CSC413/2516 Lecture 11:

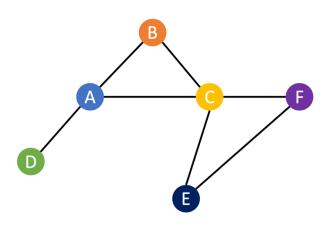
Additional architectures: GNNs, UNet, MedSAM

Bo Wang

The missing piece

- Tabular data: Linear Models, MLP
- Sequence data (e.g., Language, speech): CNN, RNN, Transformer
- Imaging data: CNN, Vision Transformer
- What about graph data?

What is a graph?

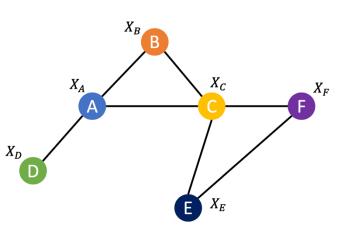


A graph is composed of

- Nodes (also called vertices)
- Edges connecting a pair of nodes presented in an adjacency matrix

A		1	1	1						
B	1		1							
C	1	1			1	1				
D	1									
Ø			1			1				
Ğ			1		1					

What is a graph?



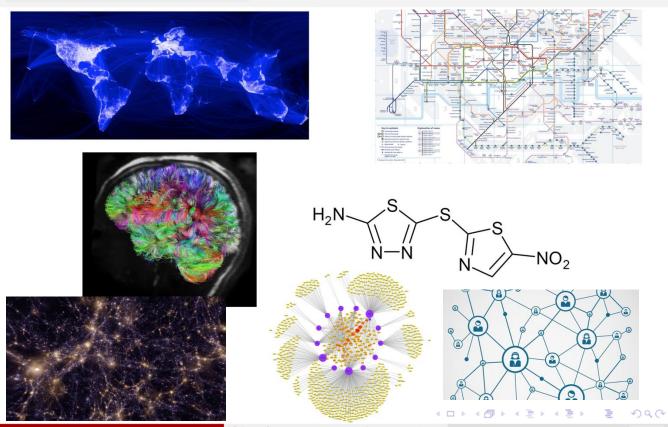
A graph is composed of

- Nodes (also called vertices)
- Edges connecting a pair of nodes presented in an adjacency matrix

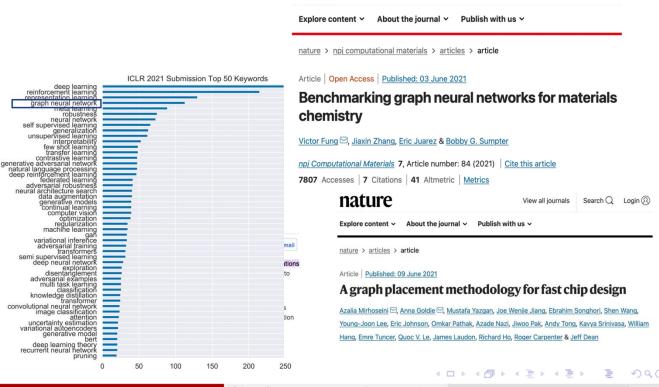
Nodes can have feature vectors

A	X_A
B	X_B
C	X_C
D	X_D
Ø	X_E
	X_F

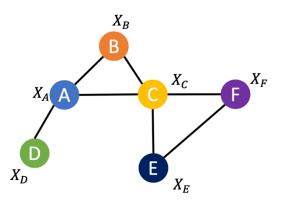
Graph is everywhere!



Graph Neural Networks (GNN) is everywhere



npi | computational materials



Given

- A graph
- Node attributes
- (part of nodes are labeled)

Find

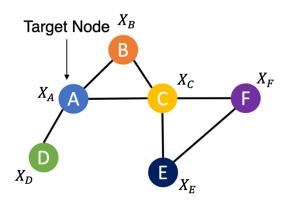
Node embeddings

Predict

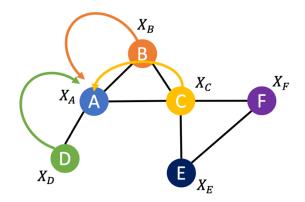
Labels for the remaining nodes

undirected unweighted graph

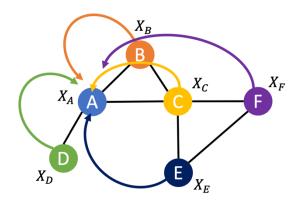




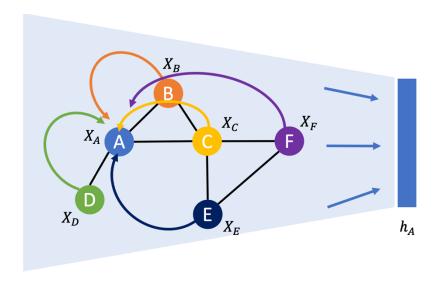
"Homophily: connected nodes are related/informative/similar"

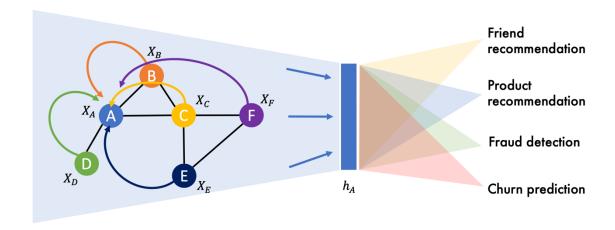


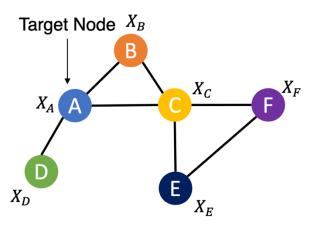
"Homophily: connected nodes are related/informative/similar"

