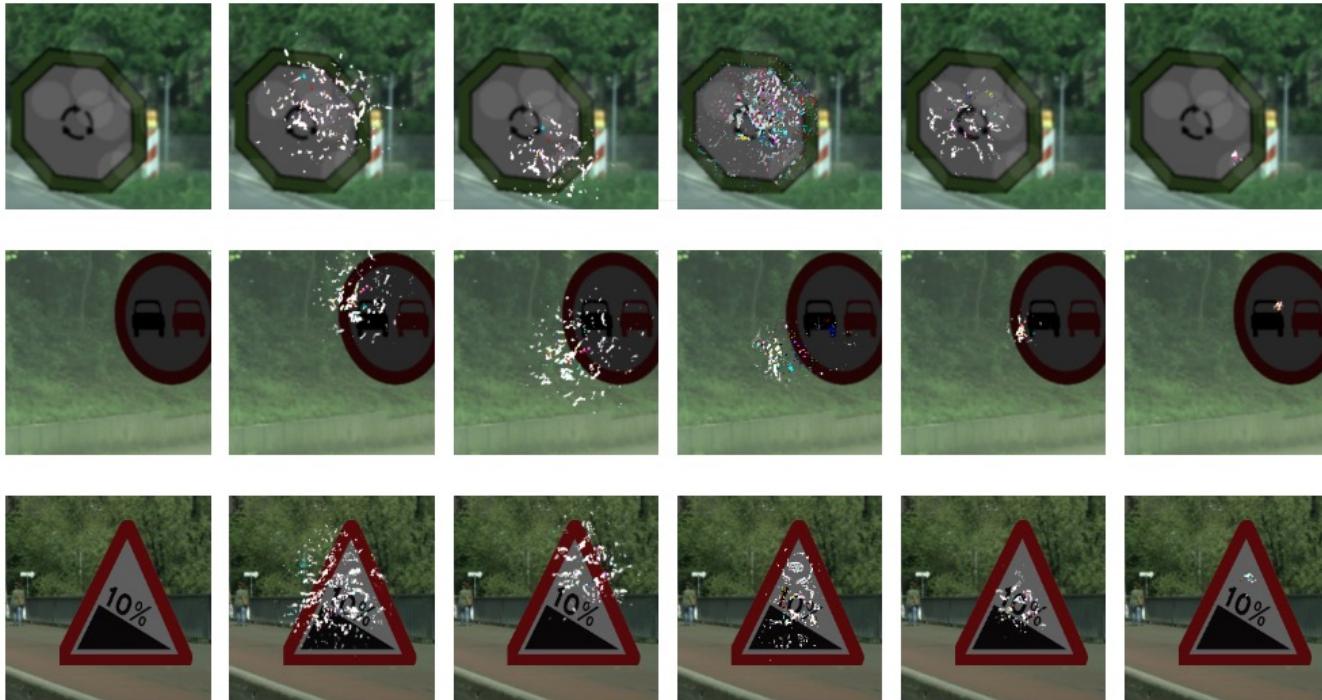
- **Diversity loss**

$$L_{div}(\mathbf{m}, \boldsymbol{\theta}) = - \sum_{j=1}^{i-1} \|\mathbf{m} \odot \boldsymbol{\theta} - \mathbf{m}_j \odot \boldsymbol{\theta}_j\|_2$$

- **Topological loss**

$$L_{topo}(\mathbf{m}) = \sum_{p \in \text{Dgm}(m) \setminus \{p^*\}} [\text{birth}(p) - \text{death}(p)]^2$$

Qualitative results



Clean Image

NC
(SP'19)

ABS
(CCS'19)

TABOR
(ICDM'19)

w/o topo.

w/ topo.

