

CSE 428 Computational Biology

Capstone

What is research

- Engineering: Solve an existing problem
- Research: Propose a new problem
 - ✓ Define the problem
 - Problem setting (input, output)
 - Benchmark for validation
 - Baselines
 - ✓ Propose the first solution (which might not be a good solution)
 - ✓ This problem cannot be trivial (Significance)
 - ✓ This problem has not been studied before (Novel)
 - ✓ Why people have never studied it before?
 - ✓ Solving this problem is feasible (Feasible)

Why interdisciplinary research is impactful

- Lots of opportunities
- New methods from domain A can solve important but unaddressed problems in domain B.
 - Apply sequence modeling to study protein sequence (protein sequence is similar to text sequence)
 - Train foundation model/LLM to study protein sequence
 - Train multi-modal LLM to jointly study protein structure and protein sequence.

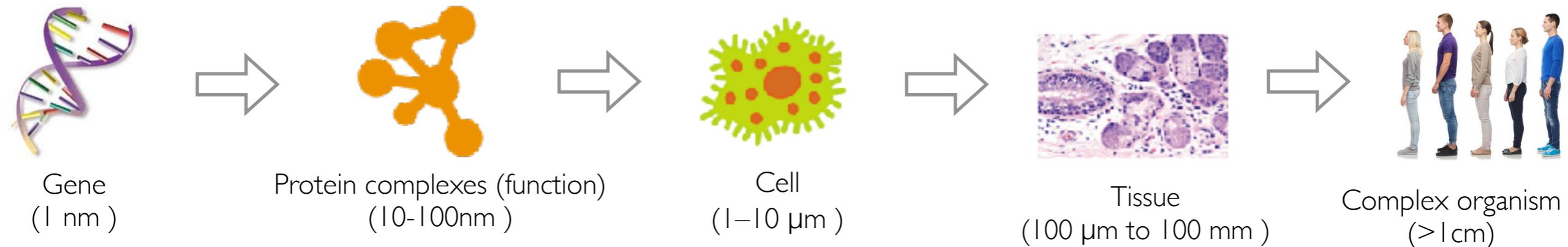
Borrow ideas from other domains

- From less novel to very novel
 - Use a method in one comp bio problem (e.g., protein structure) to solve another comp bio problem (e.g., chromatin structure)
 - Use a new ML technique from CV/NLP to solve a comp bio problem (CSE428 will focus on this)
 - Use a method in other subjects (quantum computing, theoretical physics) to solve a comp bio problem

What can you learn from research

- Career path for a CS student
 - SDE (no need to have PhD degree):
 - Prompt GPT4 for something.
 - Machine learning engineer (PhD degree is a big plus)
 - Fine-tune GPT4 for something: where to get the fine-tune data, which fine-tune techniques to use
 - Need substantial research ability to understand and modify existing algorithm
 - Research scientist/faculty (PhD is required)
 - Develop OpenAI GPT4
 - It is all about research
- CSE 428 will be at the scope of Machine learning engineer

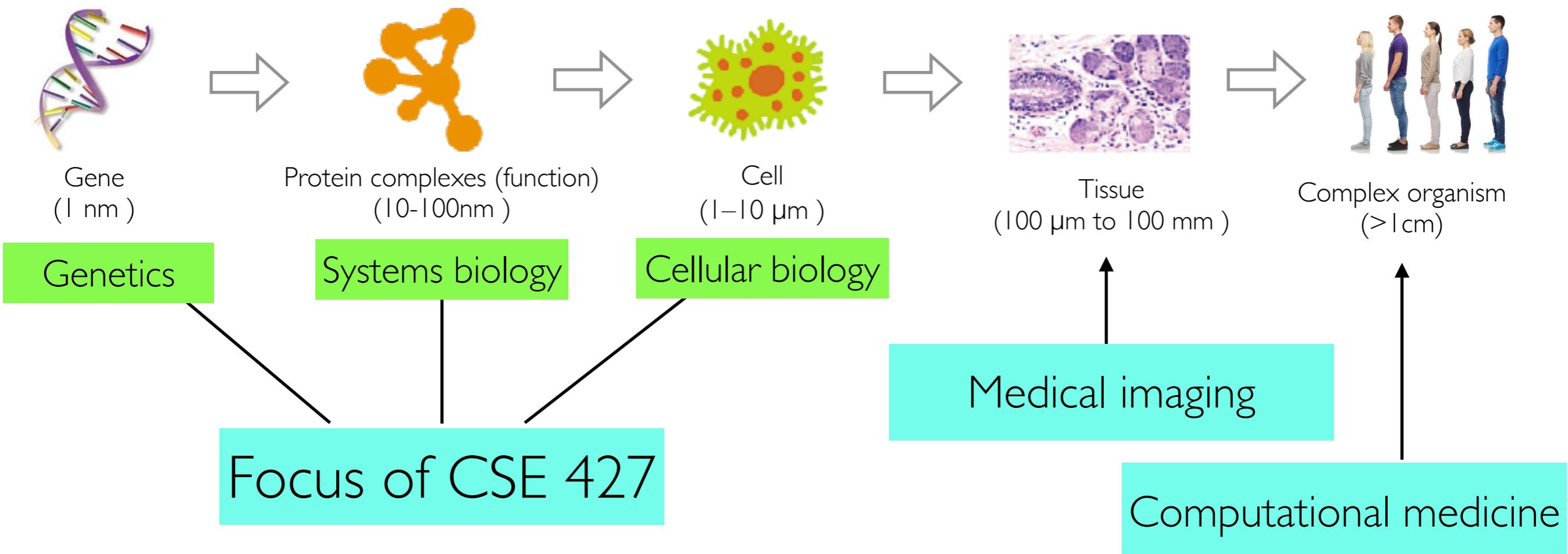
CSE427: Computational methods for biology at different scales



A rich hierarchy of biological subsystems at multiple scales: genotypic variations in nucleotides (1 nm scale) -> proteins (1–10 nm) -> protein complexes (10–100 nm), cellular processes (100 nm) -> phenotypic behaviors of cells (1–10 μ m), tissues (100 μ m to 100 mm), -> complex organisms (>1 m).

source: Yu, Michael Ku, et al. "Translation of genotype to phenotype by a hierarchy of cell subsystems." *Cell systems* 2.2 (2016): 77-88.

Computational methods for biology at different scales



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CSE 428 projects

- Option 1: define your own project and work by yourself
- Option 2: work on a suggested topic
 - Option 2A: pick a paper from Su-In Lee, Sara Mostafavi, Bill Noble
 - Option 2B: pick a paper from my lab (will introduce later)
 - Understand everything of the paper!
 - Reproduce some key results
 - Try to improve and modify the model

What you need to submit

- A course report
- A Jupyter notebook commit to the course GitHub
 - Mark down of a pipeline from reading data to produce prediction/analyses.

Schedule and grading

1. Three presentations
2. course project presentation (60%), final report (40%)

Tentative Schedule

Date	Topic
4/1	Welcome/overview. Introduction to CSE428. (Sheng)
4/8	Project topic presentation (first half)
4/15	Project topic presentation (second half)
4/22	Working time
4/29	Mid-term project idea presentation (first half)
5/6	Mid-term project idea presentation (second half)
5/13	Working time
5/20	Working time
5/27	Final project presentation (first half)
6/3	Final project presentation (second half)

First presentation: decide on a paper

- Choose one paper
- Focus on the significance
 - Why is this problem important
 - Why are you interested in this project.
- 5 minutes per student.
- More instruction later based on the number of students

How to read papers

- This is the most important thing
 - One researcher spends 3 hours per day to read paper
- Read new papers (2023-) and papers published in top journals/conferences
 - Nature, Science, Cell, Recomb, ISMB
- Tips for how to read papers
 - Focus less on the background, introduction and motivation
 - Focus more on the problem setting (input, output)
 - Focus more on the datasets for evaluation (size, accessible, simulated data or real data)
- The more you read, the faster you will read.
- Ultimate goal: you can “predict” what method/dataset/evaluation this paper will do after reading the abstract

Pick the problem to work on

- Only work on the frontier methods
- Don't be ambitious!
- Only work on problem that an existing paper has worked on and you can fully understand that paper
- Only work on problem that you can clearly evaluate

Pick the problem to work on

- Pick a paper from Profs from Allen School
 - Su-In Lee, Sara Mostafavi, Sheng Wang, Bill Noble
- Read at least three papers in the first week
 - Each student will do a presentation next week
 - Significance
 - Innovation
 - Methods and evaluation
 - Why do you like this paper?

How to borrow ideas from other domains

- Find the commonality by understanding the problem setting
 - Problem A in computer vision has the same problem setting as Problem B in comp bio.
 - Talk to people work in CV/NLP

Experiments

1. Don't implement your ideas first
2. First, reproduce the results from baselines
3. Test baselines on new datasets and examine the performance
4. If the performance is bad, figuring out the reason

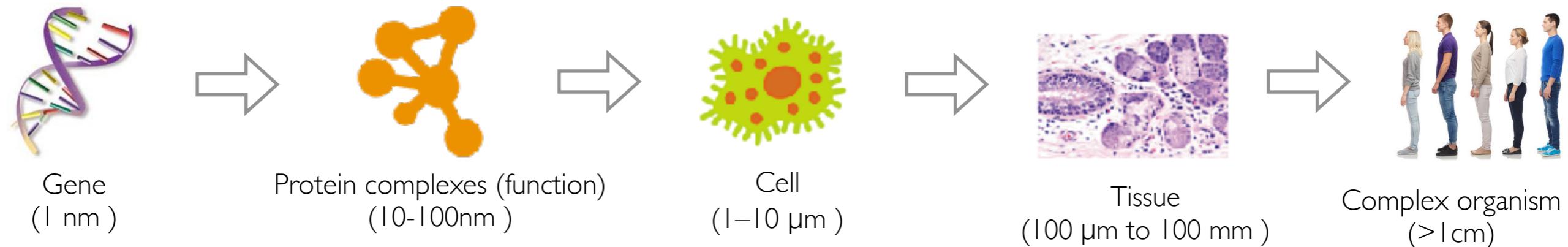
Uniqueness of comp bio research

- Interdisciplinary subject
 - Communication is very important
 - Understand biologists/doctors' needs
 - Clearly explain our methods
- New subject
 - Lots of opportunities
 - Less well-defined benchmarks

Reflection on my research career

- 2009-2013 Undergrad in CS, Peking university
- 2013-2018 PhD in CS, UIUC
- 2018-2020 Postdoc in Medicine, Stanford
- Most important thing is choosing the research area.

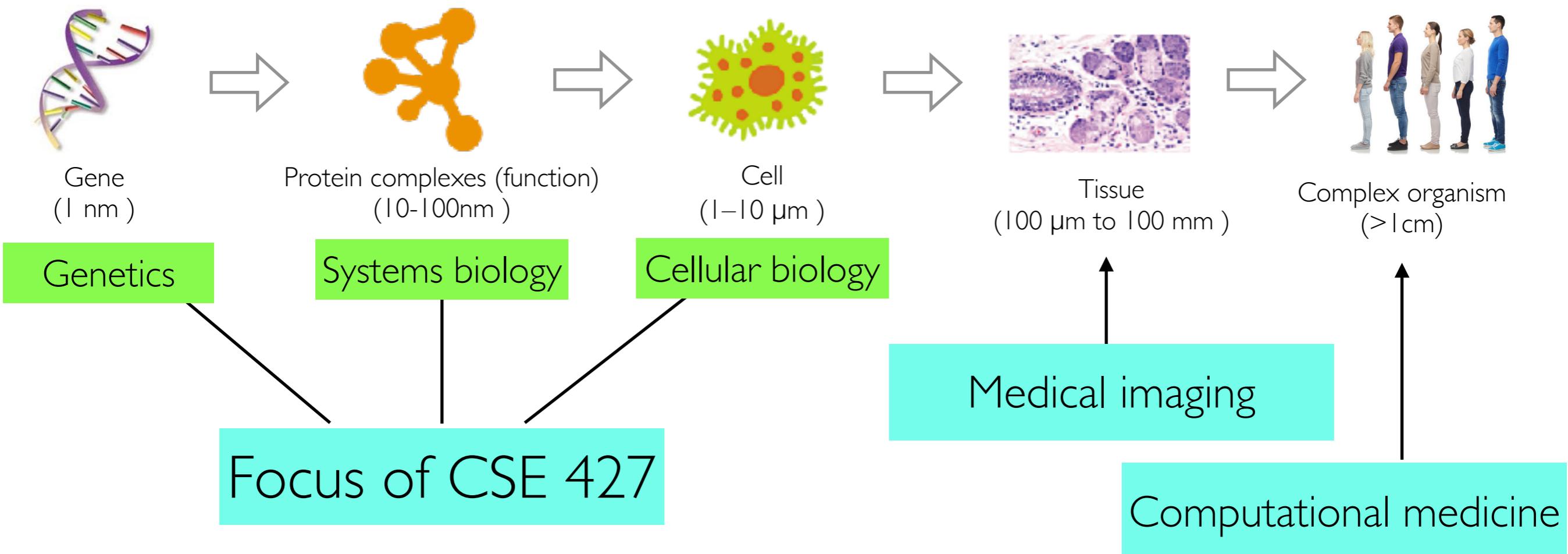
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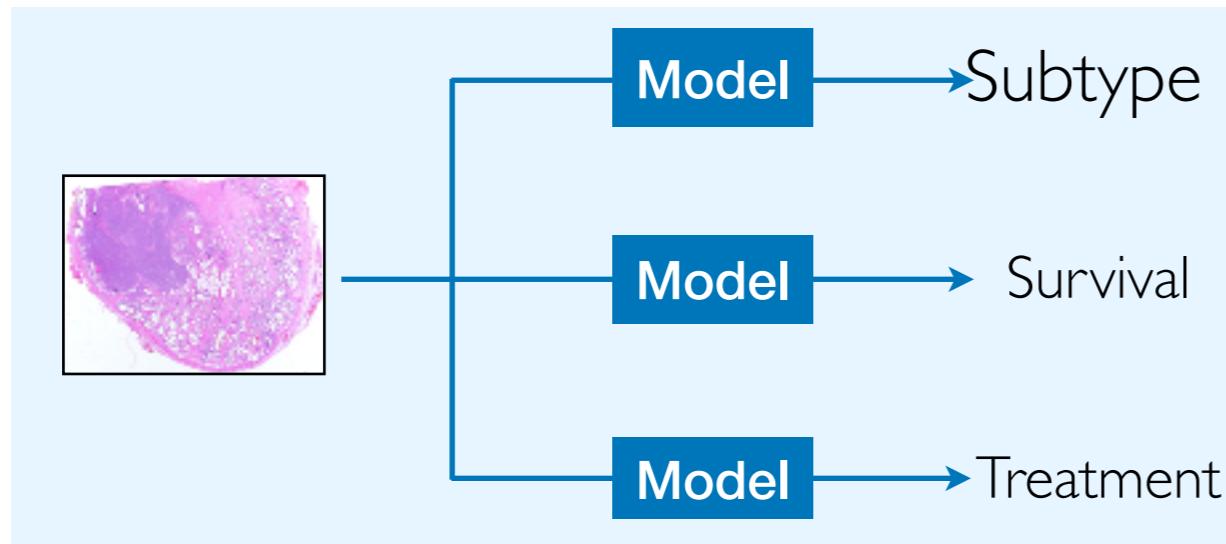
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Computational methods for biology at different scales

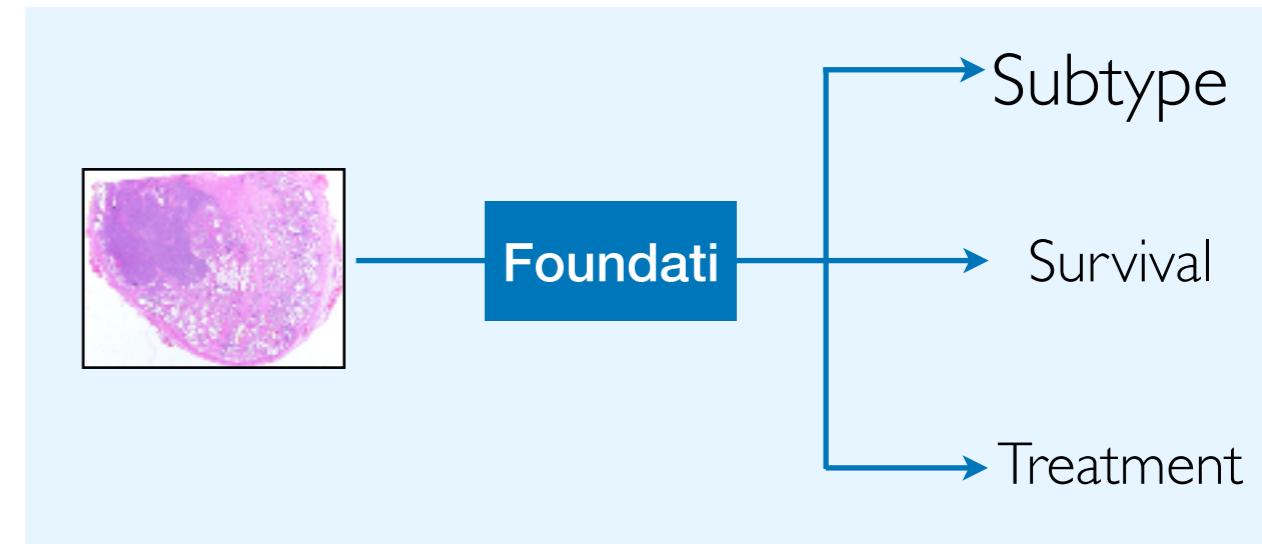


Four paradigms in AI for Medicine

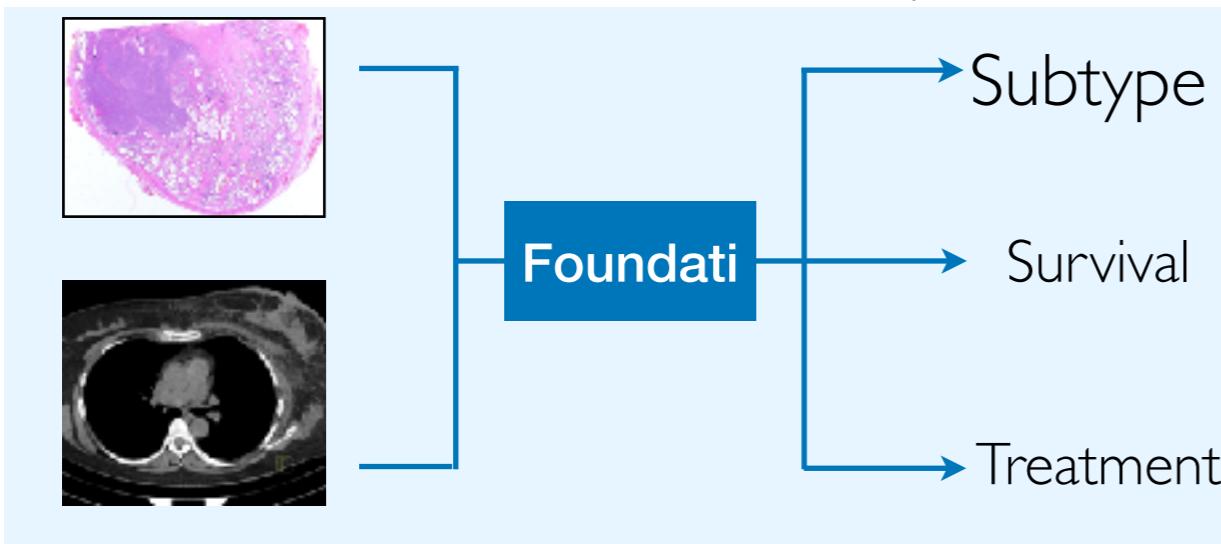
Deep learning (2012)
One model for one task



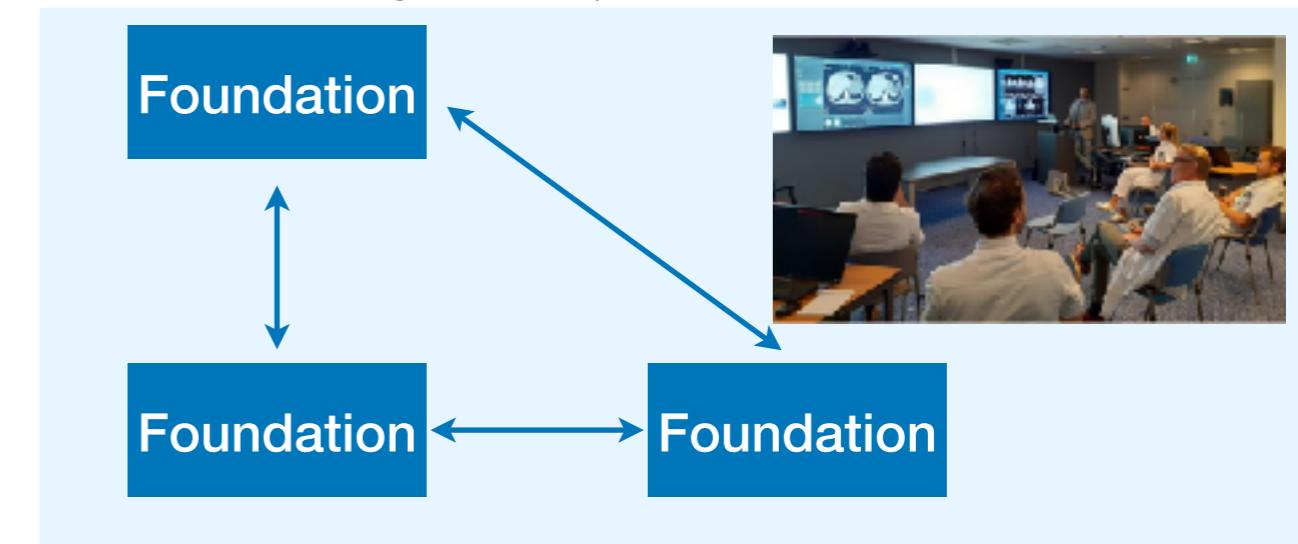
Foundation model (2022)
One model for all tasks