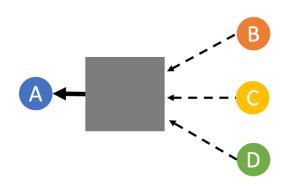


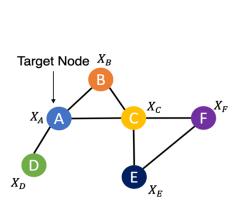
"Homophily: connected nodes are related/informative/similar"

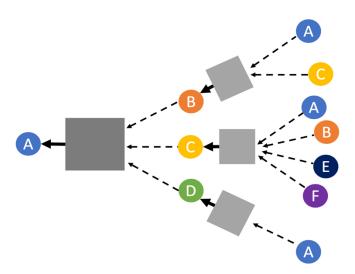










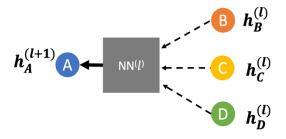


1. Aggregate messages from neighbors

 $h_v^{(l)}$: node embedding of v at l-th layer $\mathcal{N}(v)$: neighboring nodes of v $f^{(l)}$: aggregation function at l-th layer $m_v^{(l)}$: message vector of v at l-th layer

$$m_A^{(l)} = f^{(l)} \left(h_A^{(l)}, \left\{ h_u^{(l)} : u \in \mathcal{N}(A) \right\} \right)$$

= $f^{(l)} \left(h_A^{(l)}, h_B^{(l)} h_C^{(l)} h_D^{(l)} \right)$



Neighbors of node A
$$\mathcal{N}(A) = \{B, C, D\}$$

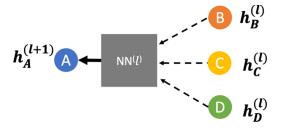
1. Aggregate messages from neighbors

$$m_A^{(l)} = f^{(l)} \left(h_A^{(l)}, \left\{ h_u^{(l)} : u \in \mathcal{N}(A) \right\} \right)$$

= $f^{(l)} \left(h_A^{(l)}, h_B^{(l)} h_C^{(l)} h_D^{(l)} \right)$

2. Transform messages

 $m{g}^{(l)}$: transformation function at l-th layer $h_A^{(l+1)} = m{g}^{(l)}(m_A^{(l)})$



Neighbors of node A $\mathcal{N}(A) = \{B, C, D\}$

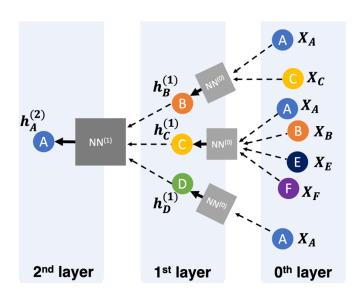
In each layer l , for each target node v :

1. Aggregate messages

$$m_v^{(l)} = \boldsymbol{f}^{(l)}\left(h_v^{(l)}, \left\{h_u^{(l)}: u \in \mathcal{N}(v)\right\}\right)$$

2. Transform messages

$$h_v^{(l+1)} = \boldsymbol{g}^{(l)}(m_v^{(l)})$$



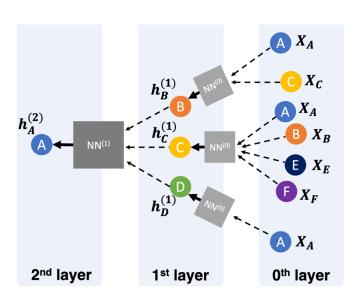
Graph Convolutional Networks^[1]

1. Aggregate messages

$$m_v^{(l)} = \frac{1}{|\mathcal{N}(v) + 1|} \sum_{u \in \mathcal{N}(v) \cup \{v\}} h_u^{(l)}$$

2. Transform messages

$$h_v^{(l+1)} = \sigma(\pmb{W}^{(l)} \circ m_v^{(l)})$$



Graph Isomorphism Networks^[2]

1. Aggregate messages

$$m_v^{(l)} = \sum_{u \in \mathcal{N}(v) \cup \{v\}} h_u^{(l)}$$

2. Transform messages

$$h_v^{(l+1)} = \sigma(\boldsymbol{W}^{(l)} \circ m_v^{(l)})$$

NN⁽¹⁾ 2nd layer 1st layer 0th layer

[2] Xu, Keyulu, et al. "How powerful are graph neural networks?."

Simplified GCN^[3]

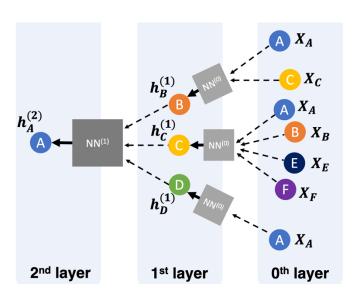
1. Aggregate messages

$$m_v^{(l)} = \frac{1}{|\mathcal{N}(v) + 1|} \sum_{u \in \mathcal{N}(v) \cup \{v\}} h_u^{(l)}$$

2. Transform messages

$$h_v^{(l+1)} = \boldsymbol{W}^{(l)} \circ m_v^{(l)}$$

[3] Wu, Felix, et al. "Simplifying graph convolutional networks."