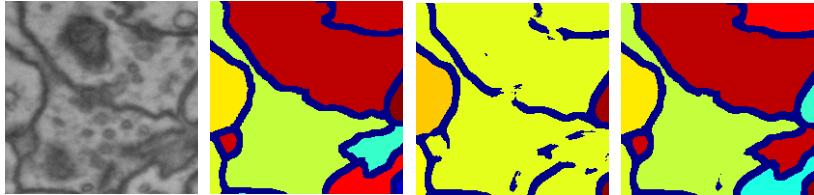
Quantitative results

- Performances comparison on the TrojAI datasets

Method	Metric	TrojAI-Round1	TrojAI-Round2	TrojAI-Round3	TrojAI-Round4
NC	AUC	0.50 ± 0.03	0.63 ± 0.04	0.61 ± 0.06	0.58 ± 0.05
ABS	AUC	0.68 ± 0.05	0.61 ± 0.06	0.57 ± 0.04	0.53 ± 0.06
TABOR	AUC	0.71 ± 0.04	0.66 ± 0.07	0.50 ± 0.07	0.52 ± 0.04
ULP	AUC	0.55 ± 0.06	0.48 ± 0.02	0.53 ± 0.06	0.54 ± 0.02
DLTND	AUC	0.61 ± 0.07	0.58 ± 0.04	0.62 ± 0.07	0.56 ± 0.05
Ours	AUC	0.90 ± 0.02	0.87 ± 0.05	0.89 ± 0.04	0.92 ± 0.06
NC	ACC	0.53 ± 0.04	0.49 ± 0.02	0.59 ± 0.07	0.60 ± 0.04
ABS	ACC	0.70 ± 0.04	0.59 ± 0.05	0.56 ± 0.03	0.51 ± 0.05
TABOR	ACC	0.70 ± 0.03	0.68 ± 0.08	0.51 ± 0.05	0.55 ± 0.06
ULP	ACC	0.58 ± 0.07	0.51 ± 0.03	0.56 ± 0.04	0.57 ± 0.04
DLTND	ACC	0.59 ± 0.04	0.61 ± 0.05	0.65 ± 0.04	0.59 ± 0.06
Ours	ACC	0.91 ± 0.03	0.89 ± 0.04	0.90 ± 0.03	0.91 ± 0.04

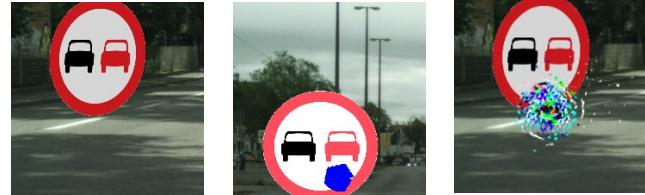
Research summary

Topology-aware deep image segmentation



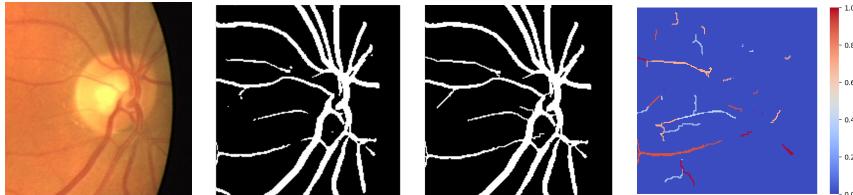
Hu et al. *NeurIPS'19, MICCAI'21, ISBI'21, ICLR'21, NeurIPS'22, ECCV'22.*

Trojan detection



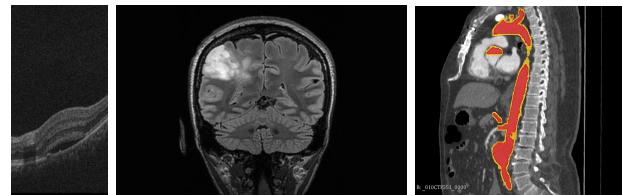
Hu et al. *ICLR'22.*

Uncertainty estimation



Hu et al. *ICLR'23, Li et al. ICLR'23.*

Biomedical applications



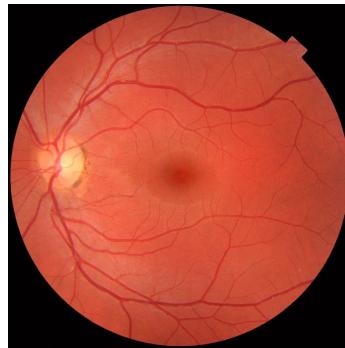
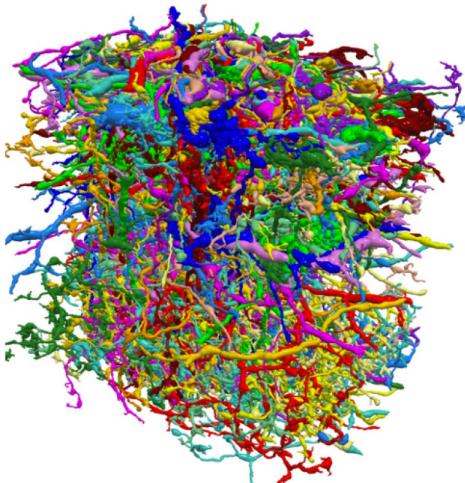
Yang et al. *under review, Konwer et al. under review.*

Data with rich structural information

- Challenges

- Complex topology/structure
- Noisy data
- Limited labels

Difficult to analyze!