Multi-modal foundation model (2023)
One model takes different inputs

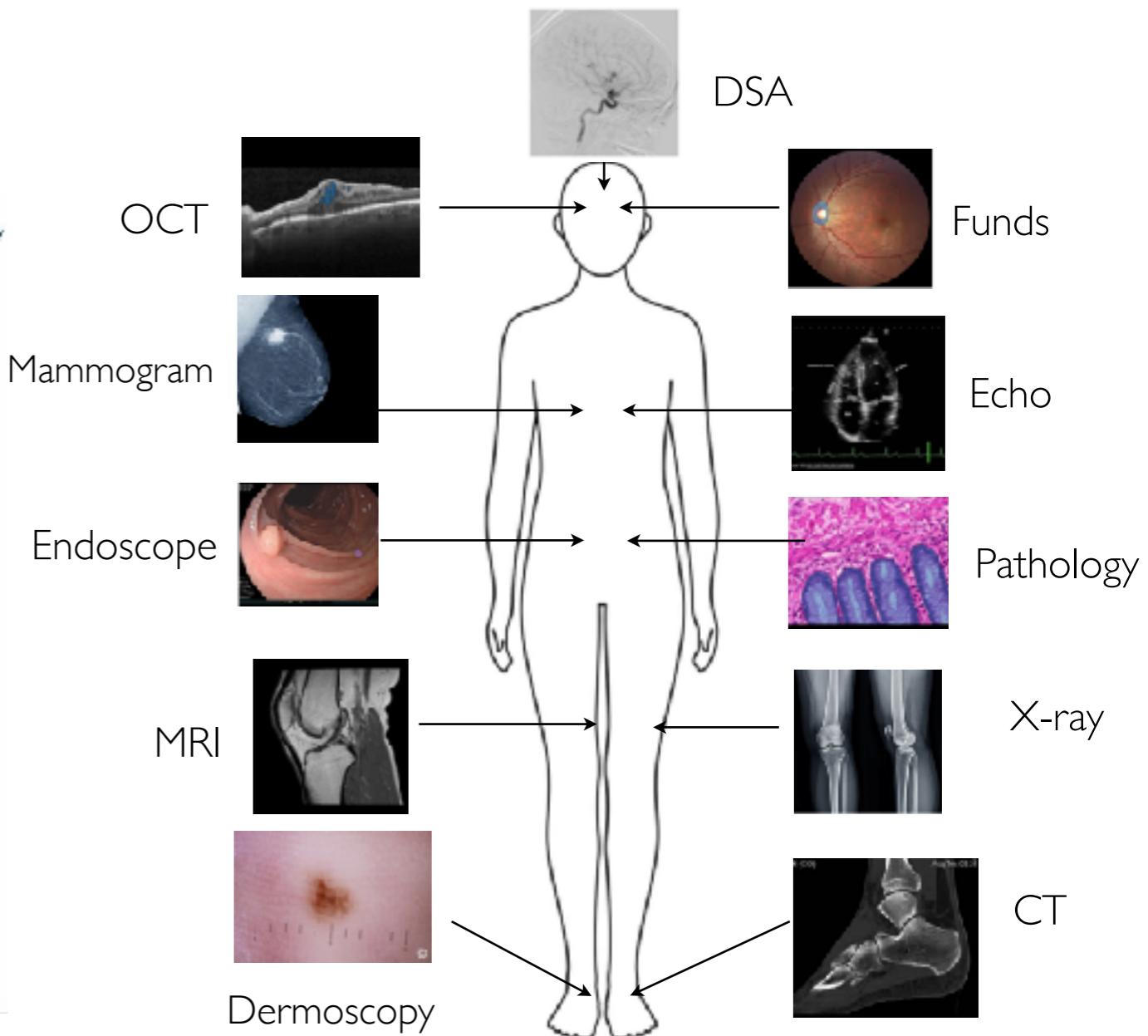
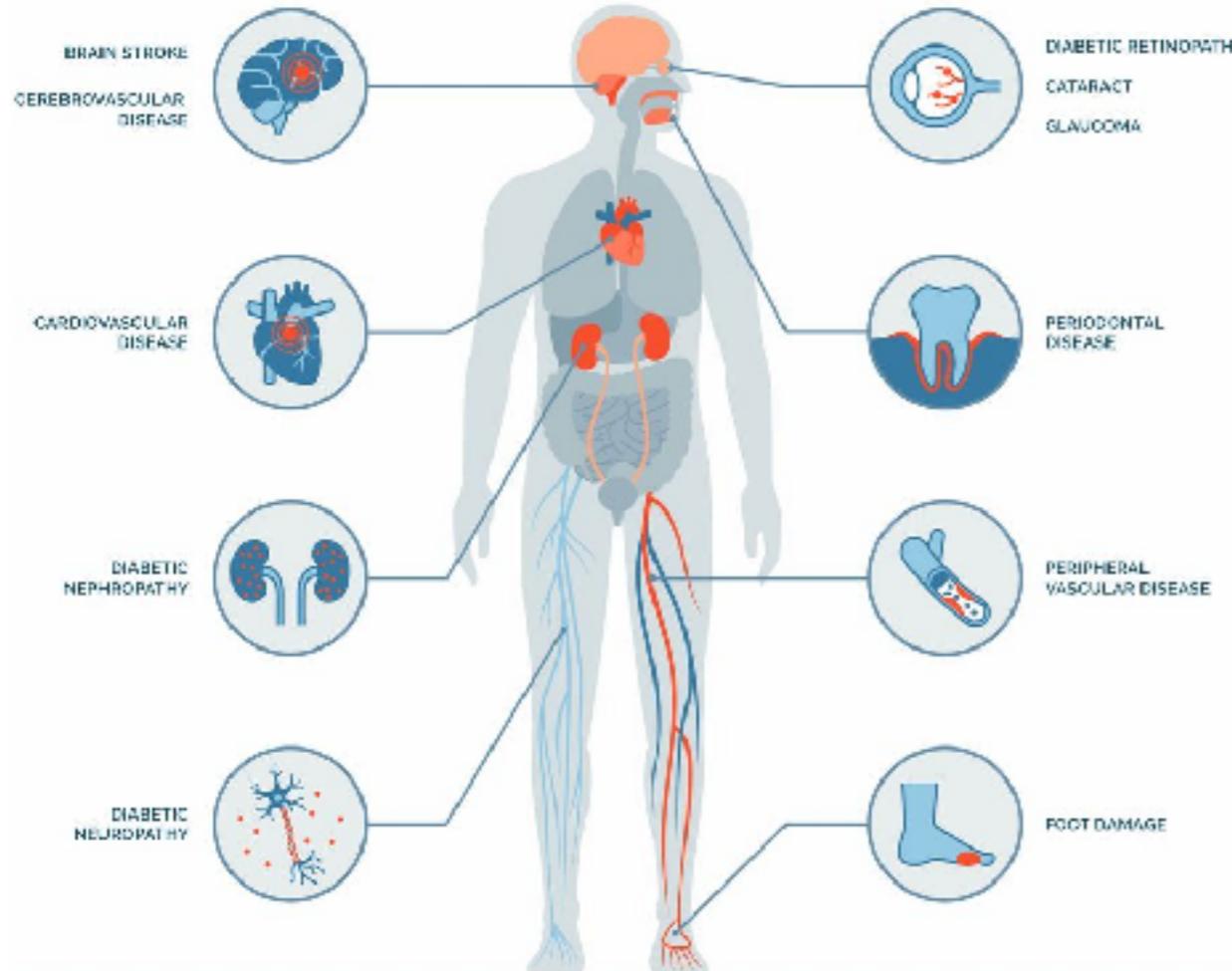


Multi-agent (2024)
Integrate multiple foundation models



Medicine is inherently multi-modal

Complication of diabetes



Today's talk: 3 parts

1. Pathology foundation model
2. 3D retinal foundation model

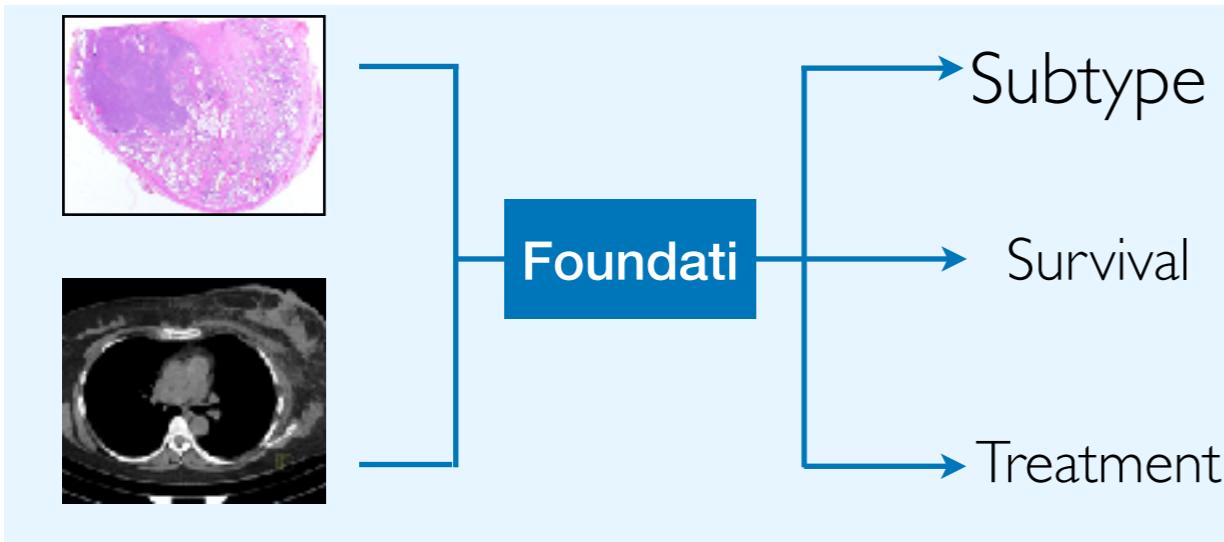


3. A multi-modal foundation model integrating 9 imaging modalities



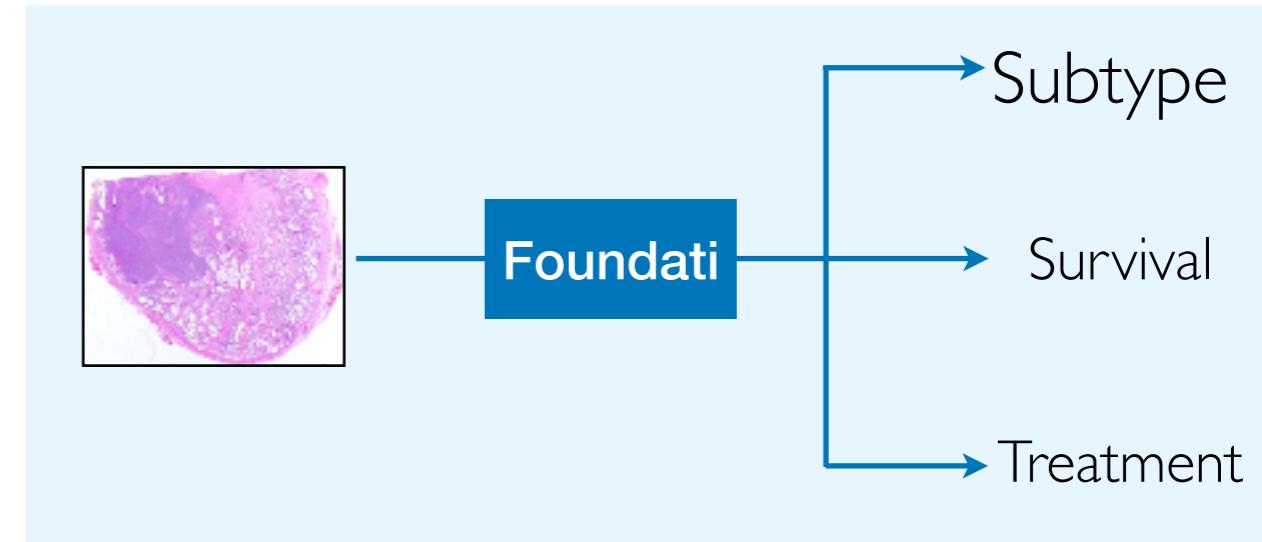
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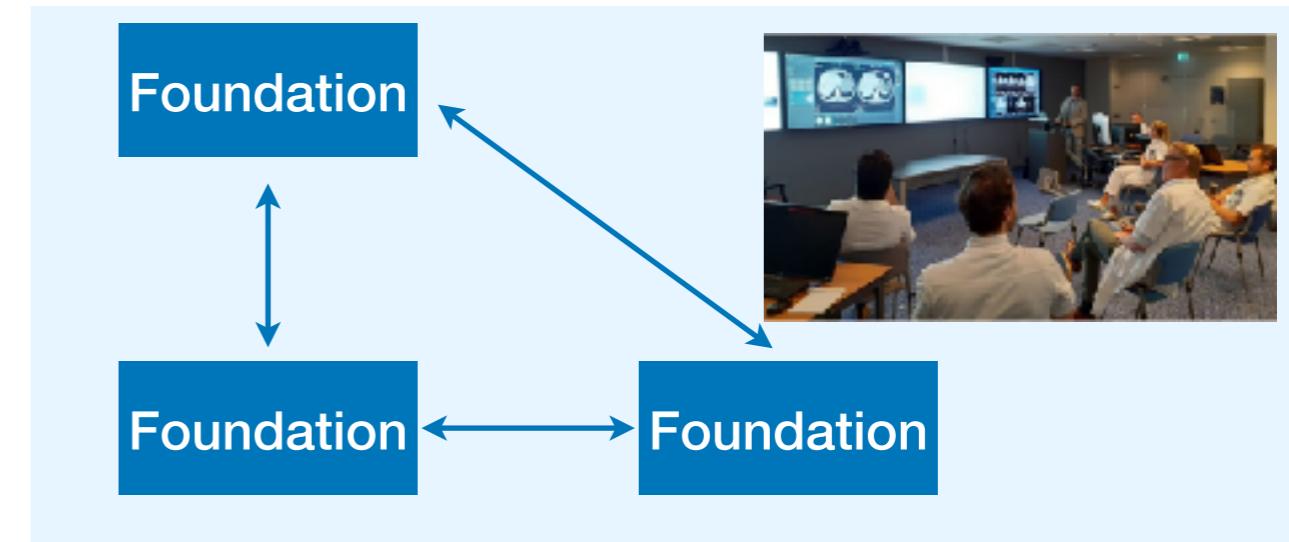
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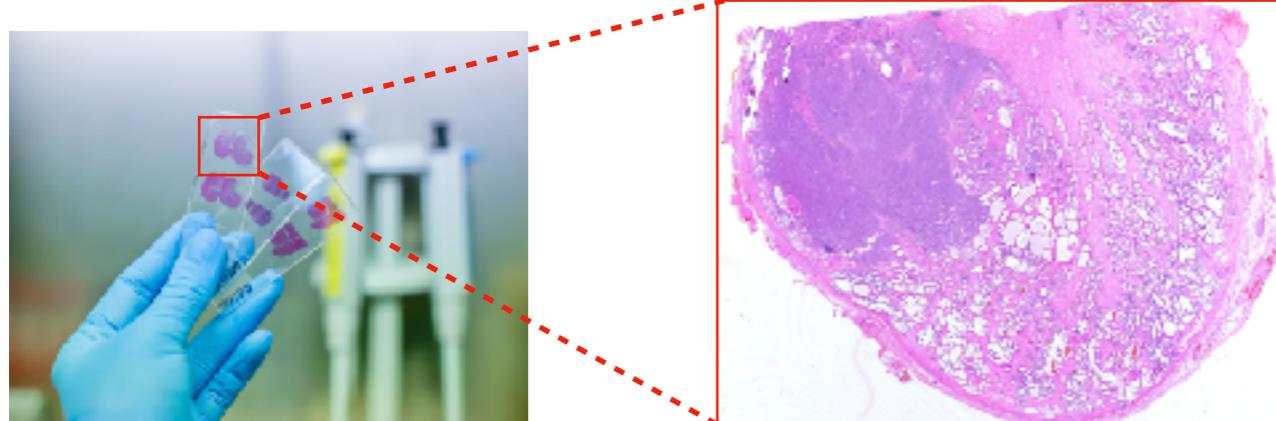


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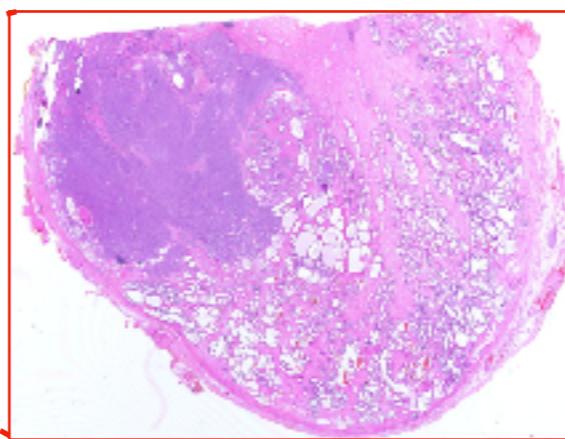
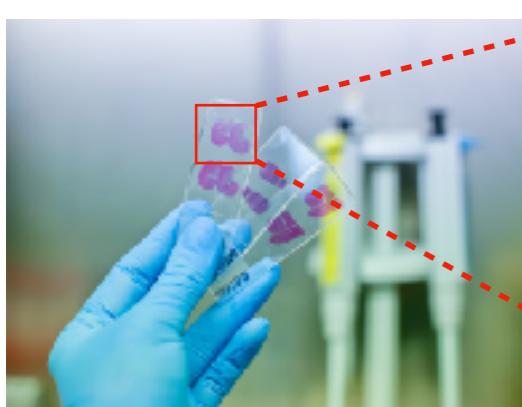


Pathology images are too large for existing AI models



Pathology images
100k by 100k pixels

Pathology images are too large for existing AI models

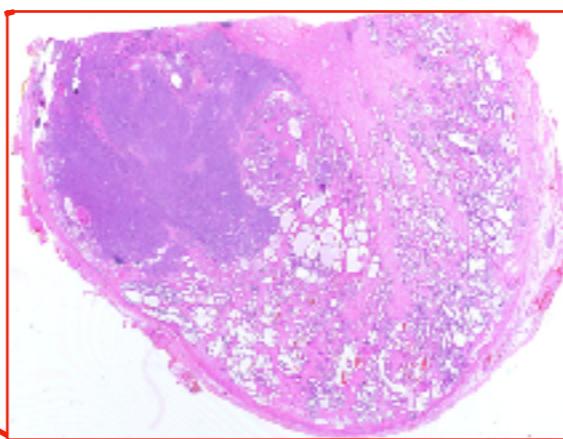
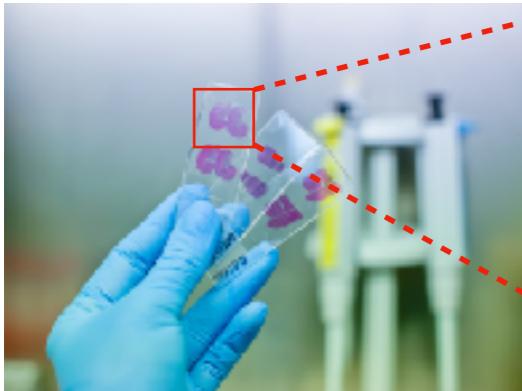


As large as a tennis court



Pathology images
100k by 100k pixels

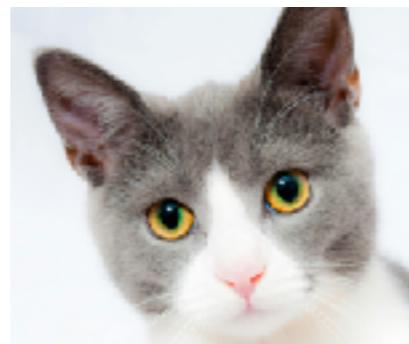
Pathology images are too large for existing AI models



As large as a tennis court



Pathology images
100k by 100k pixels



As large as a tennis ball



Images handled by existing AI models
256 by 256 pixels

Long-context modeling: ChatGPT is good at understanding long documents

You
sample-pdf-with-images.pdf
PDF

summarize this document

ChatGPT
The document contains various sections of elaborate and expressive prose, primarily employing a stream of consciousness style. It features an extensive use of ornate and descriptive language, covering topics from daily experiences to abstract thoughts. Key themes include observations of social interactions, personal reflections, and detailed descriptions of surroundings and emotional states. The narrative appears non-linear and fragmented, resembling a collection of thoughts rather than a structured story.