In each layer l:

Aggregate over neighbors

$$m_v^{(l-1)} = f^{(l)}\left(h_v^{(l-1)}, \left\{h_u^{(l-1)}: u \in \mathcal{N}(v)\right\}\right)$$

Core part of GNNs

Transform messages

$$h_v^{(l)} = \boldsymbol{g}^{(l)}(m_v^{(l-1)})$$

1-layer MLP is commonly used

- GCN^[1]
 - Average embeddings of neighboring nodes

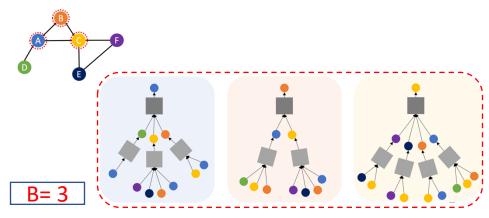
$$m_{v}^{(l)} = \frac{1}{|\mathcal{N}(v) + 1|} \sum_{u \in \mathcal{N}(v) \cup \{v\}} h_{u}^{(l)} + h_{v}^{(l+1)} = \sigma(\mathbf{W}^{(l)} \circ m_{v}^{(l)})$$

$$h_{v}^{(l)} = \sigma(\mathbf{W}^{(l)} \circ (\frac{1}{|\mathcal{N}(v) + 1|} \sum_{u \in \mathcal{N}(v) \cup \{v\}} h_{u}^{(l-1)}))$$

• GCN^[1]

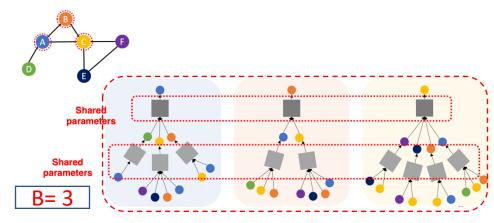
Can we use batch-mode?

$$h_v^{(l)} = \sigma(\boldsymbol{W}^{(l)} \circ (\frac{1}{|\mathcal{N}(v)+1|} \sum_{u \in \mathcal{N}(v) \cup \{v\}} h_u^{(l-1)}))$$



• GCN^[1]

$$h_v^{(l)} = \sigma(\boldsymbol{W}^{(l)} \circ (\frac{1}{|\mathcal{N}(v)+1|} \sum_{u \in \mathcal{N}(v) \cup \{v\}} h_u^{(l-1)}))$$



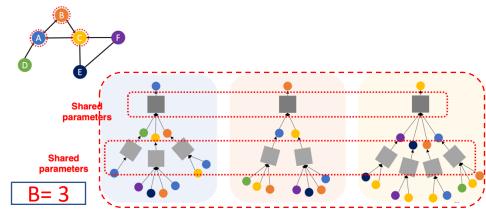
• GCN^[1]

$$h_{v}^{(l)} = \sigma(\mathbf{W}^{(l)} \circ (\frac{1}{|\mathcal{N}(v)+1|} \sum_{u \in \mathcal{N}(v) \cup \{v\}} h_{u}^{(l-1)}))$$

$$\mathbf{H}^{(l)} = \sigma((\mathbf{A} + \mathbf{I}) \mathbf{H}^{(l-1)} \mathbf{W}^{(l)})$$

Node embedding matrix

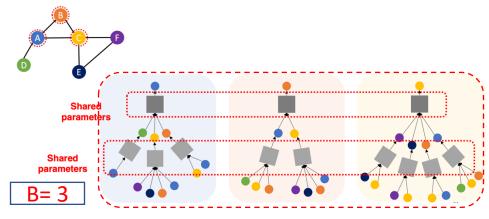
(row-normalized) Adjacency matrix

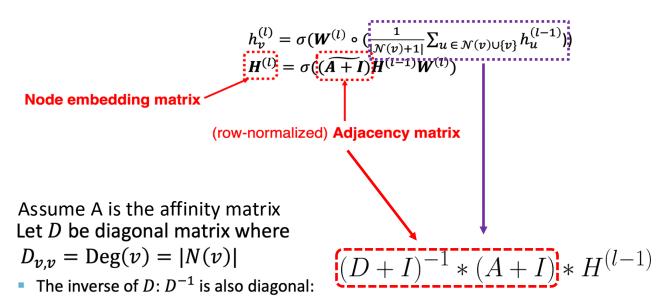


• GCN^[1]

$$h_v^{(l)} = \sigma(\boldsymbol{W}^{(l)} \circ (\frac{1}{|\mathcal{N}(v)+1|} \sum_{u \in \mathcal{N}(v) \cup \{v\}} h_u^{(l-1)}))$$

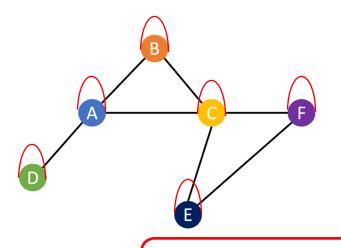
$$\boldsymbol{H}^{(l)} = \sigma((\boldsymbol{A}+\boldsymbol{I})\boldsymbol{H}^{(l-1)}\boldsymbol{W}^{(l)})$$
Fixed Trainable





 $D_{v,v}^{-1} = 1/|N(v)|$

$$\widetilde{A+I} = (D+I)^{-1} * (A+I) \longrightarrow \widetilde{A} = D^{-1} * A$$