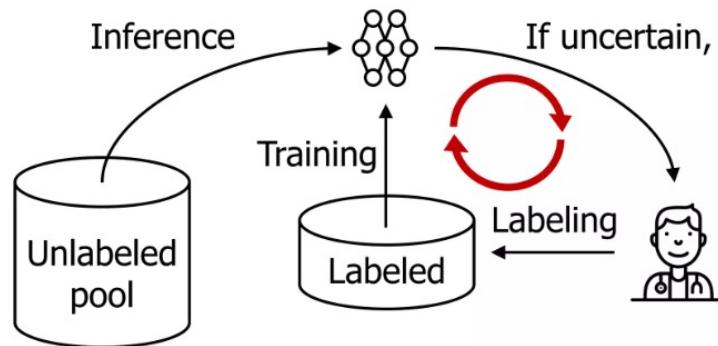
Career goal

- **Develop principled methods**
 - Model the intrinsic structures of data
 - Use topological/structural priors
- **Different types of scenarios/data**
 - Imperfect data: Medical imaging, general data science
 - Different types of data: Point cloud, Graph
 -

Direction 1: Imperfect data

- Annotations are difficult to obtain
 - Leverage information from unlabeled data
 - Crowd counting, cell detection ...

Active Learning

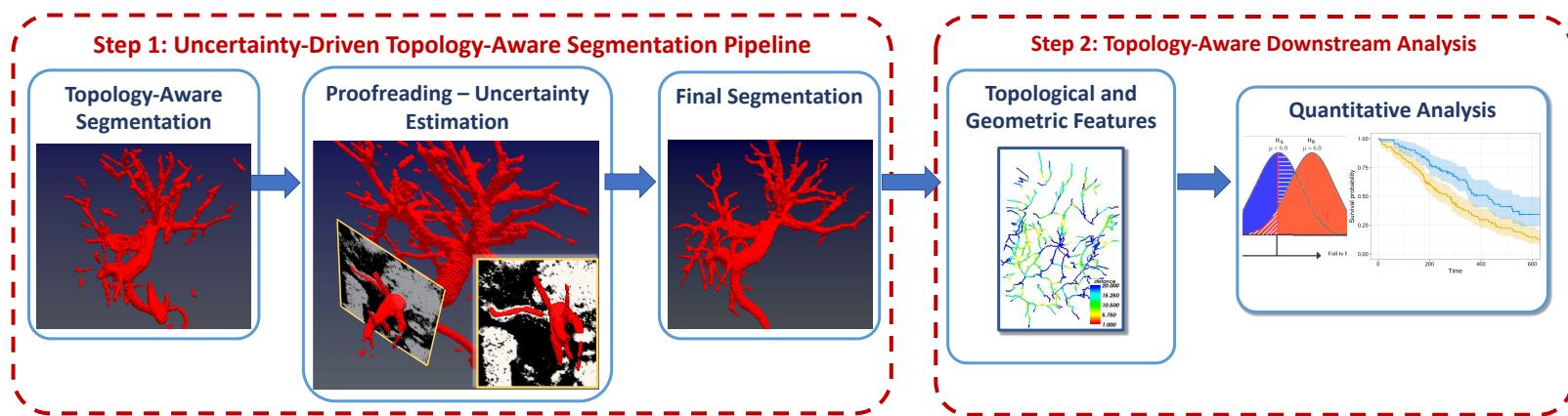


Yoo et al. CVPR'19.

*Explore the structures
within unlabeled data!*

Direction 2: Deep learning based quantification analysis

- Combine topology-aware segmentation and uncertainty estimation
 - Interactive annotation/proofreading
 - Downstream topology-aware analysis
 - Neurons, vasculatures, digital pathology images, etc.

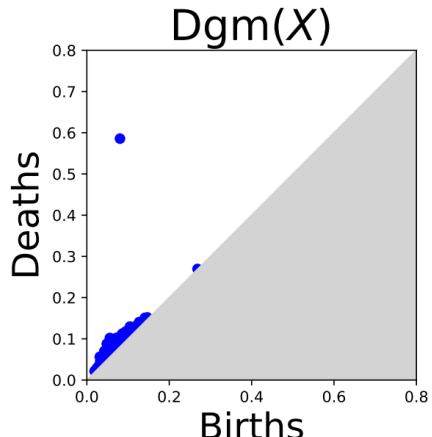
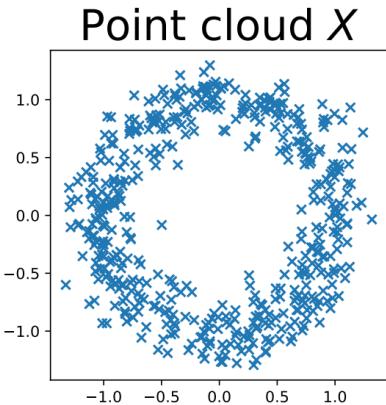