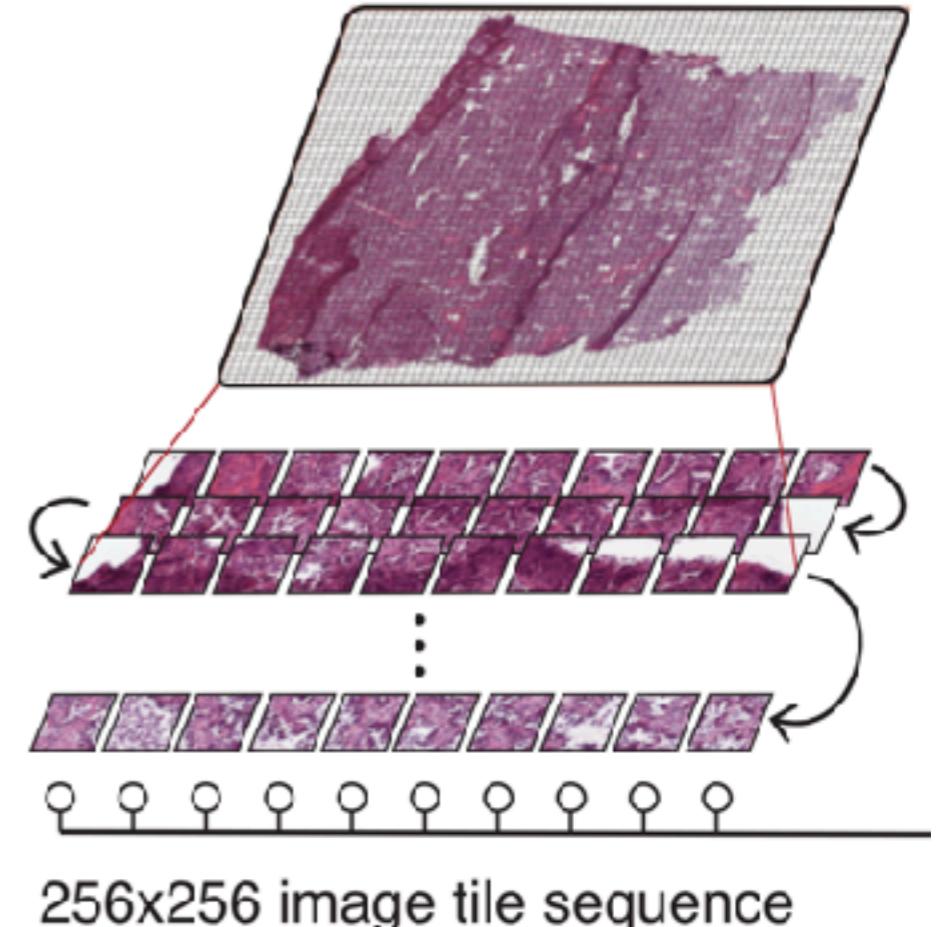
undo redo back forward

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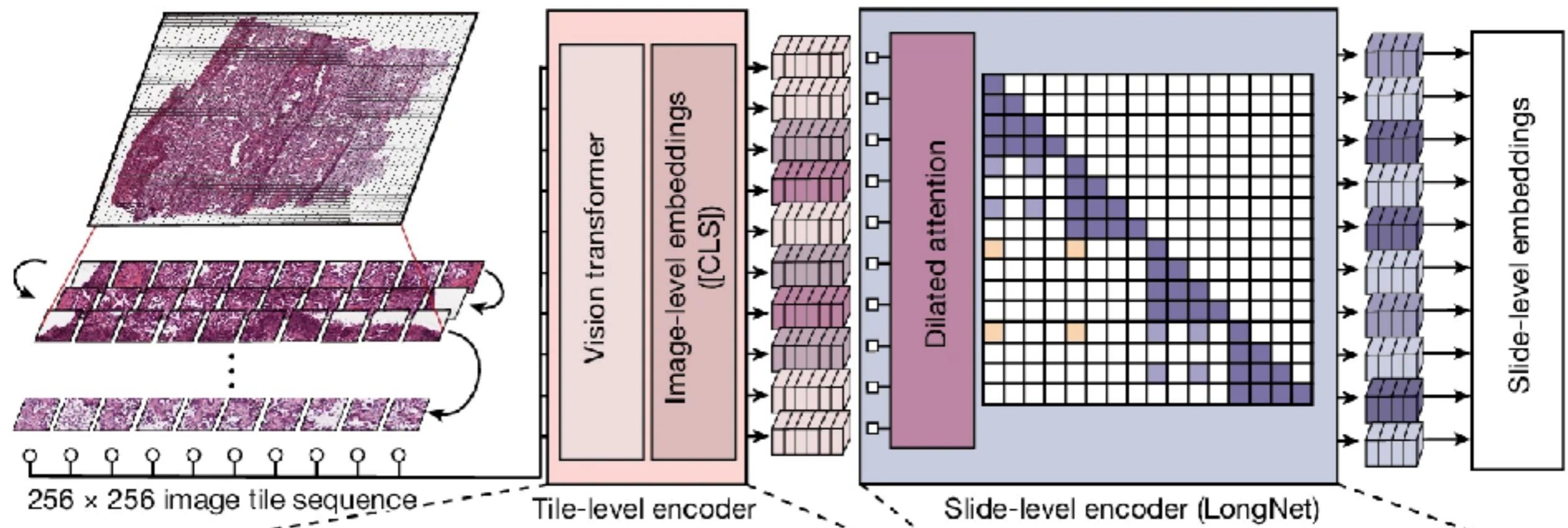
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Use LongNet to model a **long sentence** of small images from a pathology slide

Tile-level encoder to capture local patterns

Slide-level encoder to capture the pattern in the whole slide



A self-supervised learning framework based on DinoV2 and
LongNet

GigaPath: A whole-slide foundation model for pathology

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Article | Open access | Published: 22 May 2024

A whole-slide foundation model for digital pathology from real-world data

Hanwen Xu, Naoto Usuyama, Jaspreet Bagga, Sheng Zhang, Rajesh Rao, Tristan Naumann, Cliff Wong, Zelalem Gero, Javier González, Yu Gu, Yanbo Xu, Mu Wei, Wenhui Wang, Shuming Ma, Furu Wei, Jianwei Yang, Chunyuan Li, Jianfeng Gao, Jaylen Rosemon, Tucker Bower, Soohye Lee, Roshanthi Weerasinghe, Bill J. Wright, Ari Robicsek, Brian Piening, Carlo Bifulco✉, Sheng Wang✉ & Hoifung Poon✉ — Show fewer authors

Nature 630, 181–188 (2024) | Cite this article

200k model downloads every month
(Hugging Face)!

Media coverage: [Forbes](#), [Yahoo](#), [Becker's hospital review](#), [Fierce biotech](#), [CTOL digital solutions](#), [HIT consultant](#), [GeekWire](#), [Cosmic log](#), [HealthXL](#), [RamaOnHealthcare](#), [Providence](#), [nikkei](#), [cryptorank](#), [deeptech](#)



Hanwen Xu
U of Washington



Naoto Usuyama
Microsoft Research



Carlo Bifulco
Providence



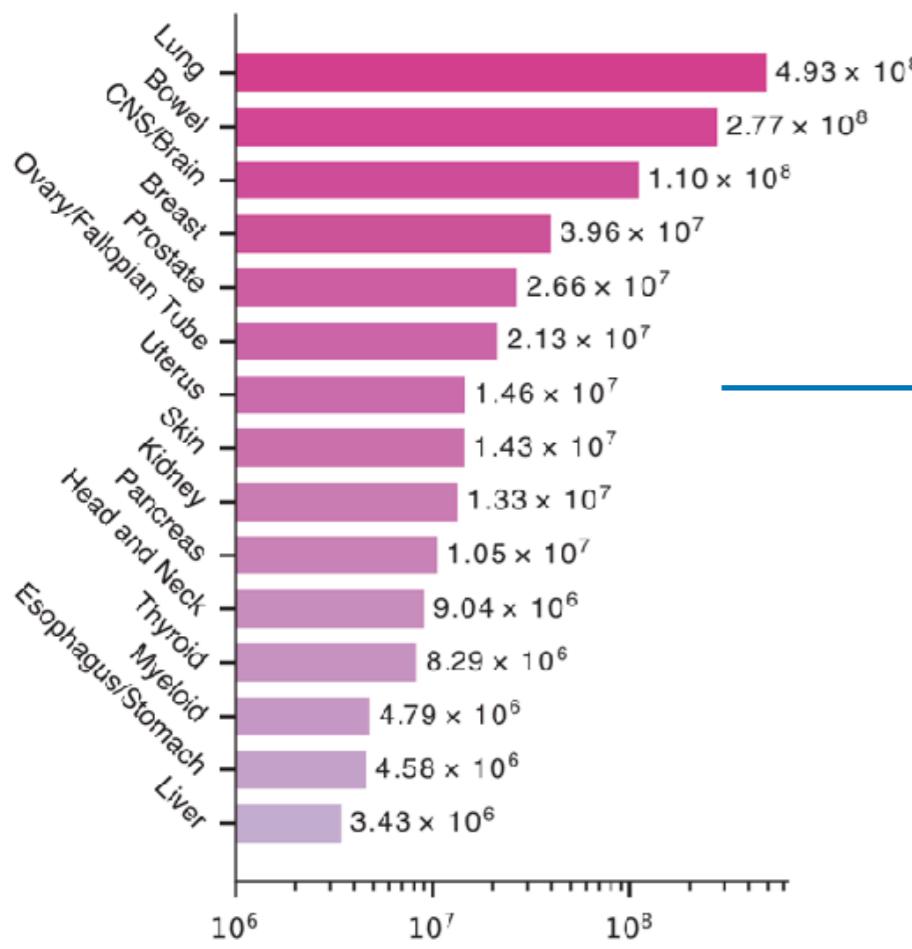
Sheng Wang
U of Washington



Hoifung Poon
Microsoft Research

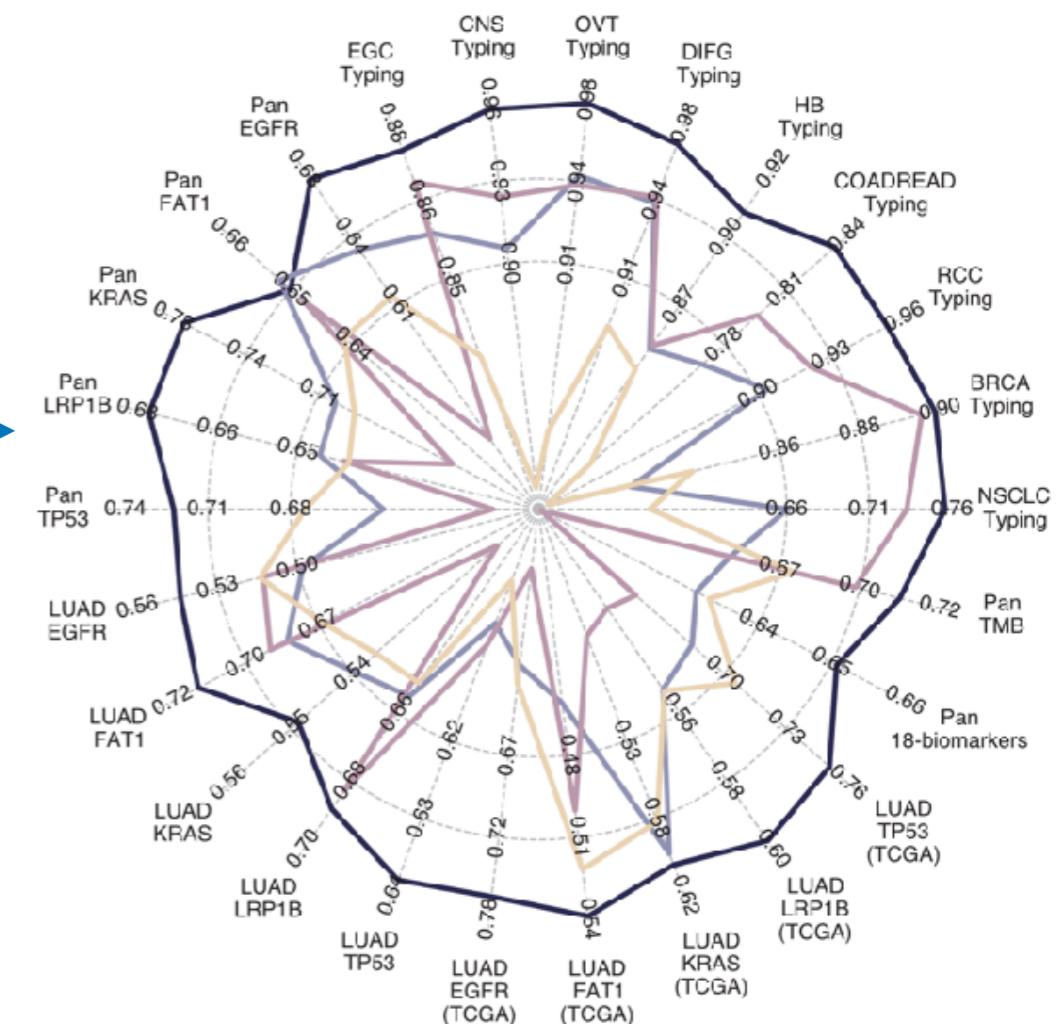
One (foundation) model fits all

30,000 patients from 28 hospitals
140k slides, 15 cancer types

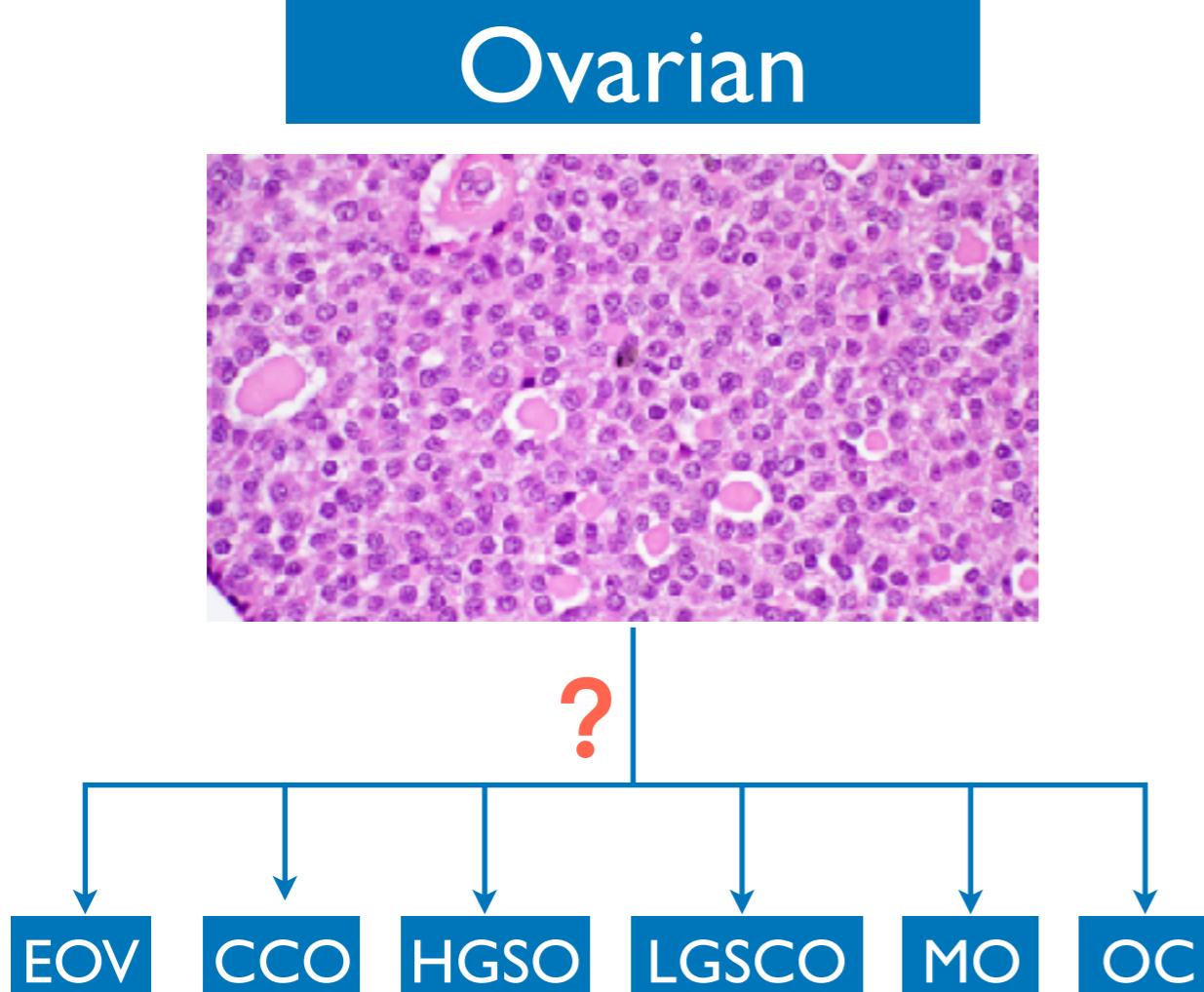


GigaPa

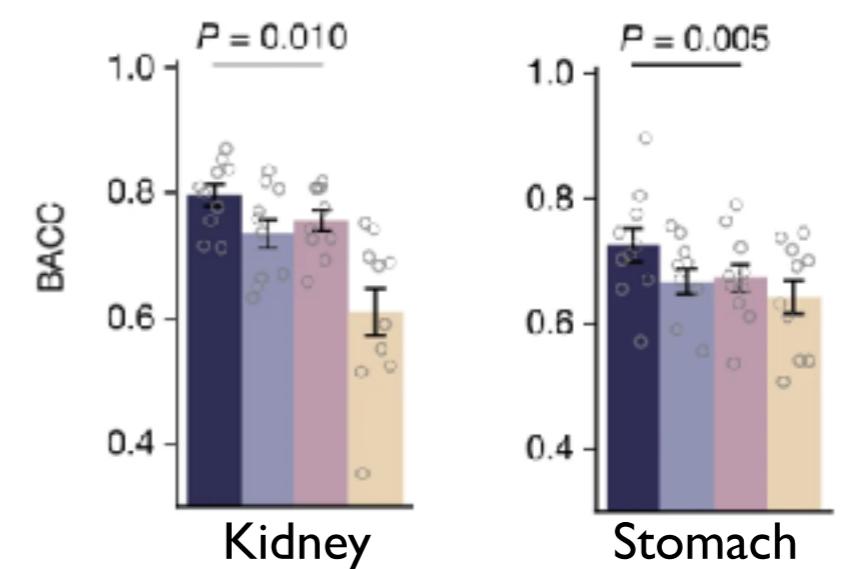
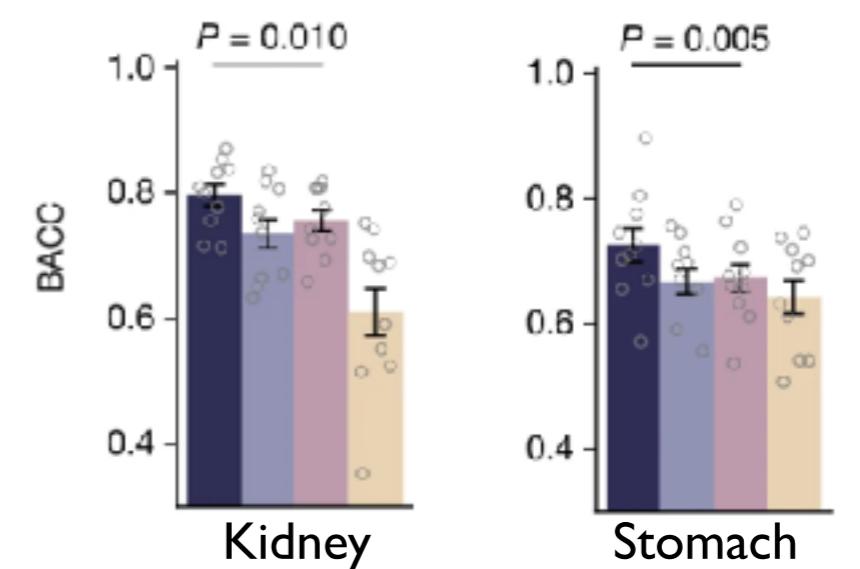
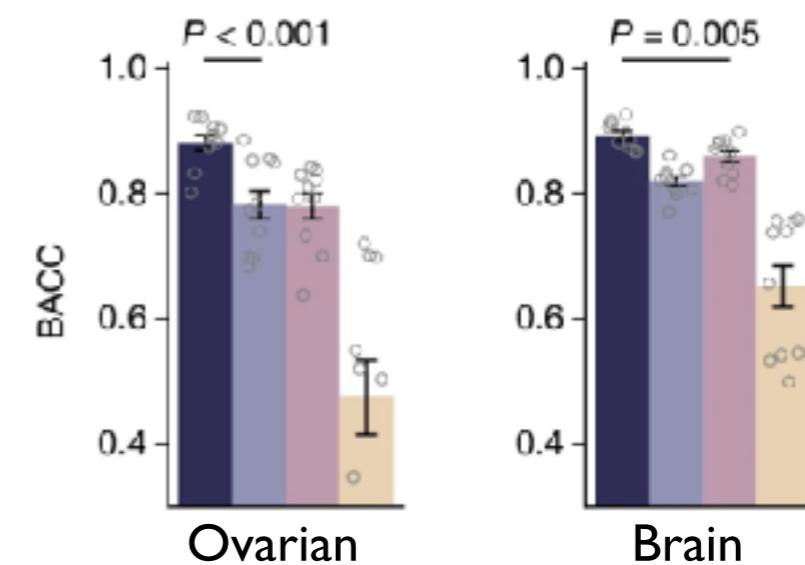
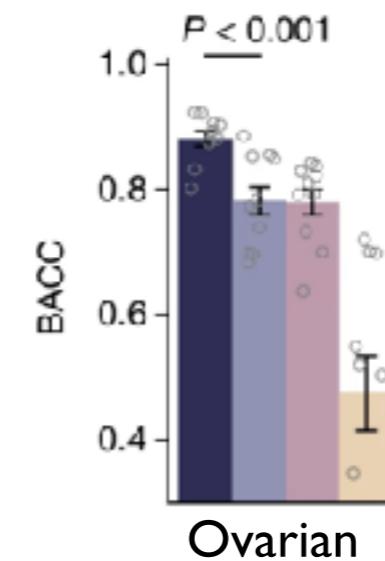
Best performance on 25 out of 26 tasks