A graph is composed of

- **Nodes** (also called vertices)
- Edges connecting a pair of nodes presented in an adjacency matrix

	⋖)	m)	U		Ш	U
A	1	1	1	1		
B	1	1	1			
C	1	1	1		1	1
D	1			1		
(3)			1		1	1
B			1		1	1

Graph Convolutional Network (GCN) -- Summary

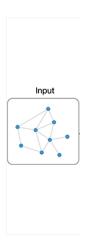
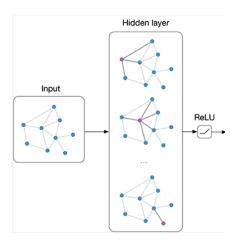


Image Credit: Defferrard et al. NIPS 2016

Graph Convolutional Network (GCN) -- Summary

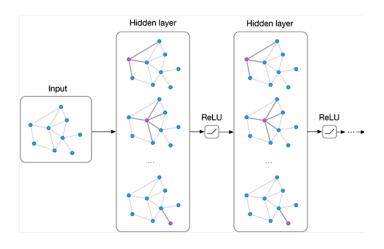


$$\operatorname{ReLU}\left(\hat{A}XW^{(0)}\right)$$

Image Credit: Defferrard et al. NIPS 2016



Graph Convolutional Network (GCN) -- Summary



$$\hat{A} \operatorname{ReLU}(\hat{A}XW^{(0)}) W^{(1)}$$

Image Credit: Defferrard et al. NIPS 2016



Graph Attention Network (optional)

- GAT^[14]
 - Different weights to different nodes in a neighborhood
 - · Multi-head attention

$$\alpha_{ij} = \frac{\exp\left(\text{LeakyReLU}\left(\vec{\mathbf{a}}^T[\mathbf{W}\vec{h}_i\|\mathbf{W}\vec{h}_j]\right)\right)}{\sum_{k \in \mathcal{N}_i} \exp\left(\text{LeakyReLU}\left(\vec{\mathbf{a}}^T[\mathbf{W}\vec{h}_i\|\mathbf{W}\vec{h}_k]\right)\right)}$$

 \vec{h}_{1} \vec{d}_{11} \vec{d}_{13} \vec{d}_{13} \vec{d}_{13} \vec{d}_{13} \vec{d}_{14} \vec{d}_{15} \vec{d}_{16} \vec{d}_{16} \vec{d}_{16}

[14] Petar Veličković., et al. "GRAPH ATTENTION NETWORKS."

How to Train GNN?

- Semi-supervised learning
 - Input node features are given for all nodes in a graph
 - Only a subset of nodes have labels

$$\min_{\Theta} \mathcal{L}(\boldsymbol{y}, f(\boldsymbol{z}_v))$$

 $oldsymbol{y}$: node label

 \mathcal{L} could be L2 if y is real number, or cross entropy if y is categorical

Node embedding z_v is a function of input graph

How to Train GNN?

Unsupervised setting:

- No node label available
- Use the graph structure as the supervision!
 - "Similar" nodes have similar embeddings

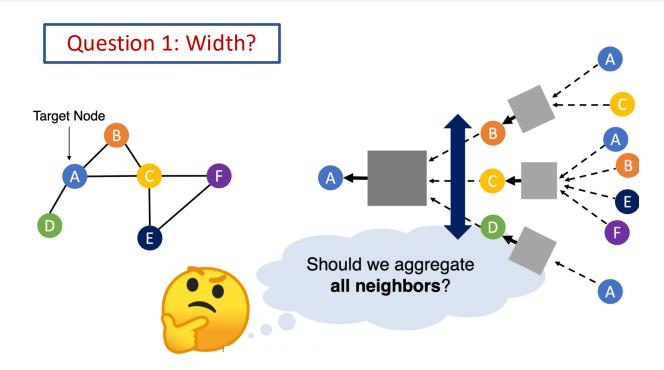
$$\mathcal{L} = \sum_{z_u, z_v} CE(y_{u,v}, DEC(z_u, z_v))$$

- Where $y_{u,v} = 1$ when node u and v are similar
- CE is the cross entropy
- DEC is the decoder such as inner product

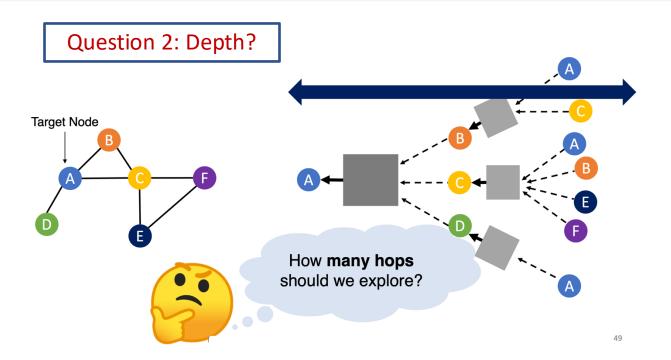
Still an active research topic!



Two interesting questions about GNN



Two interesting questions about GNN

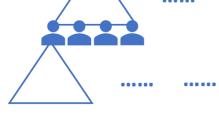


Question 1: Width?