Direction 3: Other types of data

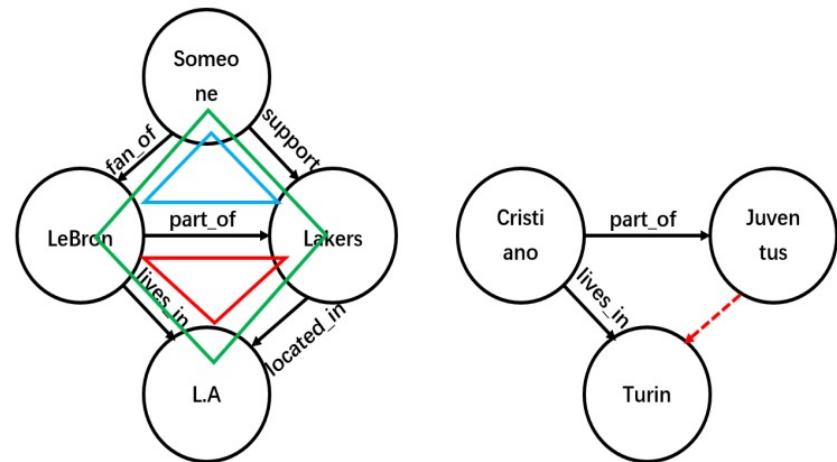
- Topology on different types of data

*Extending topology non-trivially
to other types of data!*

Point Cloud



Graph



de Surrel, Thibault, et al. "RipsNet: a general architecture for fast and robust estimation of the persistent homology of point clouds." **TAGL Workshops** (2022).

Yan, Zuoyu, et al. "Cycle Representation Learning for Inductive Relation Prediction." **ICML** (2022).

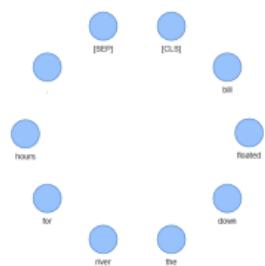
Direction 4: Topo attention in NLP/LLM

• Topology of attention connectivity

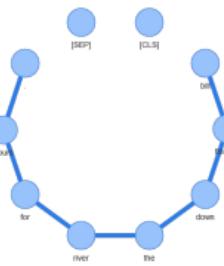
- Prune number of heads
- Robust against adversarial attacks

Using TDA to analyze the structures of neural networks!

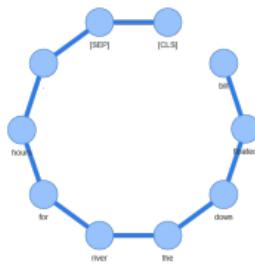
$t = 0.0$



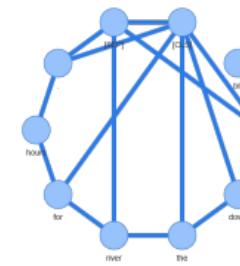
$t = 0.005$



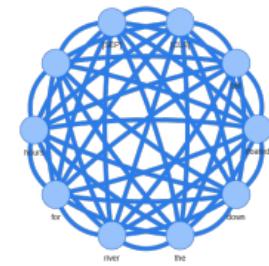
$t = 0.1$



$t = 0.9999$



$t = 1.0$



Reference

- **Hu, Xiaoling**, et al. "Topology-preserving deep image segmentation." *NeurIPS* (2019).
- **Hu, Xiaoling**, et al. "Topology-aware segmentation using discrete Morse theory." *ICLR* (2021, **Spotlight**).
- Yang, Jiaqi*, **Hu, Xiaoling***, et al. "3D topology-preserving segmentation with compound multi-slice representation." *ISBI* (2021).
- Yang, Jiaqi*, **Hu, Xiaoling***, et al. "A topological-attention convlstm network and its application to em images." *MICCAI* (2021).
- **Hu, Xiaoling**, et al. "Trigger hunting with a topological prior for trojan detection." *ICLR* (2022).
- Gupta, Saumya*, **Hu, Xiaoling***, et al. "Learning topological interactions for multi-class medical image segmentation." *ECCV* (2022, **Oral**).
- **Hu, Xiaoling**. "Topology-aware image segmentation with homotopy warping." *NeurIPS* (2022).
- **Hu, Xiaoling**, et al. "Deep statistic shape model for myocardium segmentation." *arXiv preprint arXiv:2207.10607* (2022).
- **Hu, Xiaoling**, et al. "Learning probabilistic topological representation using discrete Morse theory." *ICLR* (2023, **Spotlight**).
- Li, Chen, **Hu, Xiaoling**, et al. "Confidence estimation using unlabeled data." *ICLR* (2023).
- Yang, Jiaqi, **Hu, Xiaoling**, et al. "Weakly supervised learning for lesion segmentation on oct images with anomaly attention mechanism." *under review*.
- Konwer, Aishik, **Hu, Xiaoling**, et al. "Enhancing modality-agnostic representations via meta-learning for brain tumor segmentation." *under review*.

Acknowledgment

Credits are due to the committee members,
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Thank you for your attention!

Q&A