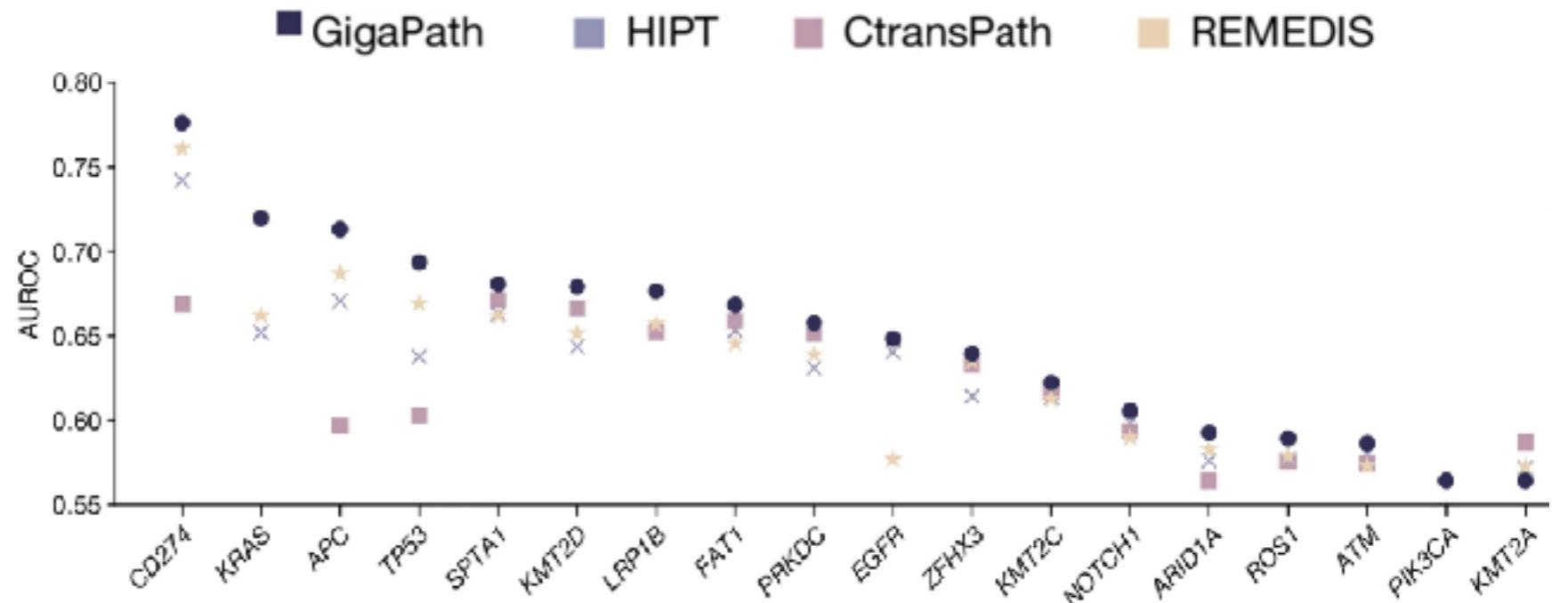
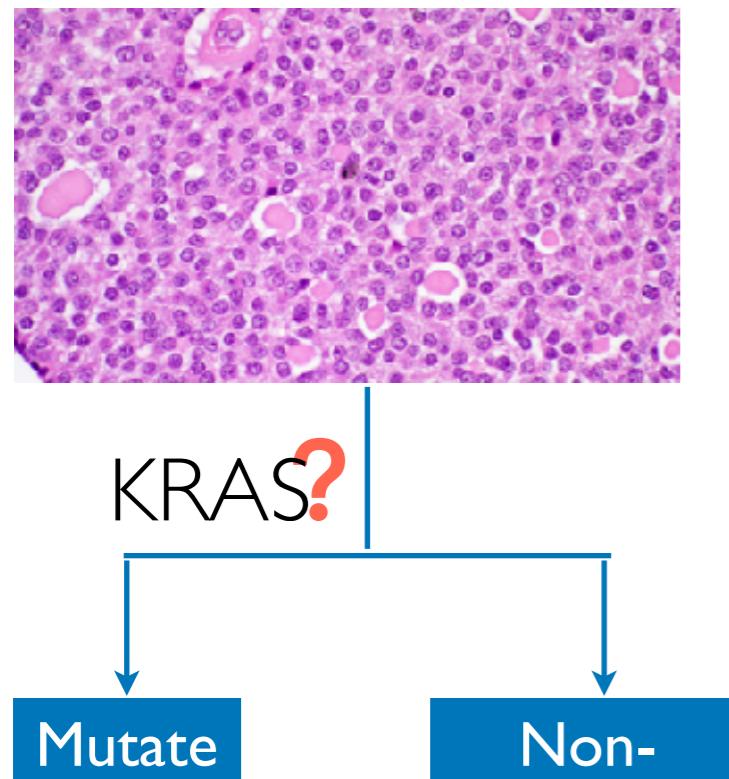
Cancer subtype classification using pathology images



■ GigaPath ■ HIPT ■ CtransPath ■ REMEDIS



Biomarker prediction using pathology images: best performance on 17 out of 18 biomarker predictions



Directly predicting treatment is too difficult

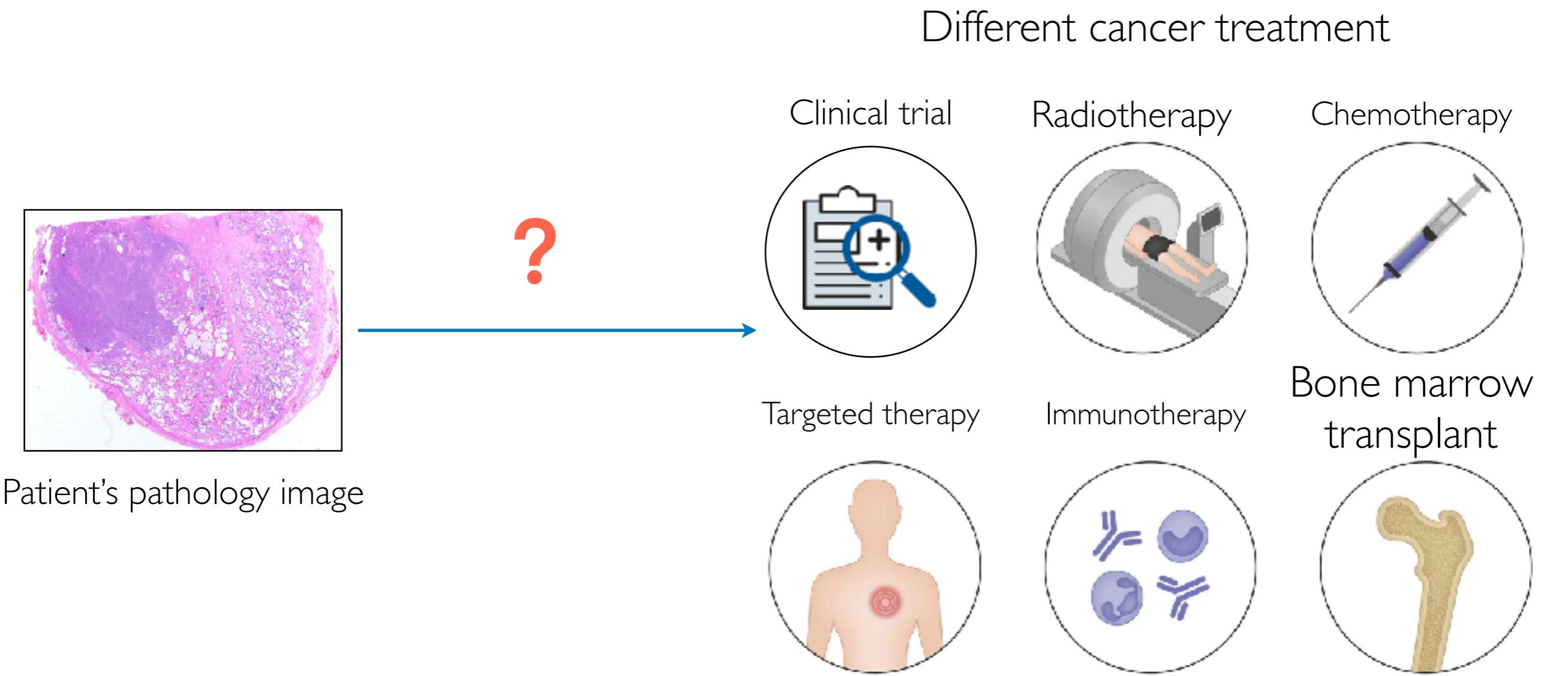


Image from IHH Healthcare Singapore

Chain-of-Thought: Decompose a complicated task into many subtasks

Standard GenAI

Model Input

Q: Roger has 5 tennis balls. He buys 2 more cans of tennis balls. Each can has 3 tennis balls. How many tennis balls does he have now?

A: The answer is 11.

Q: The cafeteria had 23 apples. If they used 20 to make lunch and bought 6 more, how many apples do they have?

Model Output

A: The answer is 27. 

Chain-of-Thought GenAI

Model Input

Q: Roger has 5 tennis balls. He buys 2 more cans of tennis balls. Each can has 3 tennis balls. How many tennis balls does he have now?

A: Roger started with 5 balls. 2 cans of 3 tennis balls each is 6 tennis balls. $5 + 6 = 11$. The answer is 11.

Q: The cafeteria had 23 apples. If they used 20 to make lunch and bought 6 more, how many apples do they have?

Model Output

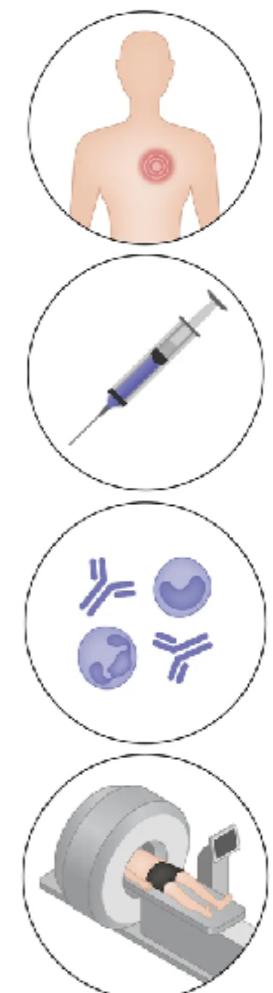
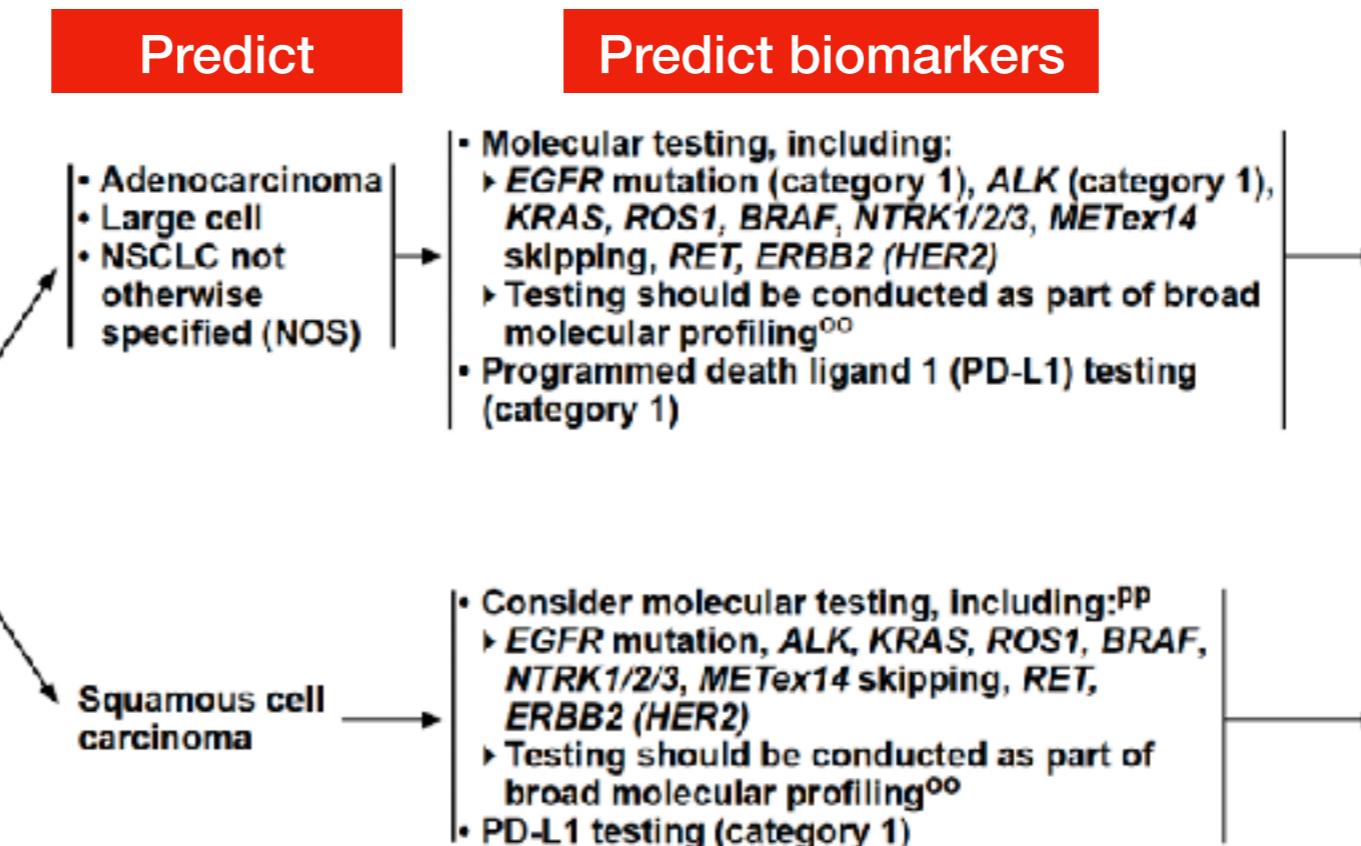
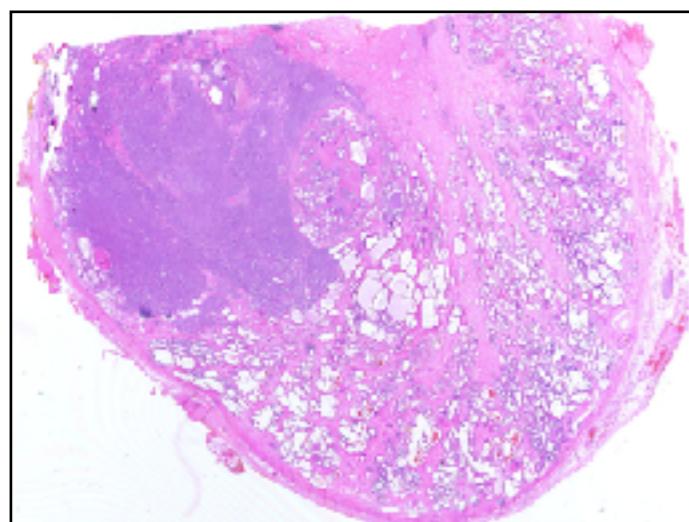
A: The cafeteria had 23 apples originally. They used 20 to make lunch. So they had $23 - 20 = 3$. They bought 6 more apples, so they have $3 + 6 = 9$. The answer is 9. 

Our idea: use Clinical Guideline as the Chain-of-Thought



National
Comprehensive
Cancer
Network®

NCCN Guidelines Version 7.2024 Non-Small Cell Lung Cancer

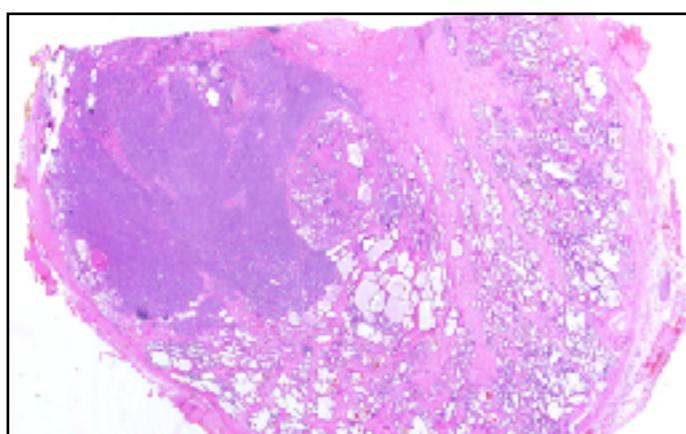


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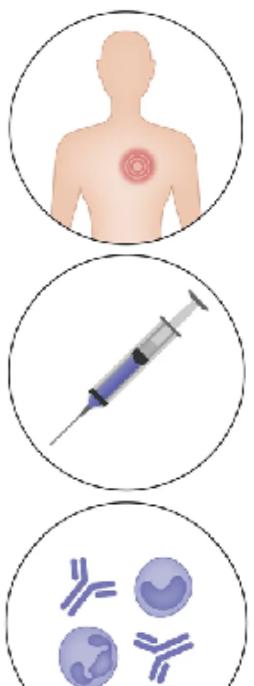
Predict

- Adenocarcinoma
- Large cell
- NSCLC not otherwise specified (NOS)

Predict biomarkers

- Molecular testing, including:
 - ▶ EGFR mutation (category 1), ALK (category 1), KRAS, ROS1, BRAF, NTRK1/2/3, METex14 skipping, RET, ERBB2 (HER2)
 - ▶ Testing should be conducted as part of broad molecular profiling^{oo}
- Programmed death ligand 1 (PD-L1) testing (category 1)

- Consider molecular testing, Including:^{PP}
 - ▶ EGFR mutation, ALK, KRAS, ROS1, BRAF,



Human-AI collaboration: Experts derive the guideline. AI makes decision on each branch.

Future implication: AI model as a clinical lab test

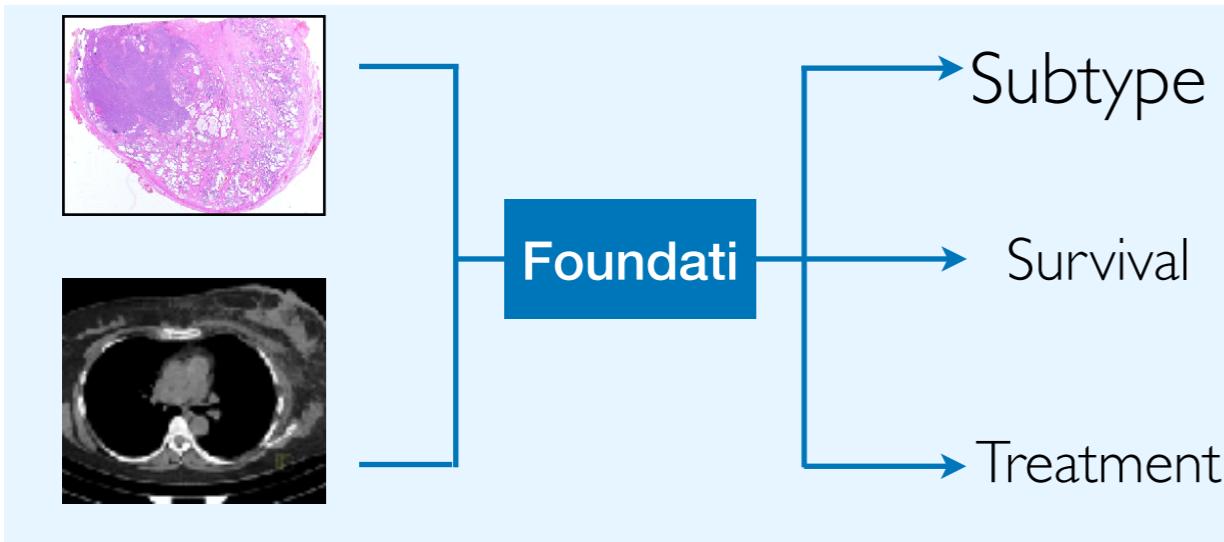
Today's talk: 3 parts

1. Pathology foundation model
2. 3D retinal foundation model
3. A multi-modal foundation model integrating 9 imaging modalities



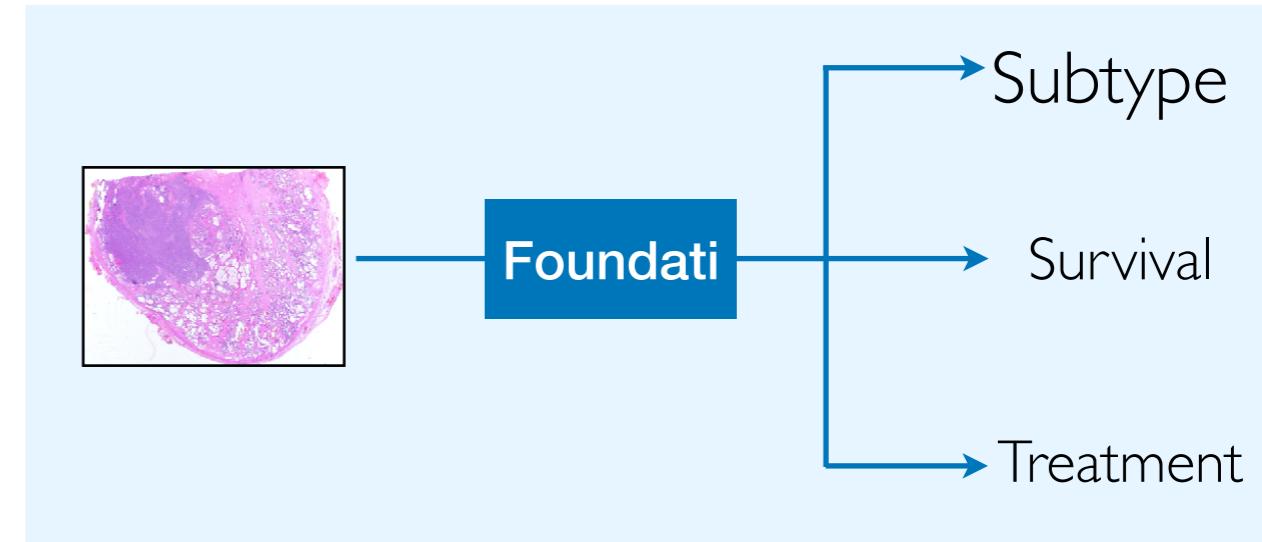
Multi-modal foundation model (2023)

One model takes different inputs



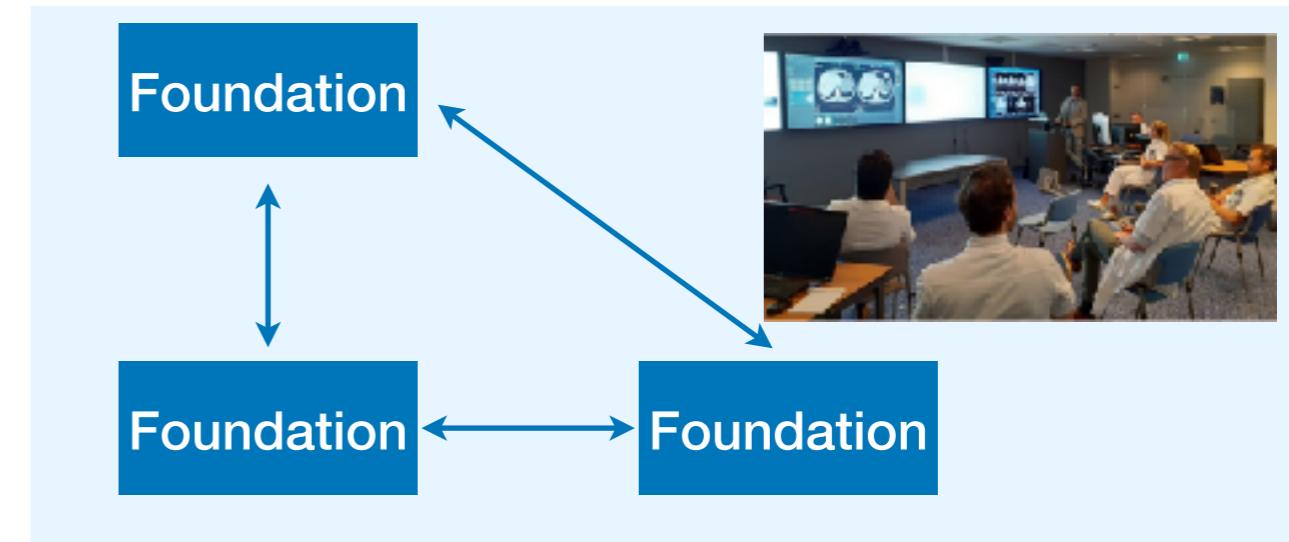
Foundation model (2022)