If we aggregate all neighbors, GNNs have scalability issues

Neighbor explosion

• In L -layer GNNs, one node aggregates information from $O(K^L)$ nodes where K is the average number of neighbors per node



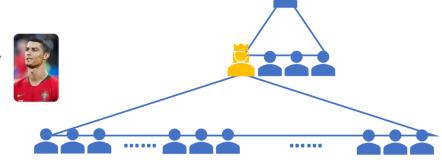
Question 1: Width?

- If we aggregate all neighbors, GNNs have scalability issues
- Neighbor explosion

Hub nodes who are connected to a huge number of nodes

Cristiano Ronaldo

Cristiano Ronaldo is currently the most-followed individual on Facebook, with over 150 million followers.



Question 1: Width?

 Limit the neighborhood expansion by sampling a fixed number of neighbors



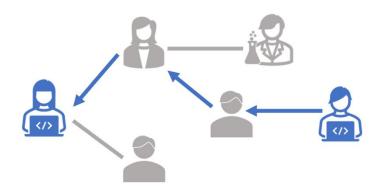
Question 1: Width?

- Random sampling
 - Assign same sampling probabilities to all neighbors
 - GraphSage^[4]
- Importance sampling
 - Assign different sampling probabilities to all neighbors
 - FastGCN^[5], LADIES^[6], AS-GCN^[7], GCN-BS^[8], PASS^[9]
- [4] Will Hamilton, et al. "Inductive representation learning on large graphs"
- [5] Jie Chen, et al. "Fastgcn: fast learning with graph convolutional networks via importance sampling"
- [6] Difan Zou, et al. "Layer-Dependent Importance Sampling for Training Deep and Large Graph Convolutional Networks"
- [7] Wenbing Huang, et al. "Adaptive sampling towards fast graph representation learning"
- [8] Ziqi Liu, et al. "Bandit Samplers for Training Graph Neural Networks"
- [9] Minji Yoon, et al. "Performance-Adaptive Sampling Strategy Towards Fast and Accurate Graph Neural Networks"



Question 2: Depth?

 Informative neighbors could be indirectly connected with a target node



Question 2: Depth?

• 2-layer or 3-layer GNNs are commonly used in real worlds

Wasn't it Deeeep Learning?

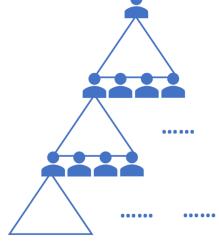


Question 2: Depth?

• When we increase the depth L more than this, GNNs face

neighbor explosion $O(K^L)$

Over-smoothing

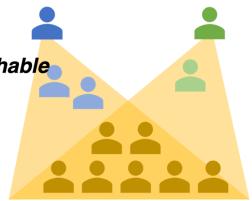


Question 2: Depth?

Over-smoothing^[10]

 When GNNs become deep, nodes share many neighbors

Node embeddings become indistinguishable

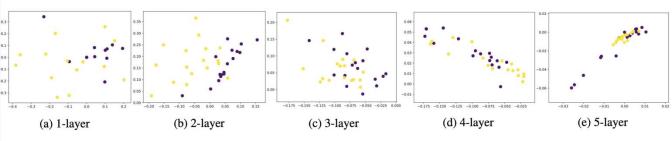


[10] Qimai Li, et al. "Deeper Insights into Graph Convolutional Networks for Semi-Supervised Learning"

Question 2: Depth?

Over-smoothing^[10]

Node embeddings of Zachary's karate club network with GNNs



[10] Qimai Li, et al. "Deeper Insights into Graph Convolutional Networks for Semi-Supervised Learning"



GNN Applications



Food Discovery with Uber Eats: Using Graph Learning to Power Recommendations





PinSage: A new graph convolutional neural network for web-scale recommender systems

Ruining He | Pinterest engineer, Pinterest Labs

Web image search gets better with graph neural networks

'n to image search uses images returned by traditional search eles in a graph neural network through which similarity signals are amazon | science nieving improved ranking in cross-modal retrieval. PUBLICATION

P-Companion: A principled framework for diversified complementary product recommendation

By Junheng Hao, Tong Zhao, Jin Li, Xin Luna Dong, Christos Faloutsos, Yizhou Sun, Wei Wang

GNN applications

- Graph-level prediction: whether the molecule is a potent **drug**^[29]
 - Execute on a large dataset of known candidate molecules
 - Select the ~ top-100 candidates from the GNN model
 - · Have chemists thoroughly investigate those

[29] Jonathan M.Stokes, et al. "A Deep Learning Approach to Antibiotic Discovery"

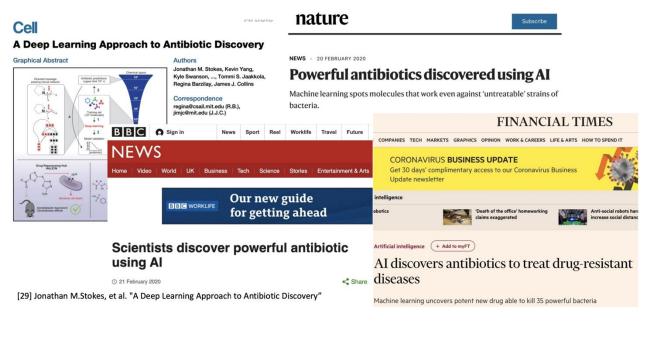


GNN applications

 Discover a previously overlooked compound that is a highly potent antibiotic^[29]

[29] Jonathan M.Stokes, et al. "A Deep Learning Approach to Antibiotic Discovery"

GNN applications

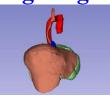


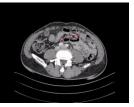
After the break

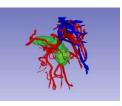
After the break: U-Net and U-mamba, MedSAM

Biomedical Image Segmentation: What and Why

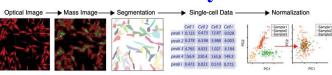




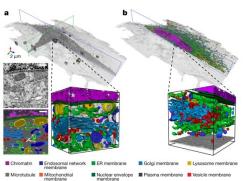




- Quantification of anatomical structures and disease progression
- ➤ Cancer microenvironment analysis



Capolupo, L et al. Science, 2022

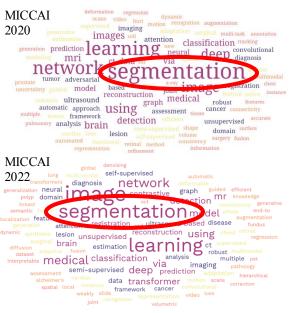


Heinrich, L. et al. Nature, 2021

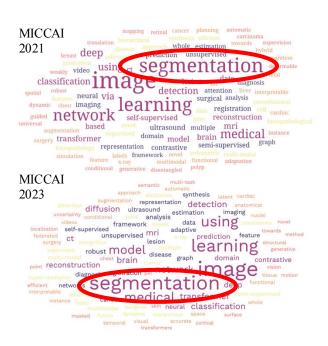
Segmentation is the core technology towards precise biomedical image analysis!

Biomedical Image Segmentation is Still an Active Research Field!

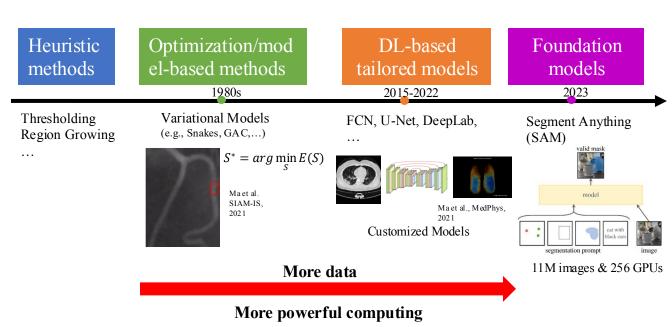
Word Cloud of paper titles in MICCAI 2020-2023



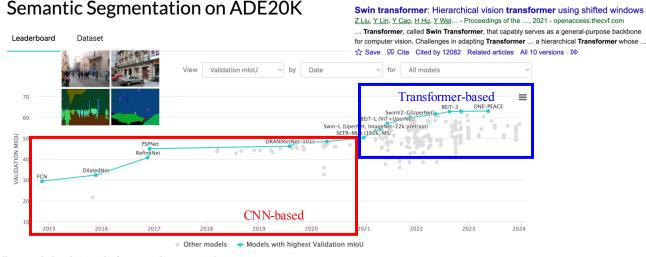
https://github.com/JunMa11/MICCAI-OpenSourcePapers



Segmentation Paradigm Over the Past Half Century



What Are the SOTA Automatic Segmentation Networks?



Fully convolutional networks for semantic segmentation

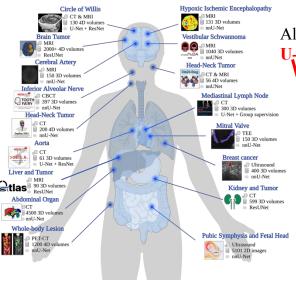
J Long, <u>E Shelhamer</u>, <u>T Darrell</u> - Proceedings of the IEEE ..., 2015 - openaccess.thecvf.com ... for per-pixel tasks like **semantic** segmentation. We show that a **fully convolutional network** (FCN) trained end-to-end, pixels-to-pixels on **semantic** segmentation exceeds the state-of-the-...

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https://paperswithcode.com/sota/semantic-segmentation-on-ade20k

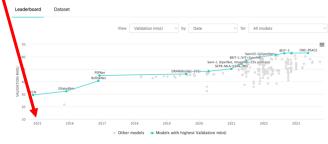
Transformer-based networks are current SOTA on the natural image segmentation benchmark.

What Are the SOTA Networks for Medical Image Segmentation?



All the winning algorithms are based on **U-Net** and its variants.

 $Semantic\,Segmentation\,on\,ADE20K$



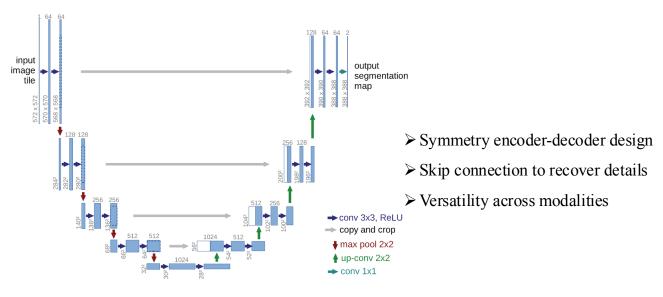
U-net: Convolutional networks for biomedical image segmentation

ORonneberger, P. Fischer, T. Brox - ... Image computing and computer ..., 2015 - Springer ... We demonstrate the application of the u-net to three different segmentation tasks. The first task is the segmentation of neuronal structures in electron microscopic recordings. An ... ☆ Save 99 Cite Cited by 96646 Related articles All 32 versions

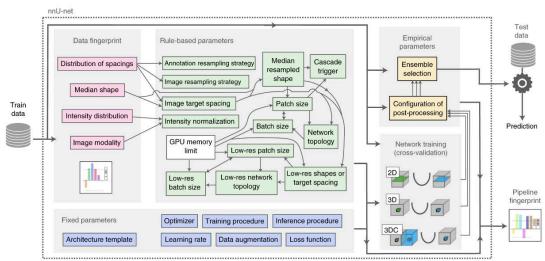
A survey of 17 segmentation challenges in MICCAI 2023

https://github.com/JunMa11/SOTA-MedSeg

What are the advantages of U-Net?