One model for all tasks



Multi-agent (2024)

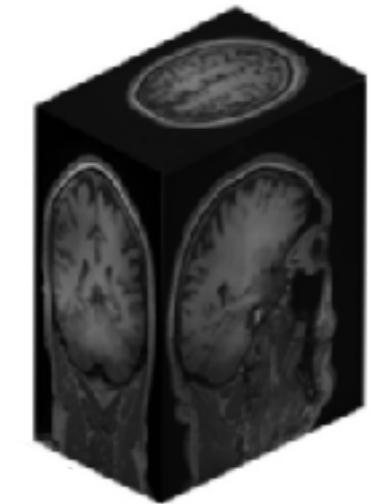
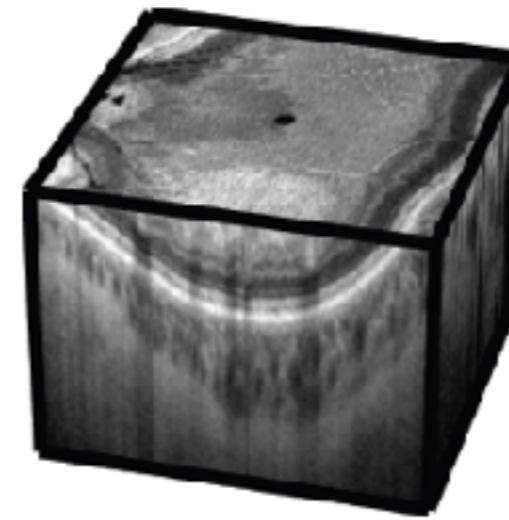
Integrate multiple foundation models



Lots of medical images are 3D

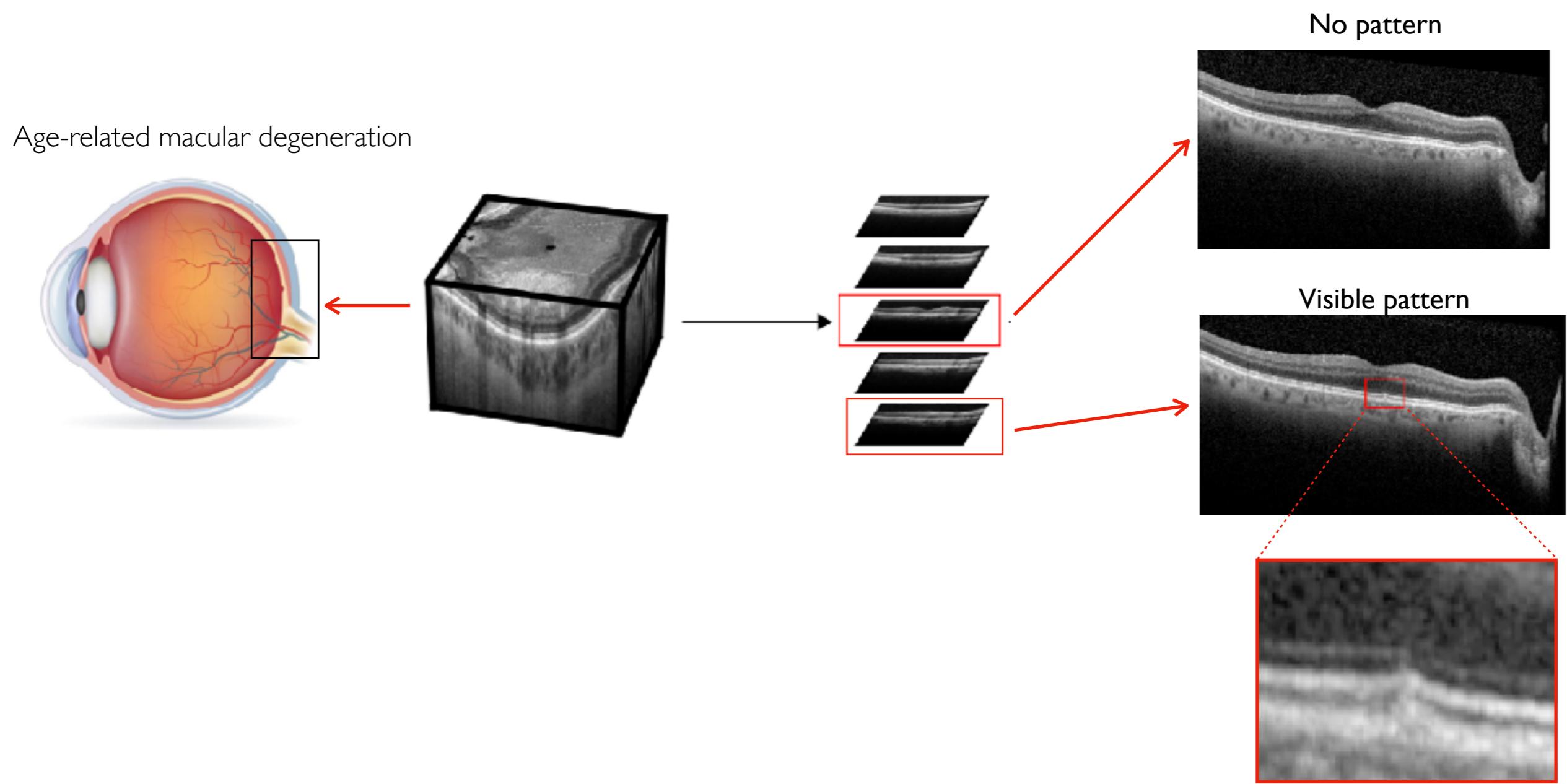


General-domain images: 2D

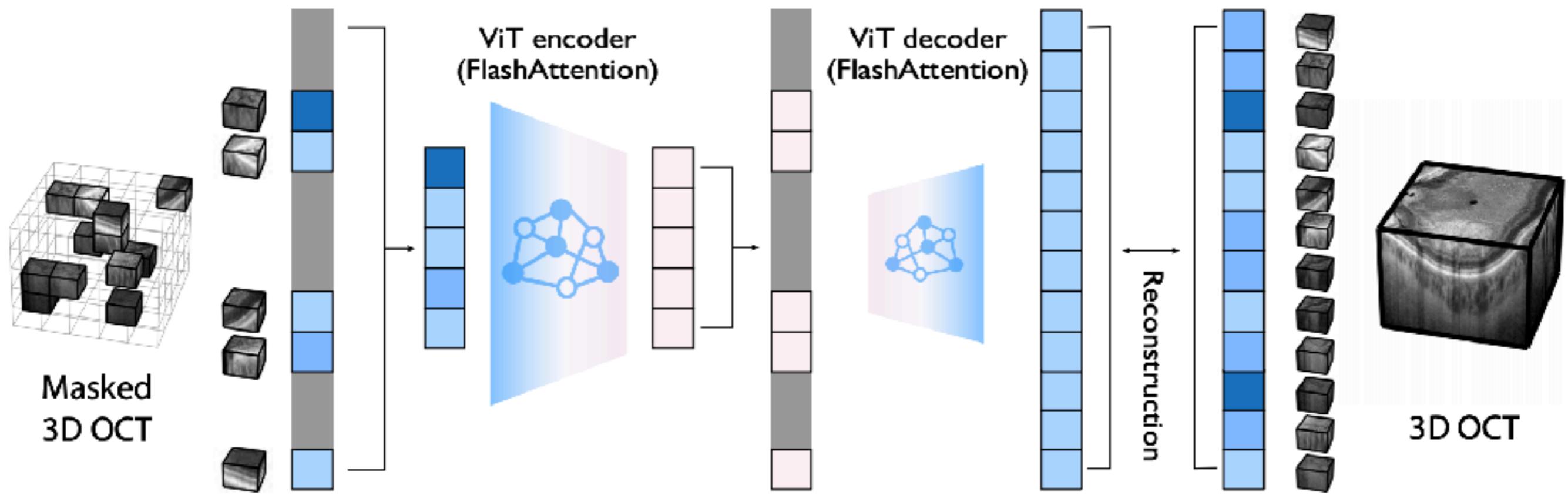


3D biomedical images: CT, MRI, OCT

Disease pattern is very small and hard to detect



A GenAI framework for 3D medical imaging: MAE + FlashAttention

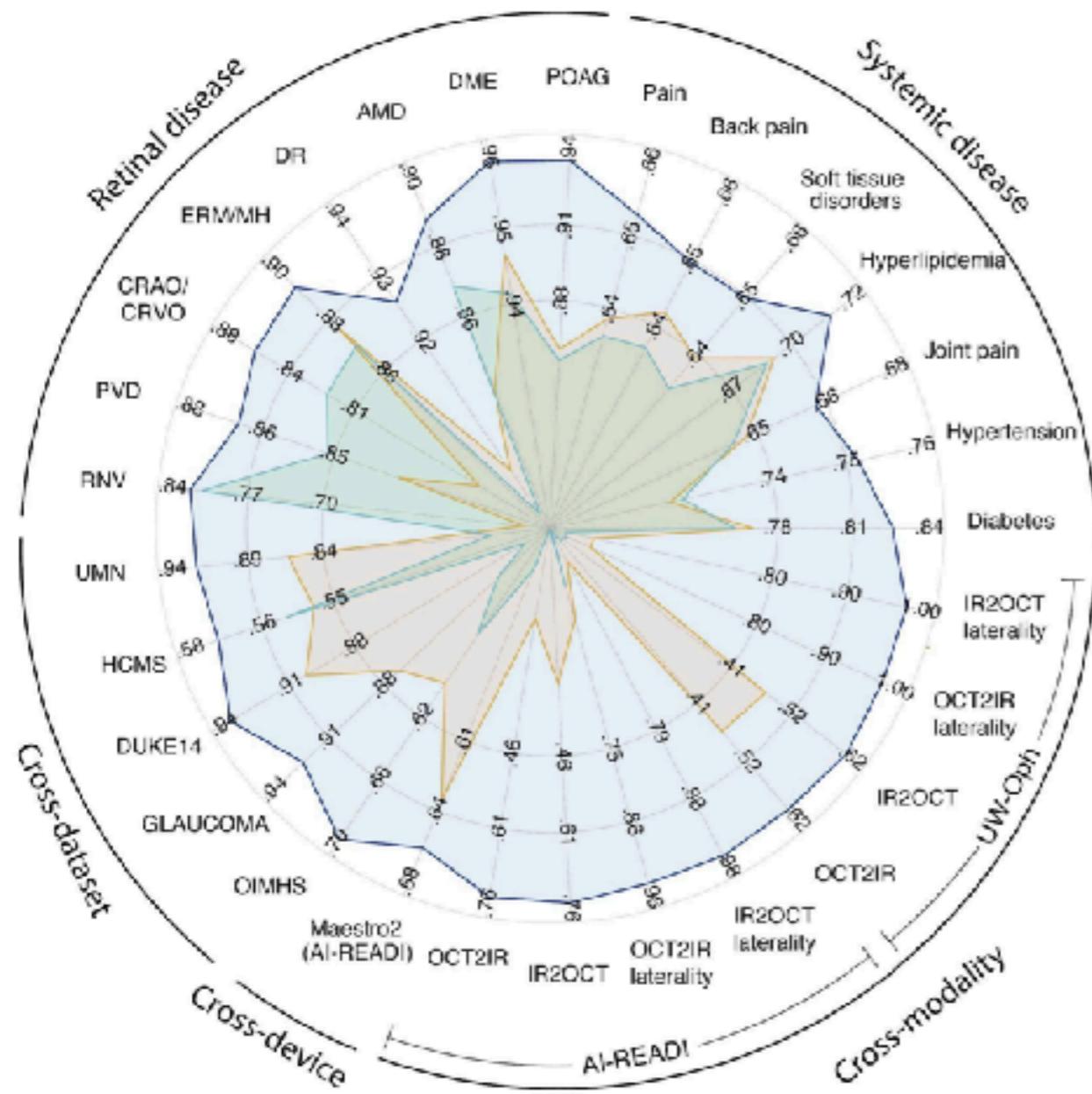


Convert a 3D volume to a **long sentence** of small cubes

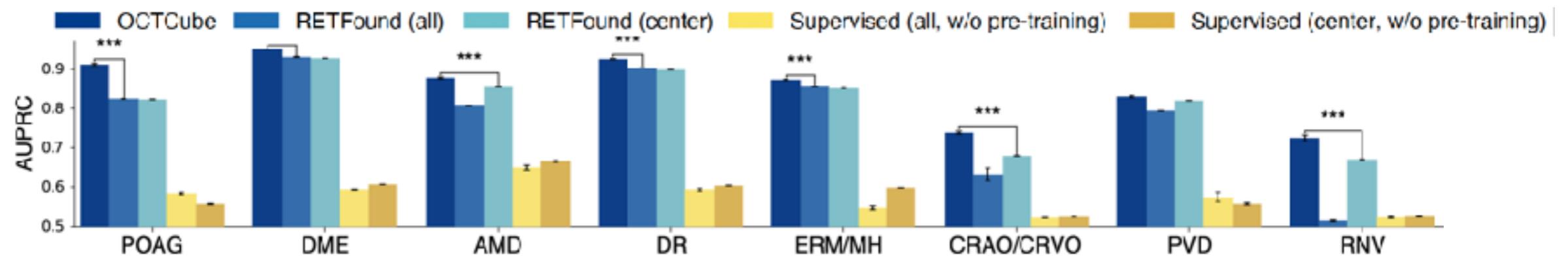
The first 3D OCT foundation model trained from 26,605 patients

Best performance on all 29 tasks

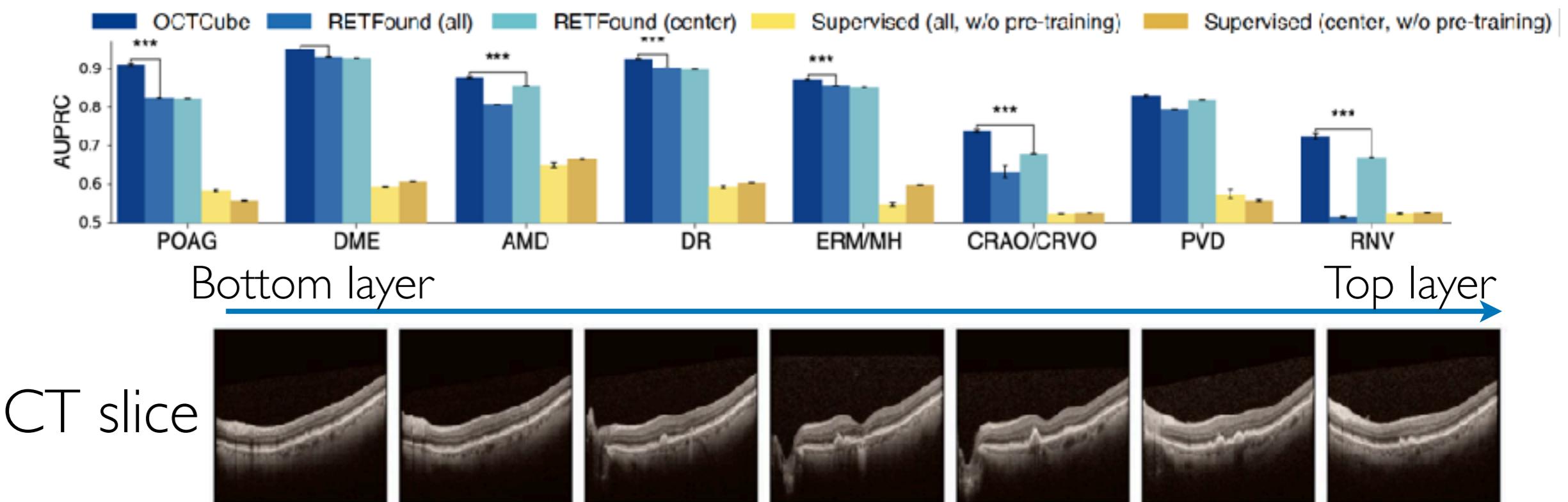
— OCTCube — RETFound (all) — RETFound (center)



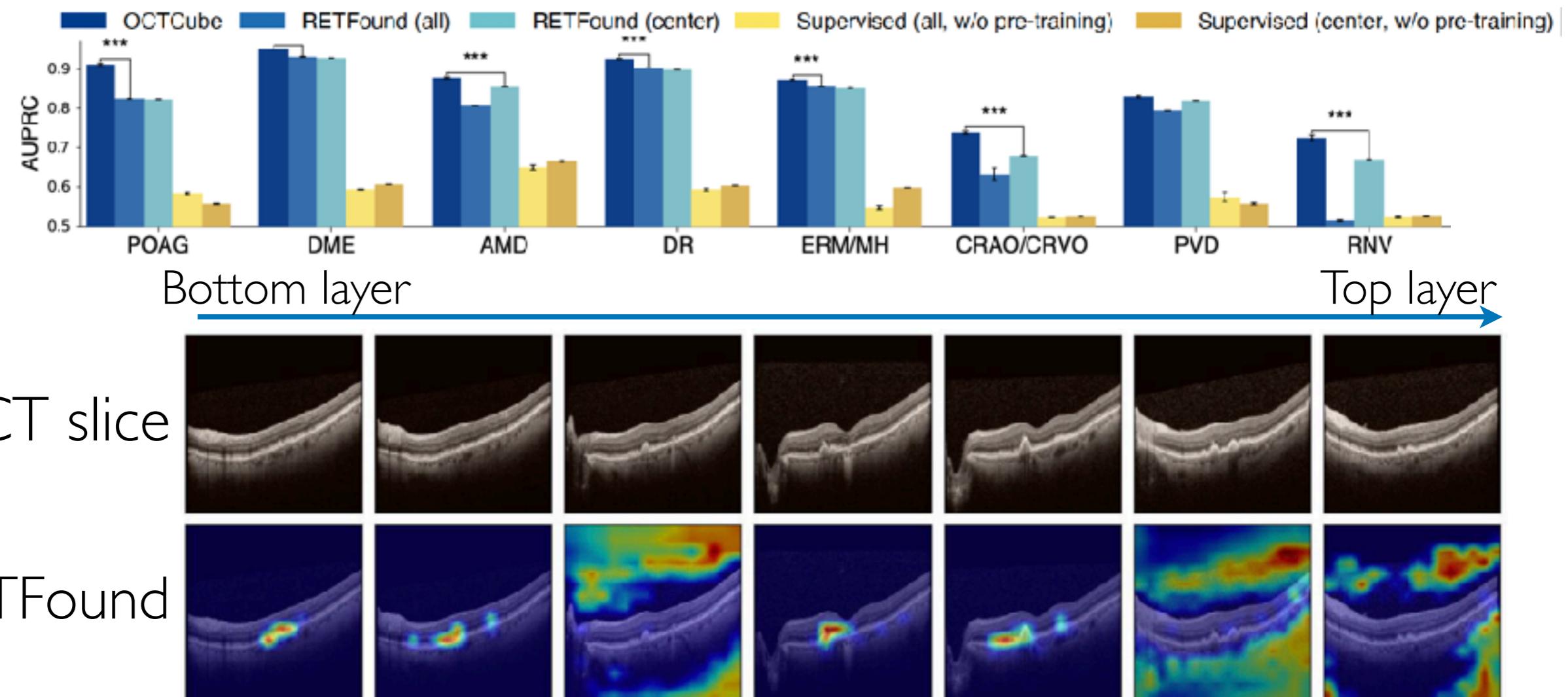
3D model offers accurate and interpretable predictions for retinal diseases