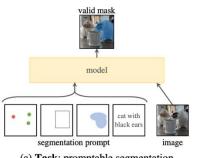


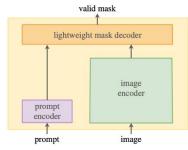
nnU-Net: Automatically config U-Net

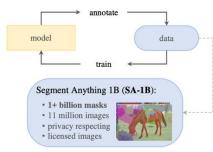


Isensee, Fabian, et al. "nnU-Net: a self-configuring method for deep learning-based biomedical image segmentation." *Nature Methods* 18.2 (2021): 203-211.

Segment Anything Model (SAM)







(a) Task: promptable segmentation

(b) Model: Segment Anything Model (SAM)

(c) Data: data engine (top) & dataset (bottom)



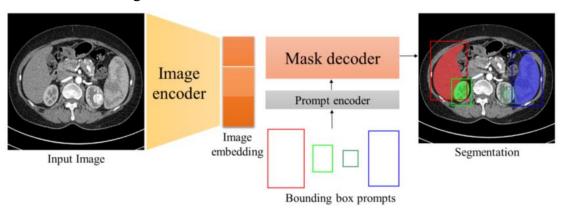




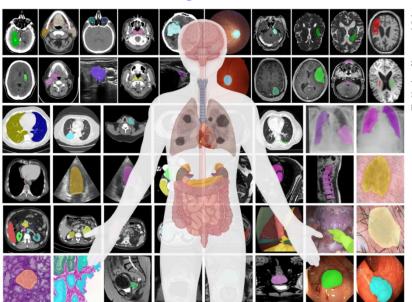
Kirillov, A., et al. "Segment anything." ICCV, 2023

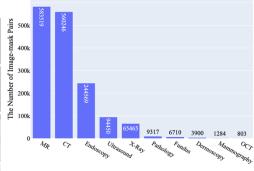
MedSAM: Pipeline

Fine-tune both image encoder and mask decoder



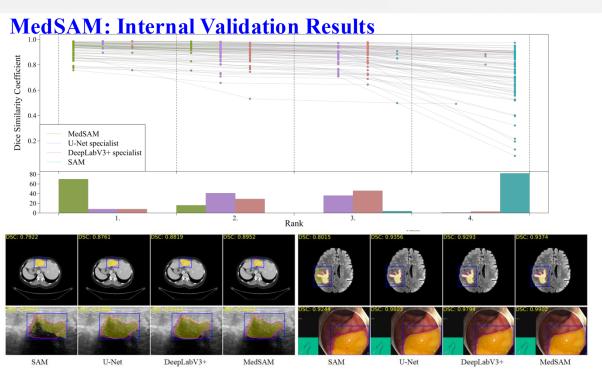
MedSAM: 1M image-mask Pairs



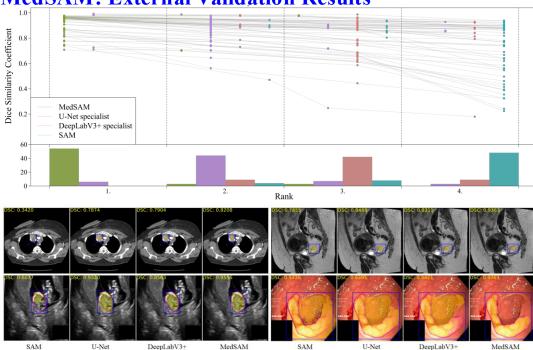


Experimental Settings

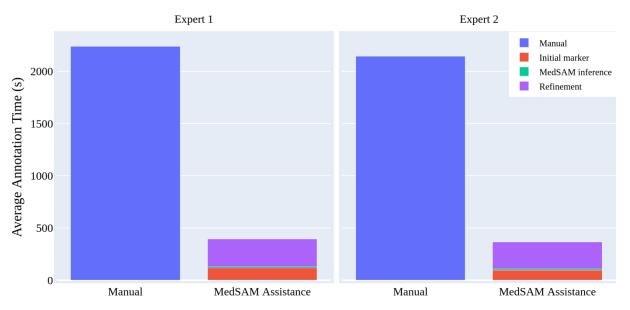
- 86 internal validation tasks
- 60 external validation tasks
- Compared to specialist U-Nets and DeepLabV3+ that are trained on each modality