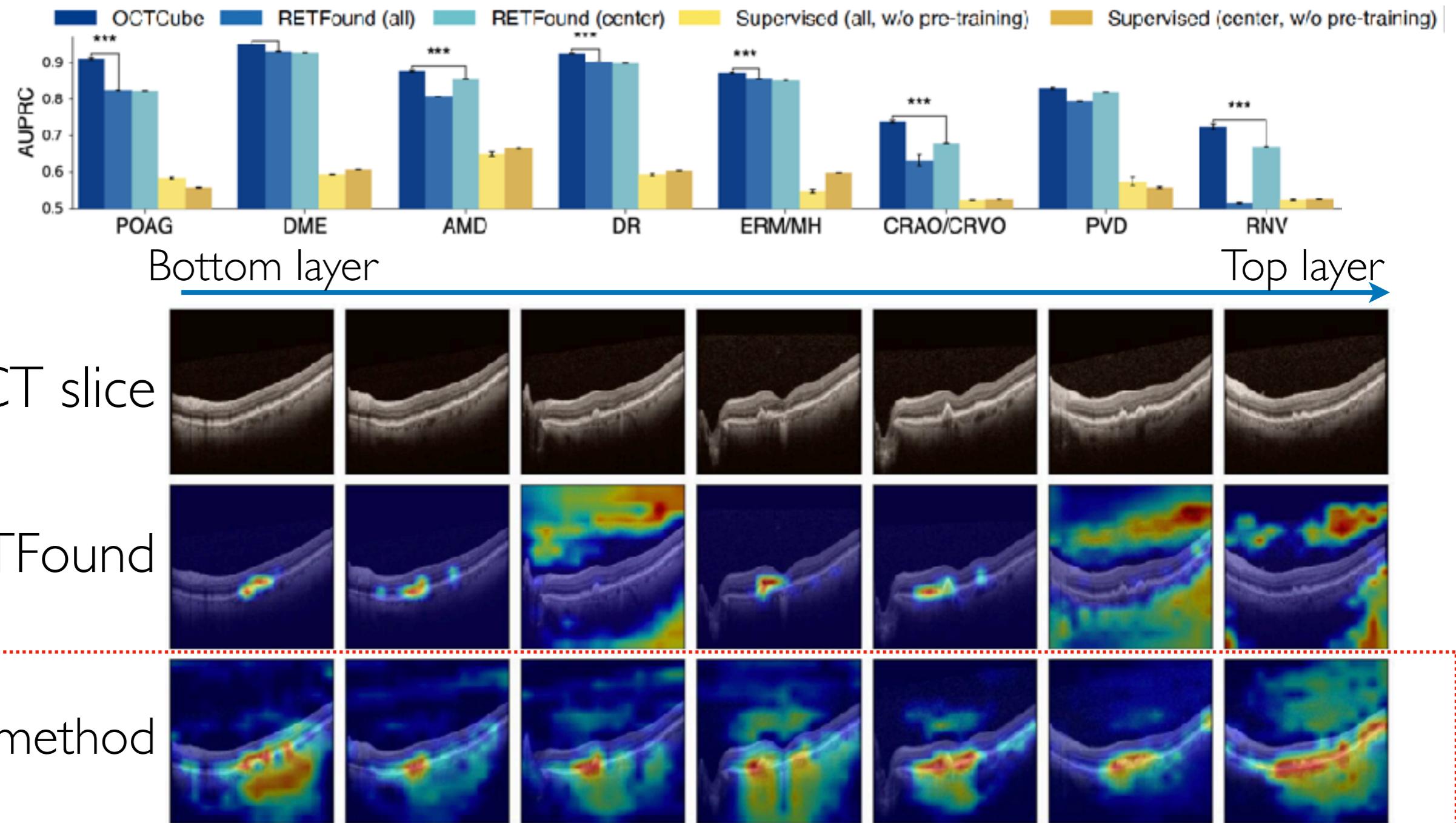
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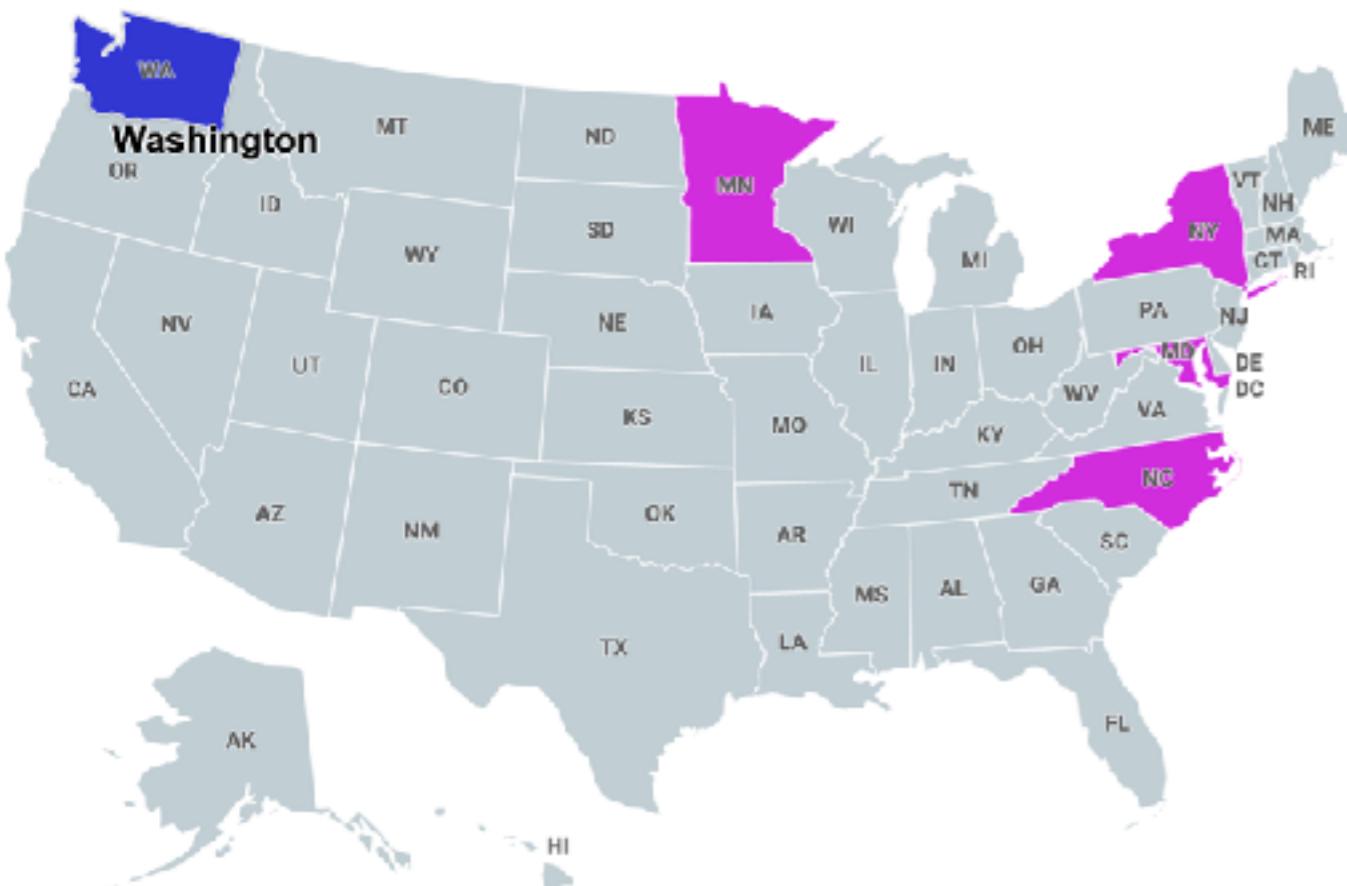
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3D model offers accurate and interpretable predictions for retinal diseases

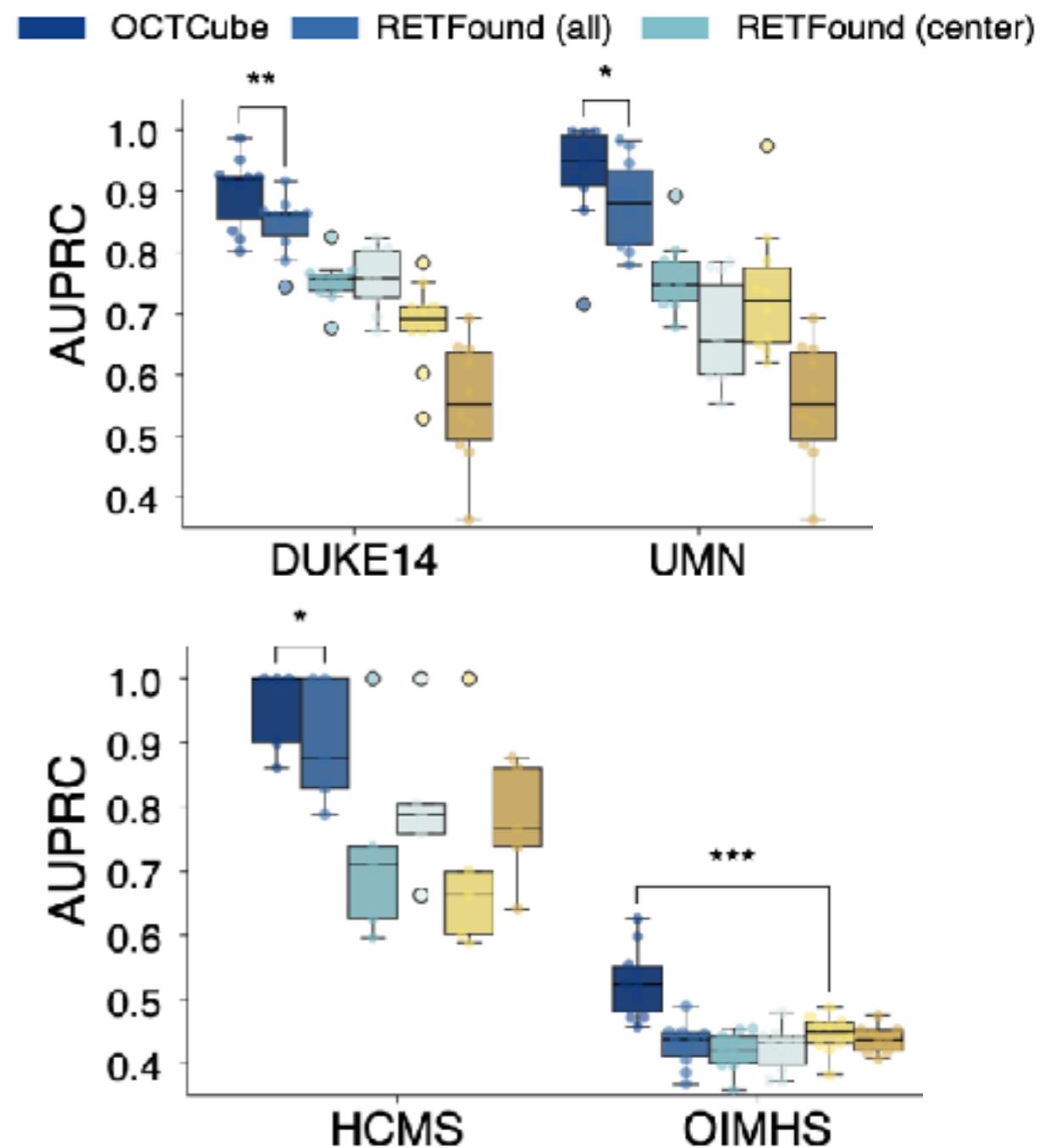


3D model is better at generalization: Cross-cohort prediction at Duke, University of Minnesota, Johns Hopkins, NYU



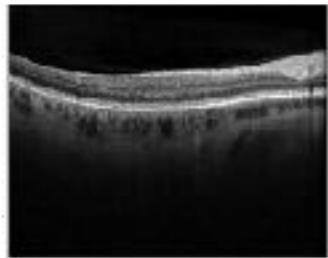
Training

Test

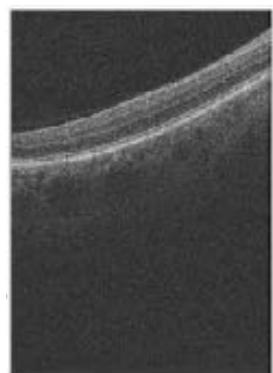


3D model enables cross-device prediction

Heidelberg Spectralis

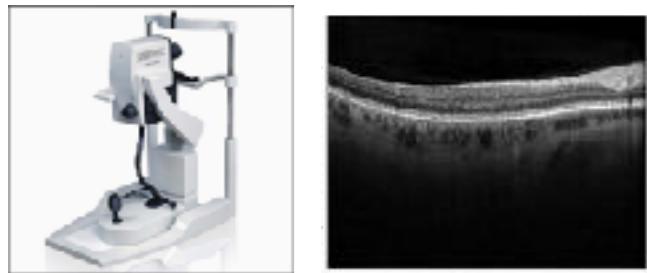


Topcon Maserstro2



3D model enables cross-device prediction

Heidelberg Spectralis



Pretrai



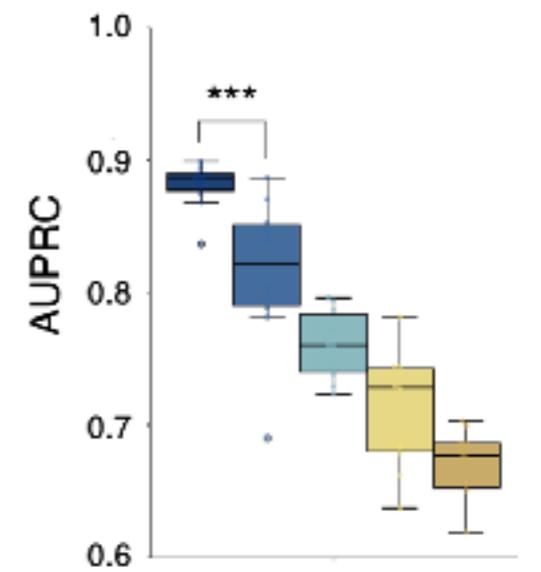
Heidelberg Spectralis

■ OCTCube ■ RETFound (all) ■ RETFound (center)

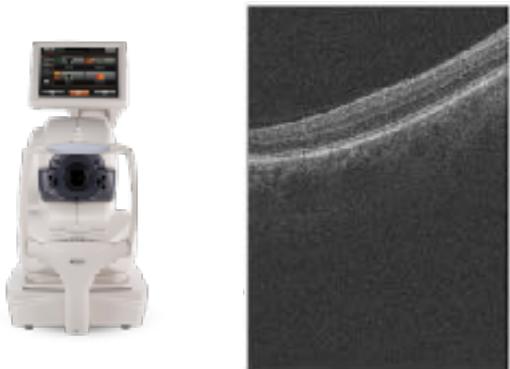
Fine-



Topcon Mastro2



Topcon Maserstro2



Pretrai

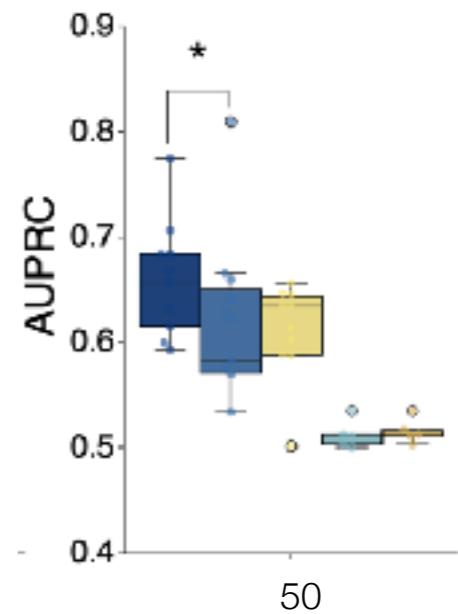


Heidelberg Spectralis

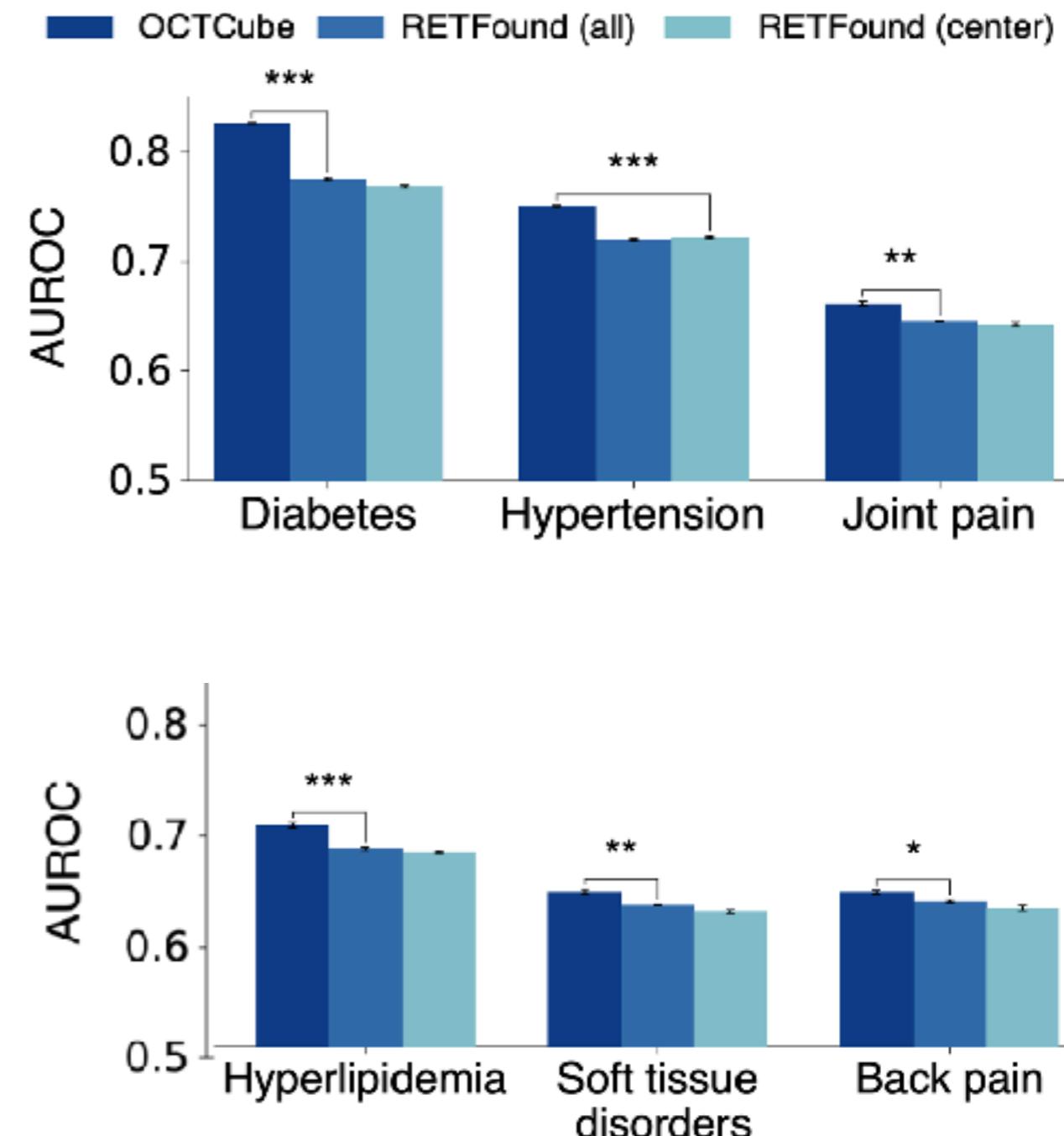
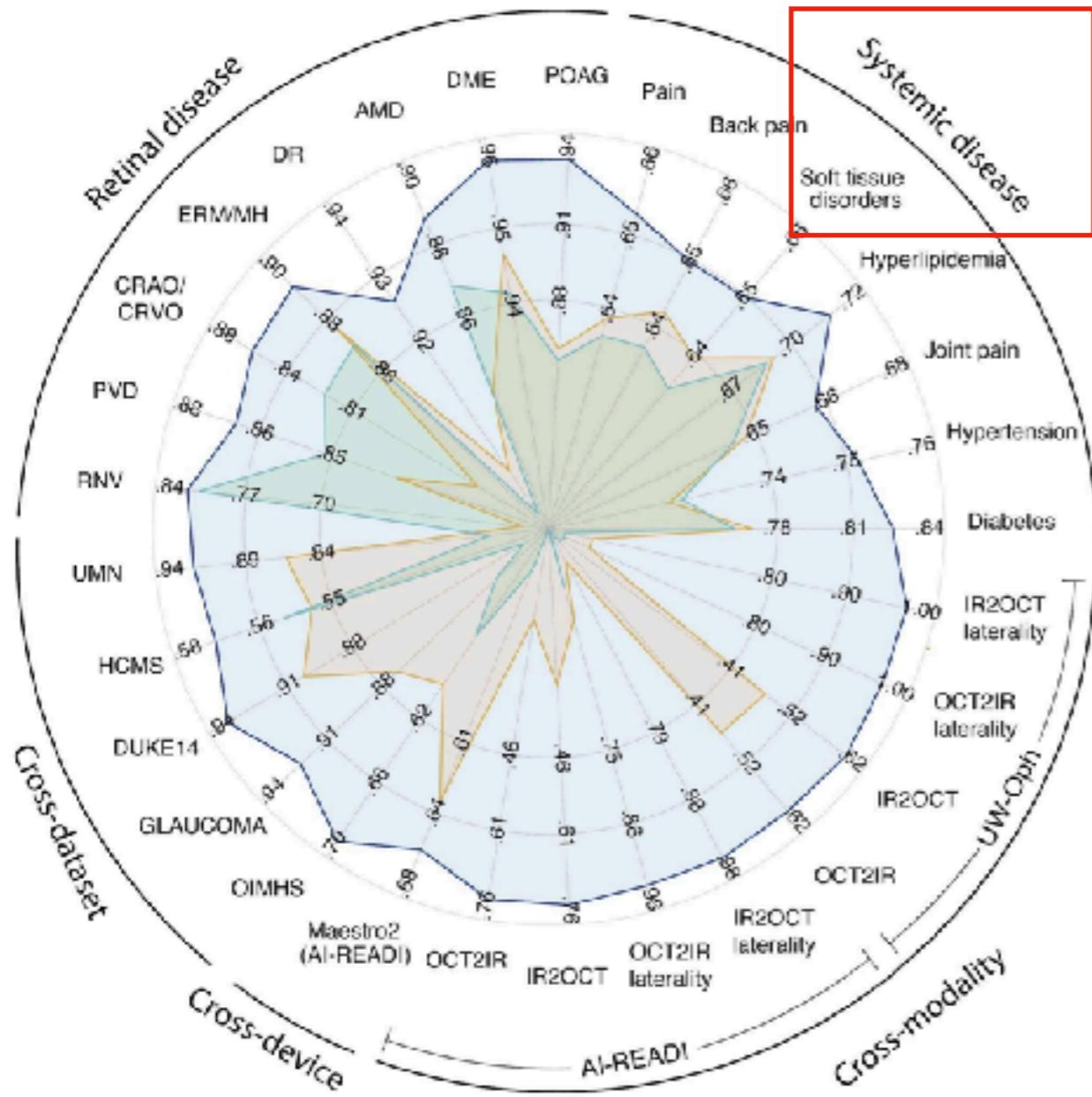
Fine-



Zeiss cirrus

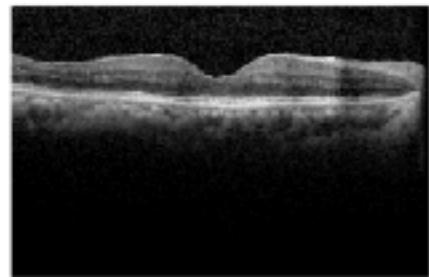


Predict systemic diseases

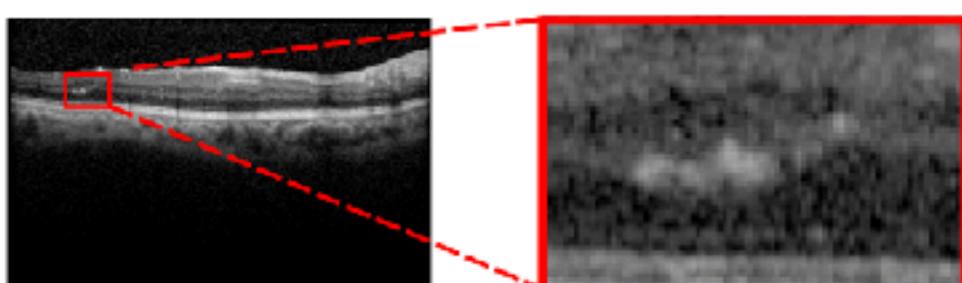
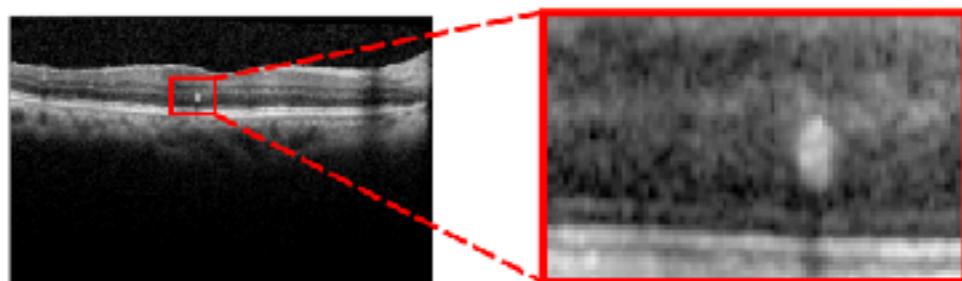


One-year early prediction of diabetes

1st visit: **2D model** cannot identify diabetes

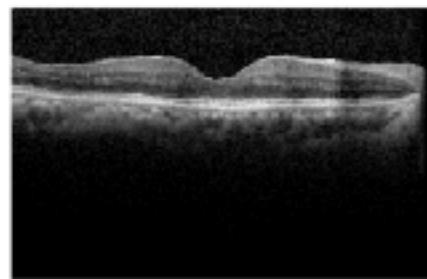


1st visit: **3D model** detects diabetes signal

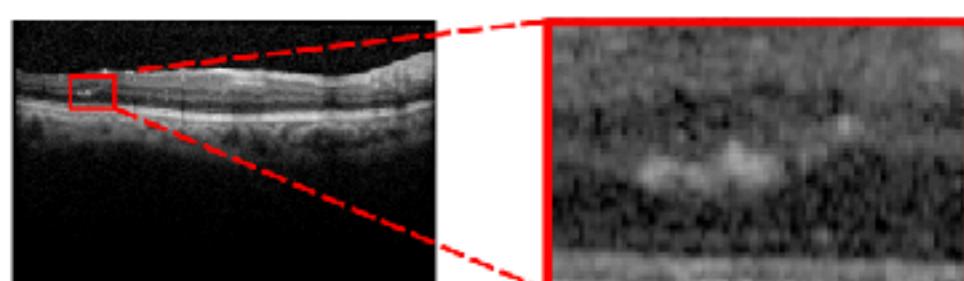
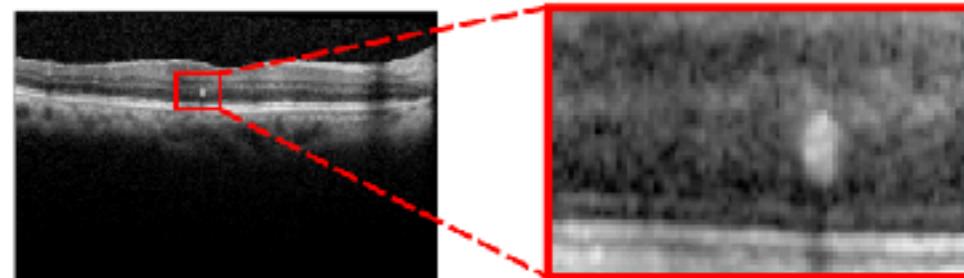


One-year early prediction of diabetes

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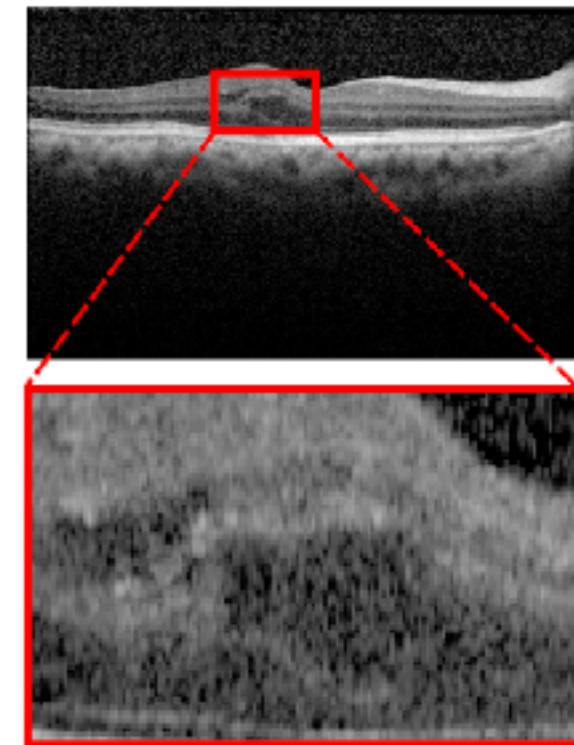
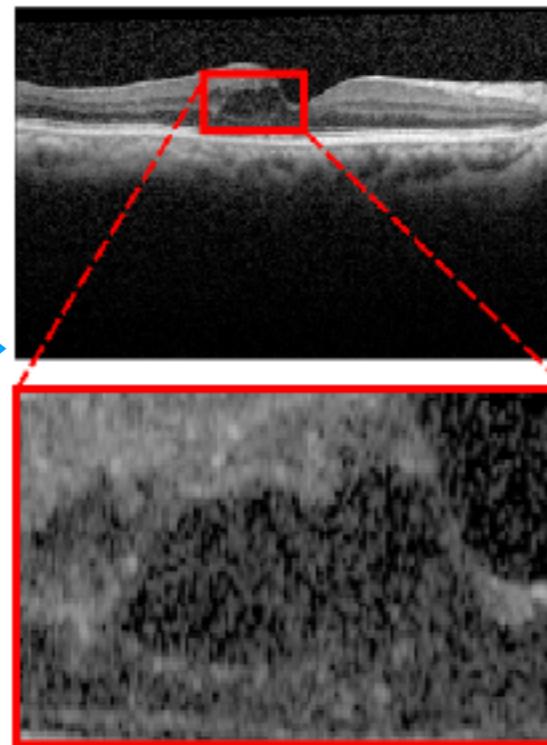


1st visit: **3D model** detects diabetes signal



I year later

2D model detects diabetes



Today's talk: 3 parts

1. Pathology foundation model
2. 3D retinal foundation model

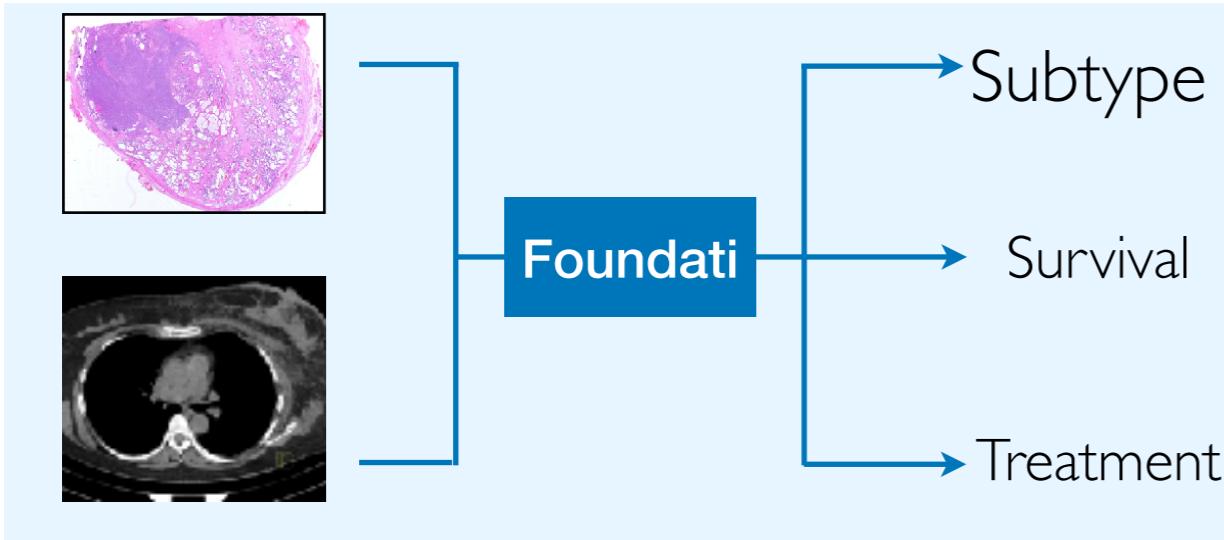


3. A multi-modal foundation model integrating 9 imaging modalities



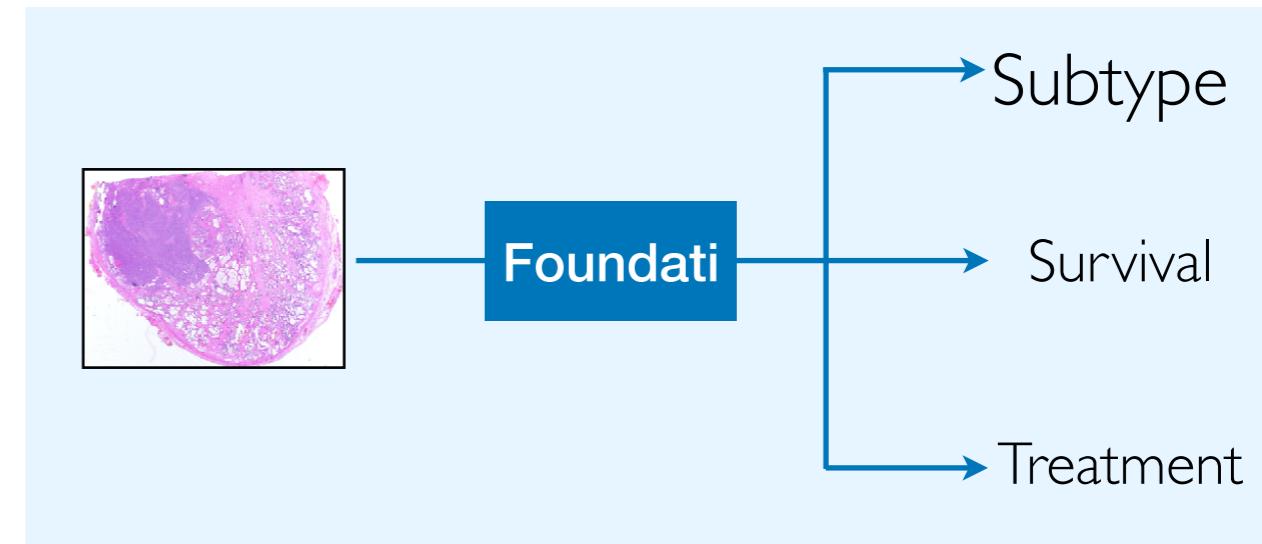
Multi-modal foundation model (2023)

One model takes different inputs



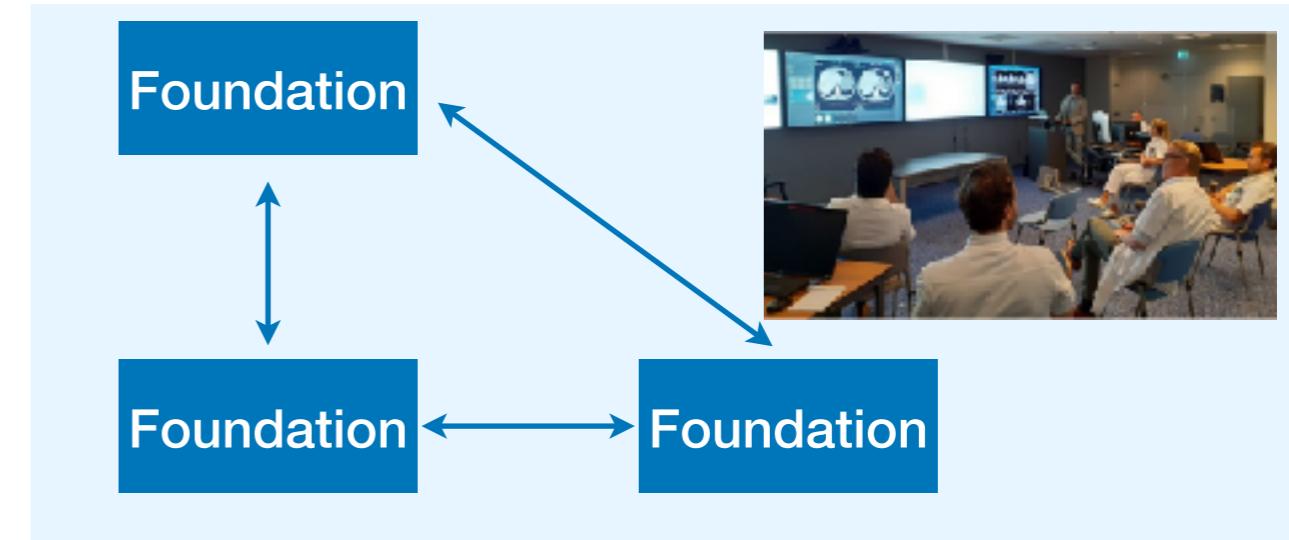
Foundation model (2022)

One model for all tasks

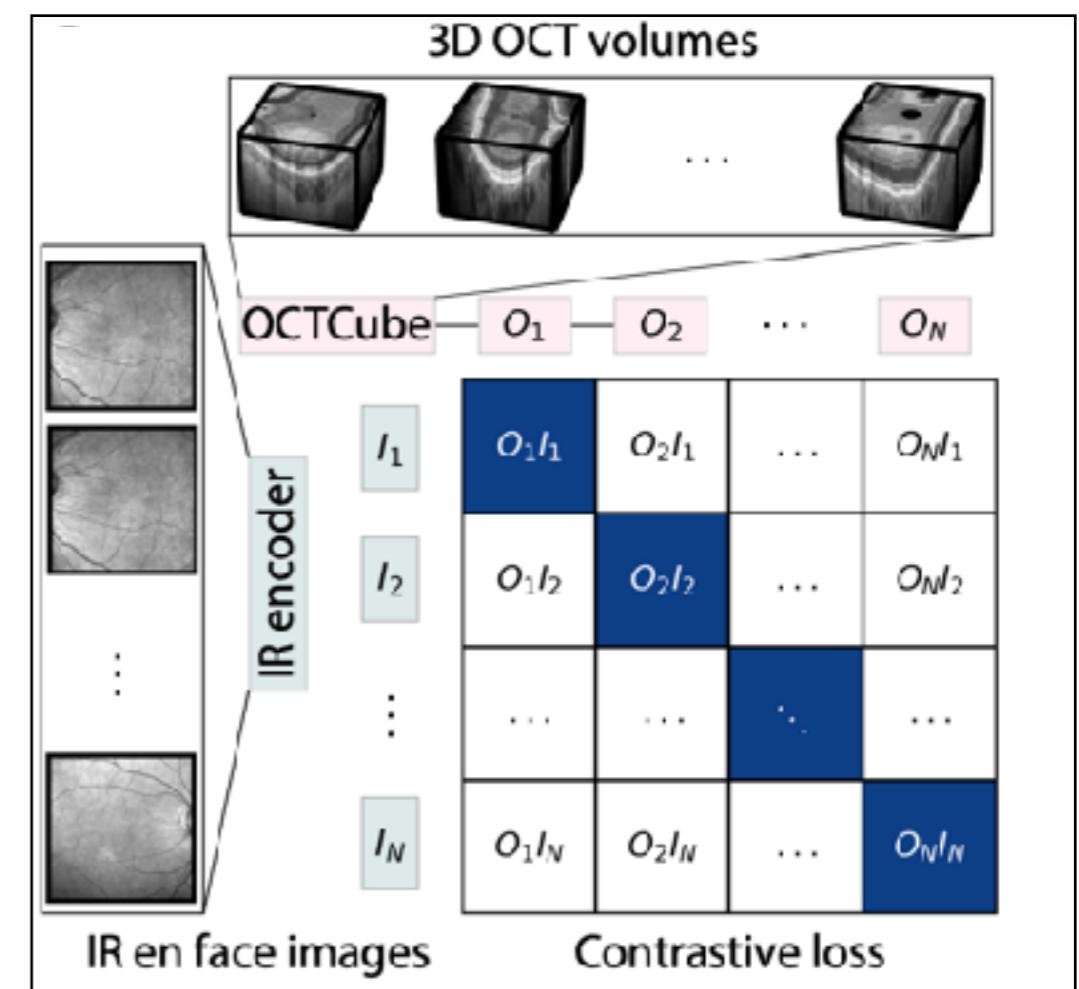
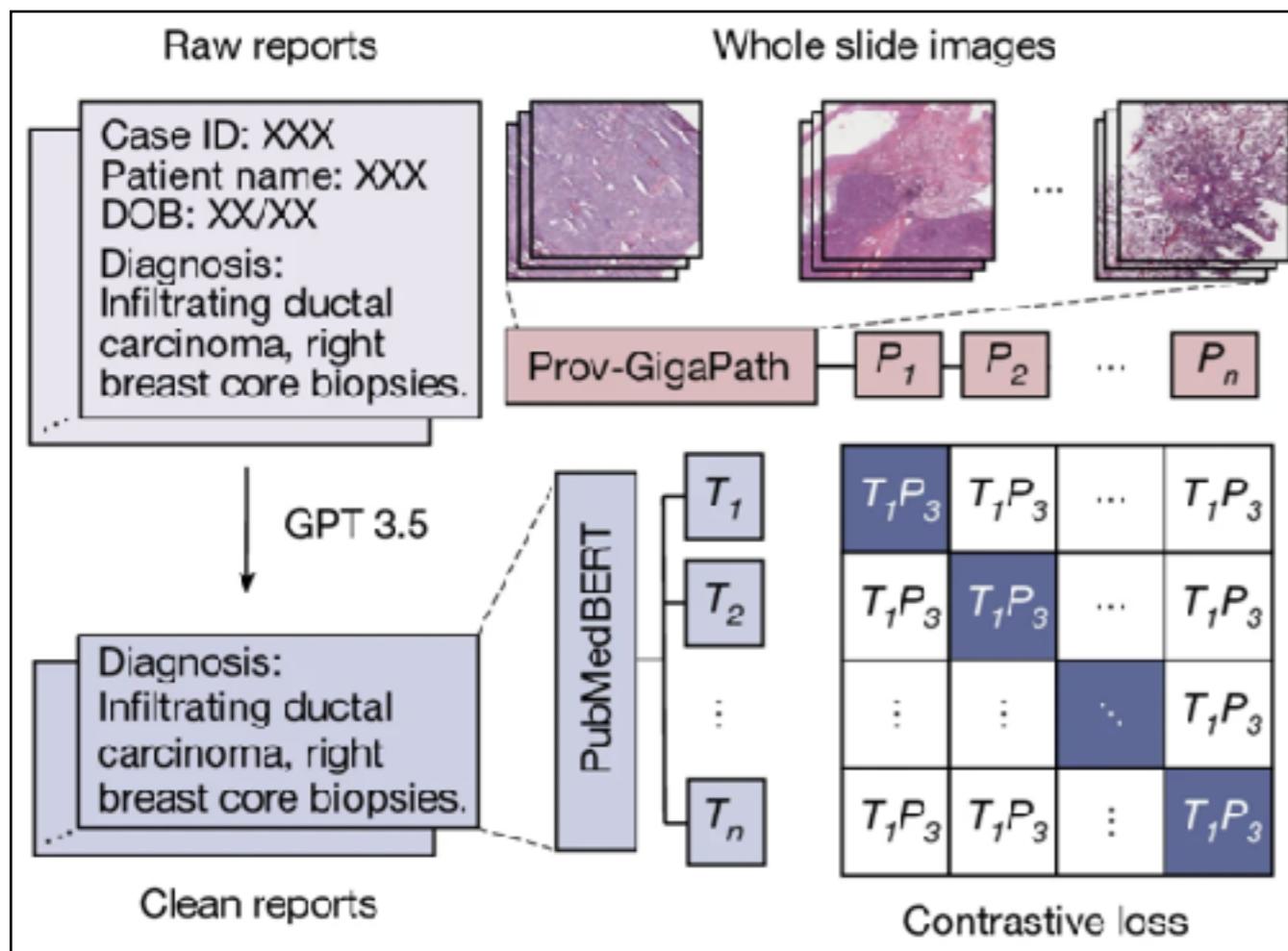


Multi-agent (2024)