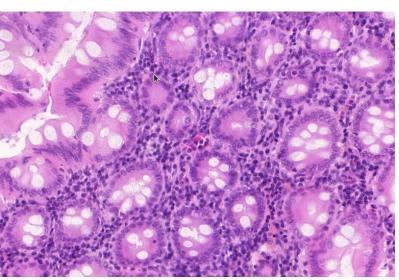
MedSAM: External Validation Results



Human Annotation Study



MedSAM: Demo

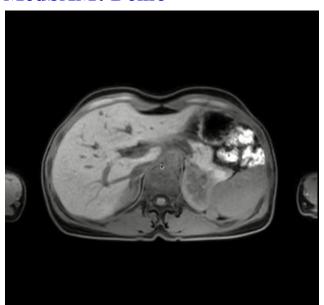


Gland Segmentation in Pathology Images

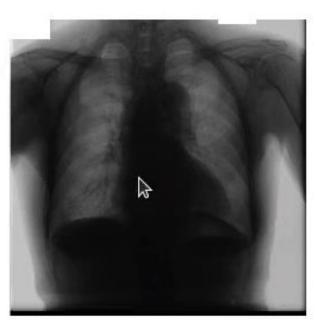


Liver and Tumor Segmentation in CT

MedSAM: Demo



Abdominal Organ Segmentation in MR

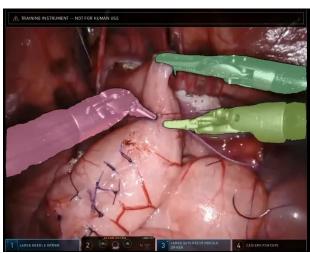


Lungs and Heart Segmentation in X-Ray

MedSAM: Demo



Tissue and Instruments Segmentation in Endoscopy Image

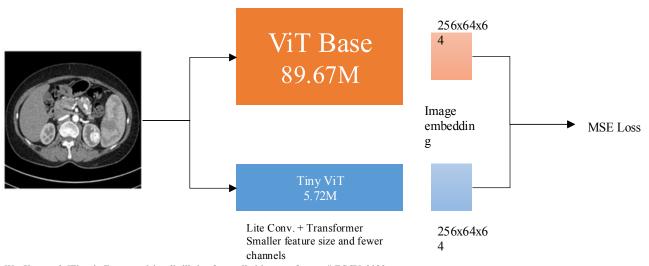


Instruments Segmentation and Tracking in Endoscopy Video

How can we make the model accessible to medical professionals?

Answer: A Lightweight MedSAM (distillation and fine-tuning)

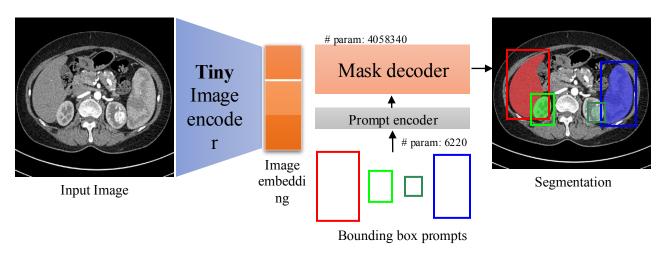
Stage 1. Distillation a small image encoder



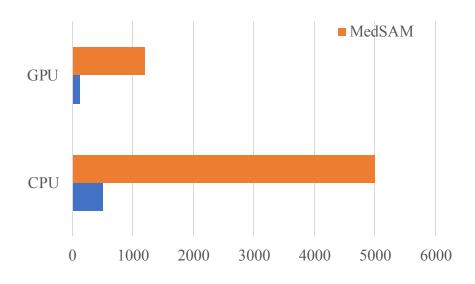
Wu, Kan, et al. "Tinyvit: Fast pretraining distillation for small vision transformers." ECCV, 2022. Zhang, Chaoning, et al. "Faster Segment Anything: Towards Lightweight SAM for Mobile Applications." arXiv preprint arXiv:2306.14289 (2023). Zhao, Xu, et al. "Fast Segment Anything" arXiv preprint arXiv:2306.12156 (2023).

Lite MedSAM: 10× Faster

Stage 2. Fine-tune the whole model

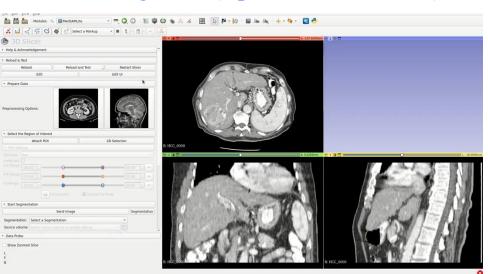


Lite MedSAM: 10× Faster



ms

3D Slicer Integration (Open-source Platform)





https://www.slicer.org/

https://github.com/bowang-lab/MedSAMSlicer

MedSAM in Community

Google Scholar (~1000 citations in eight months)

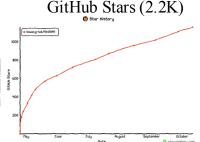


https://www.nature.com > ... > articles

Segment anything in medical images - Nature

by J Ma · 2024 · Cited by 975 — We introduce MedSAM, a deep learning-powered foundation model designed for the segmentation of a wide array of anatomical structures and lesions ...





MedSAM in HuggingFace

Segment medical images with MedSAM

In this notebook, we're going to perform inference with MedSAM, a fine-tuned version of the SAM (segment-anything model) by Meta Al on the medical domain (thereby greatly improving its performance),

- · Original repo
- · Hugging Face docs.

https://github.com/NielsRogge/Transformers-

Tutorials/blob/master/SAM/Run inference with MedSAM using Hugging Face Transforme rs.ipvnb

MedSAM in napari

I integrated MedSam into napari FYI #36

O Closed Karol-G opened this issue on May 5 - 2 comments