Integrate multiple foundation models

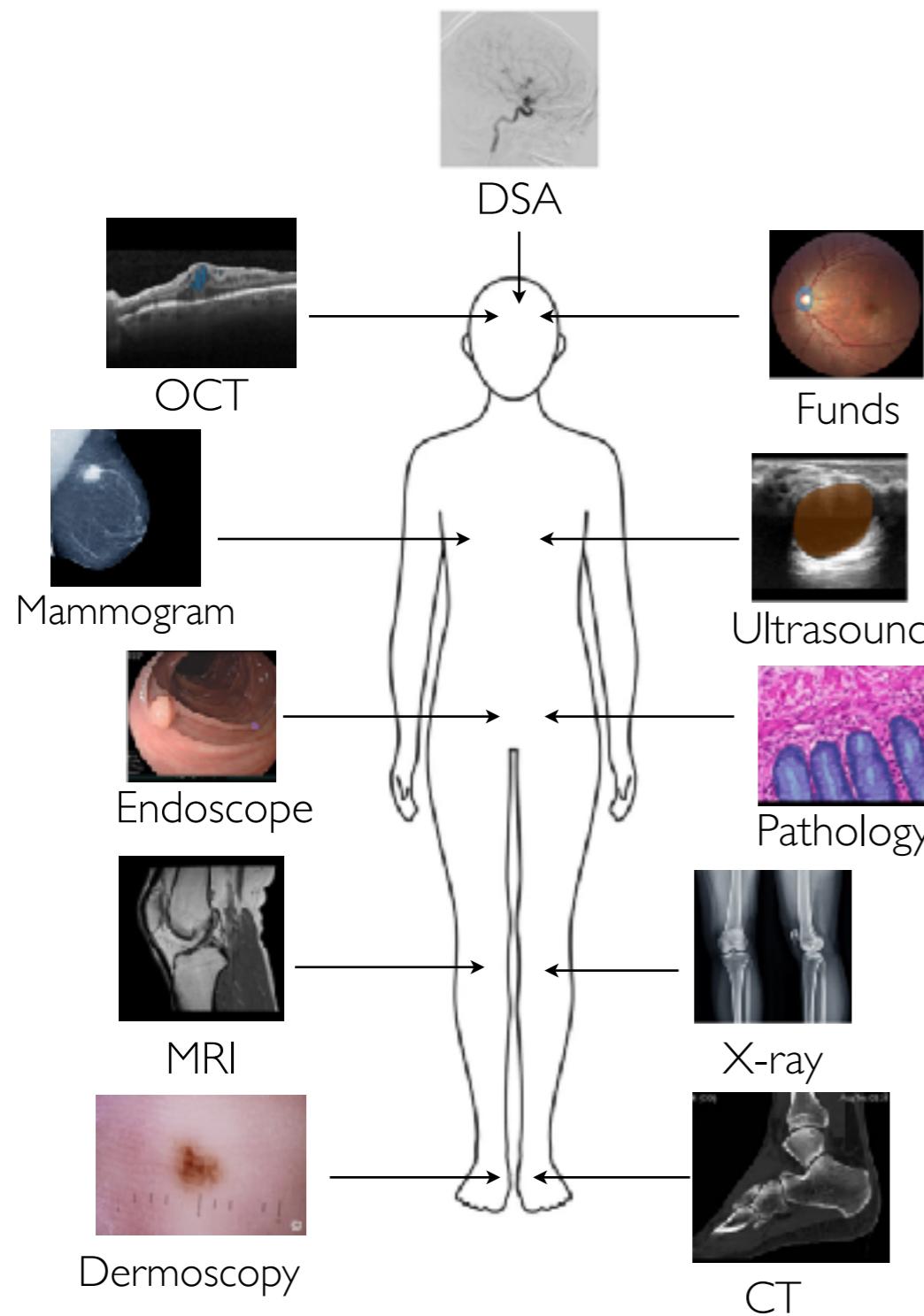


Multi-modality analysis in GigaPath and OCTCube



Medical report + Pathology image

OCT image + IR image



Existing cross-modal framework is
Limited to two modalities

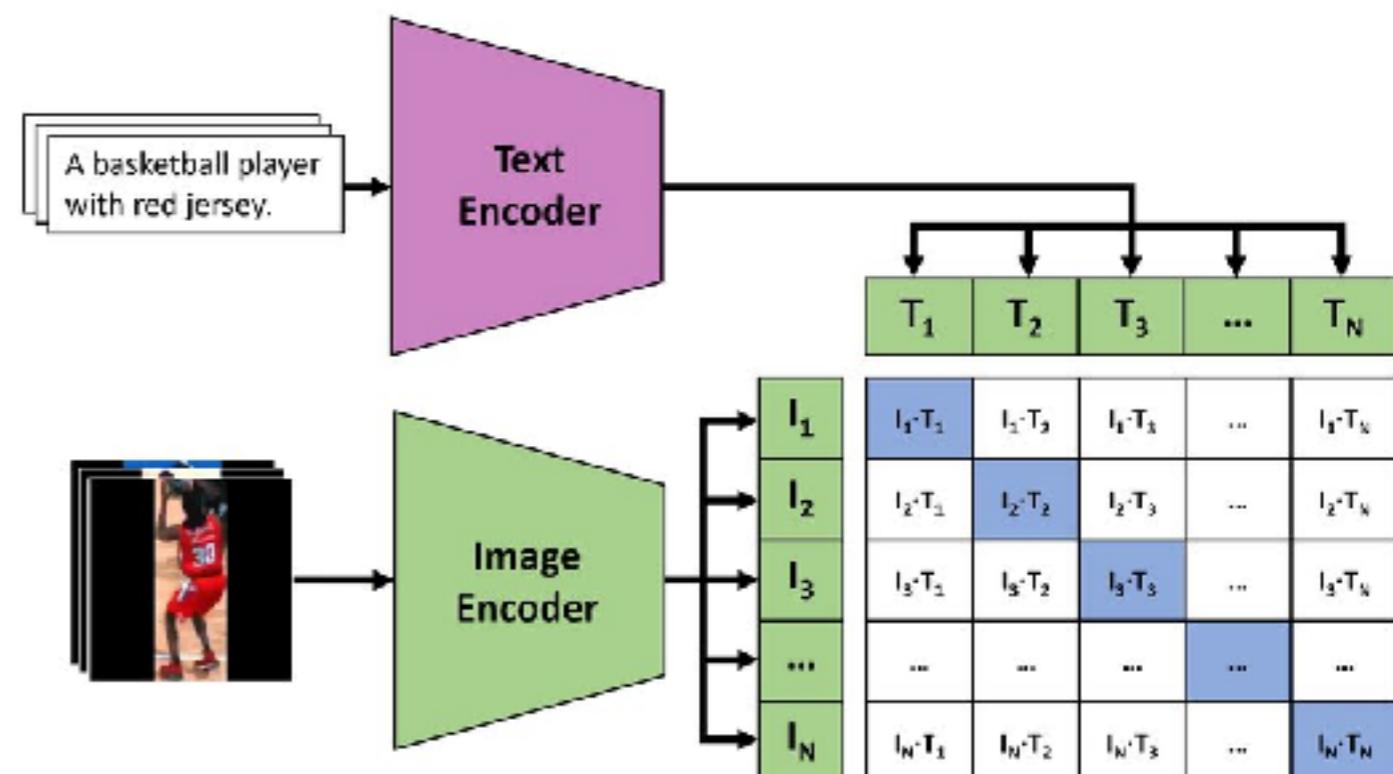
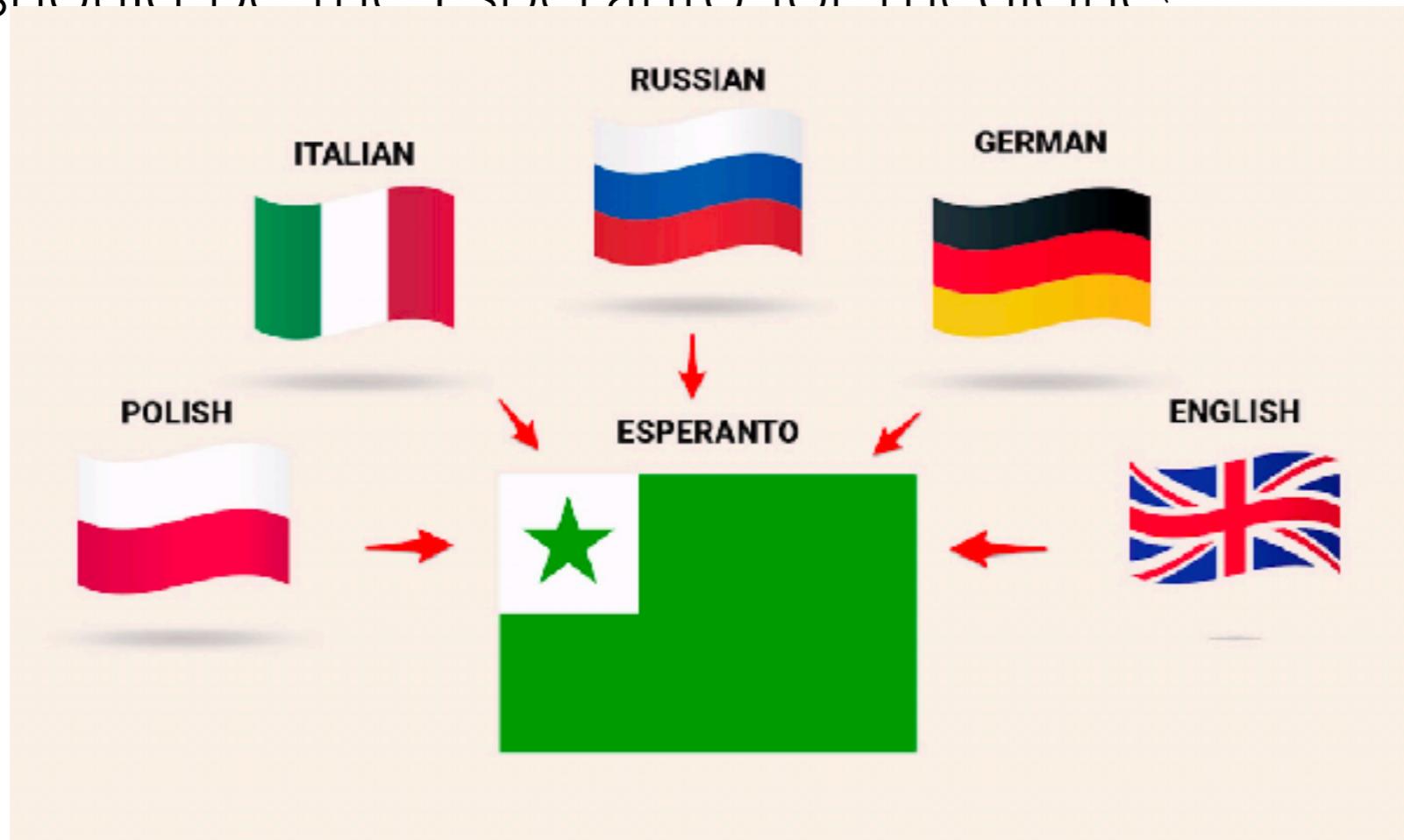


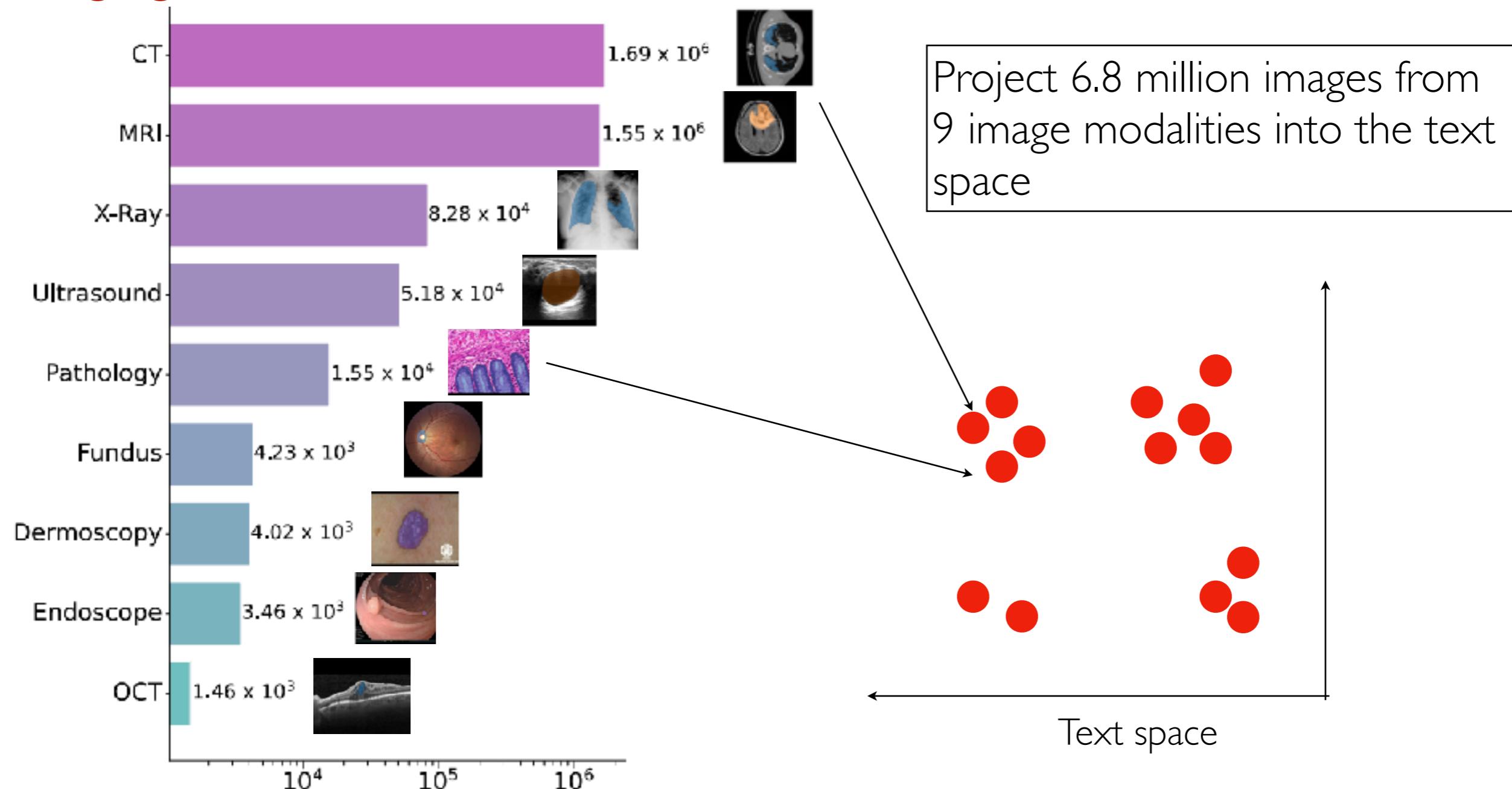
Image from CLIP-Reldent

Our solution for integrating all image modalities

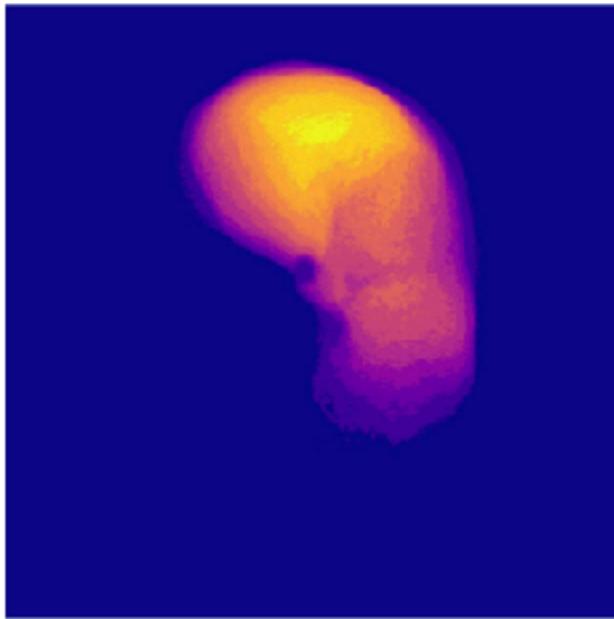
- Build one foundation model for each modality, then project different models into the same space
- What should be the Esperanto for medicine?



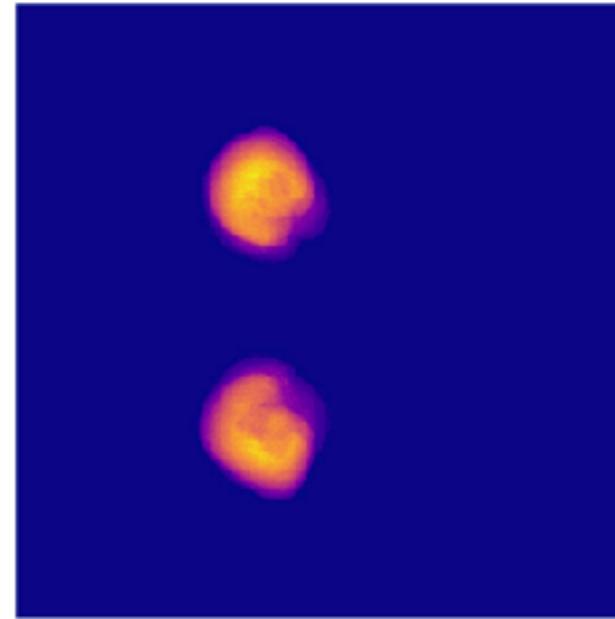
BiomedParse: use human language as the Esperanto to integrate medical imaging modalities



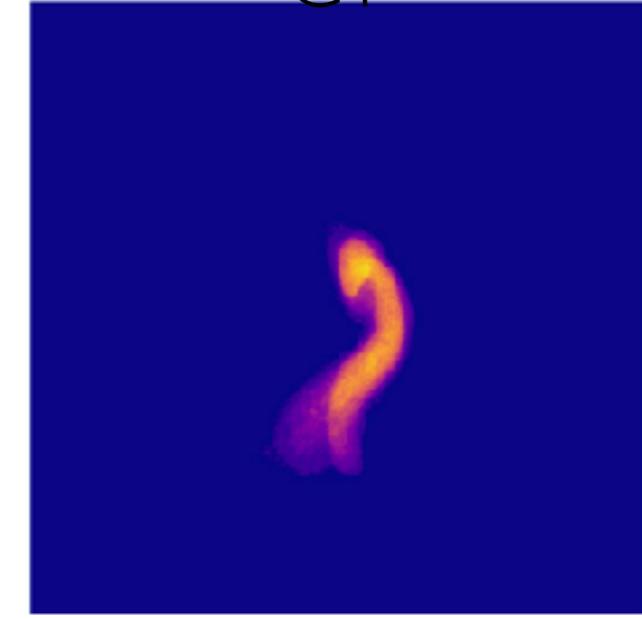
Liver in abdomen CT



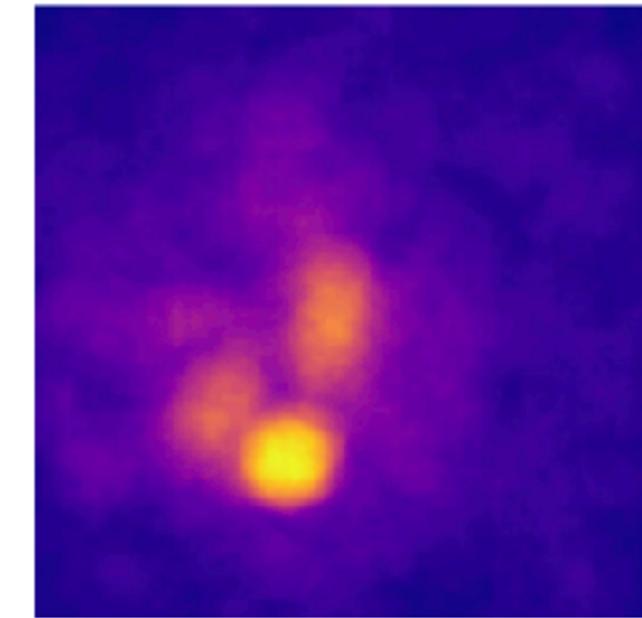
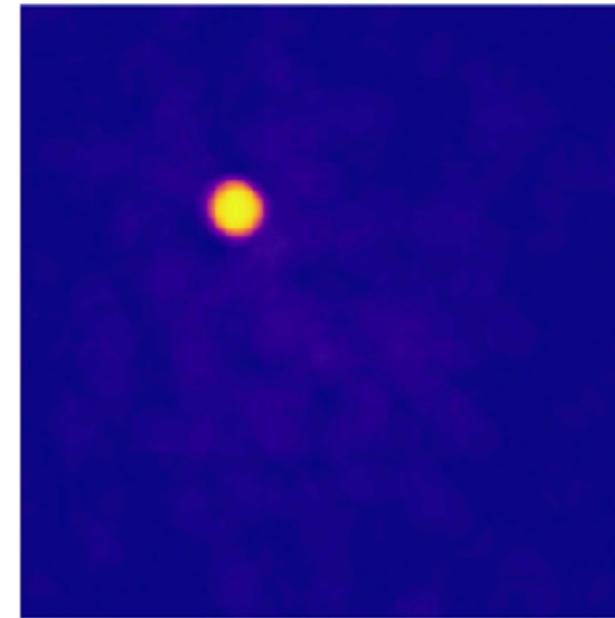
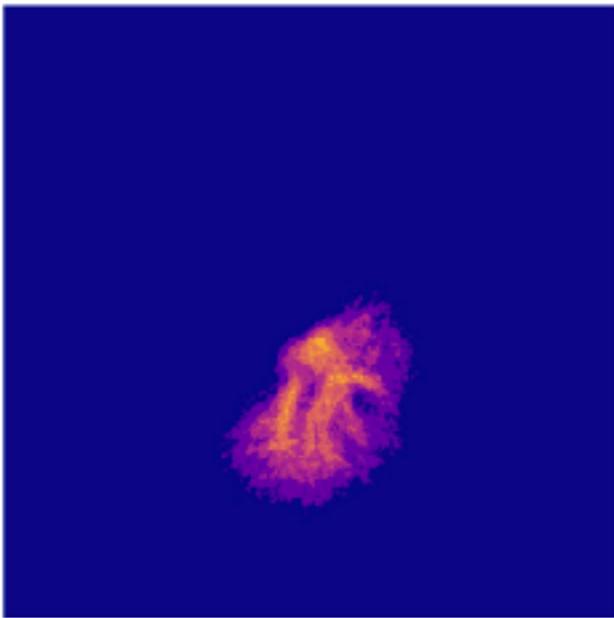
Kidney in abdomen CT



Pancreas in abdomen
CT



Liver vessel in abdomen CT | Inflammatory cells in pathology | Neoplastic cells in pathology



A foundation model for joint segmentation, detection and recognition across 9 modalities

nature methods

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Article | Published: 18 November 2024

A foundation model for joint segmentation, detection and recognition of biomedical objects across nine modalities

[Theodore Zhao](#), [Yu Gu](#), [Jianwei Yang](#), [Naoto Usuyama](#), [Ho Hin Lee](#), [Sid Kiblawi](#), [Tristan Naumann](#),
[Jianfeng Gao](#), [Angela Crabtree](#), [Jacob Abel](#), [Christine Moung-Wen](#), [Brian Piening](#), [Carlo Bifulco](#), [Mu Wei](#)
✉, [Hoifung Poon](#) ✉ & [Sheng Wang](#) ✉

[Nature Methods](#) (2024) | [Cite this article](#)

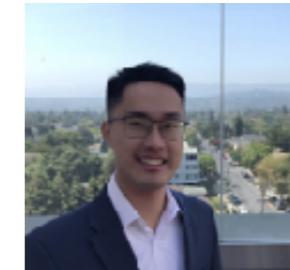
Available as open-source model on Azure AI and Hugging Face



Theodore Zhao



Aiden Gu



Sheng Wang
U of Washington



Mu Wei



Hoifung Poon

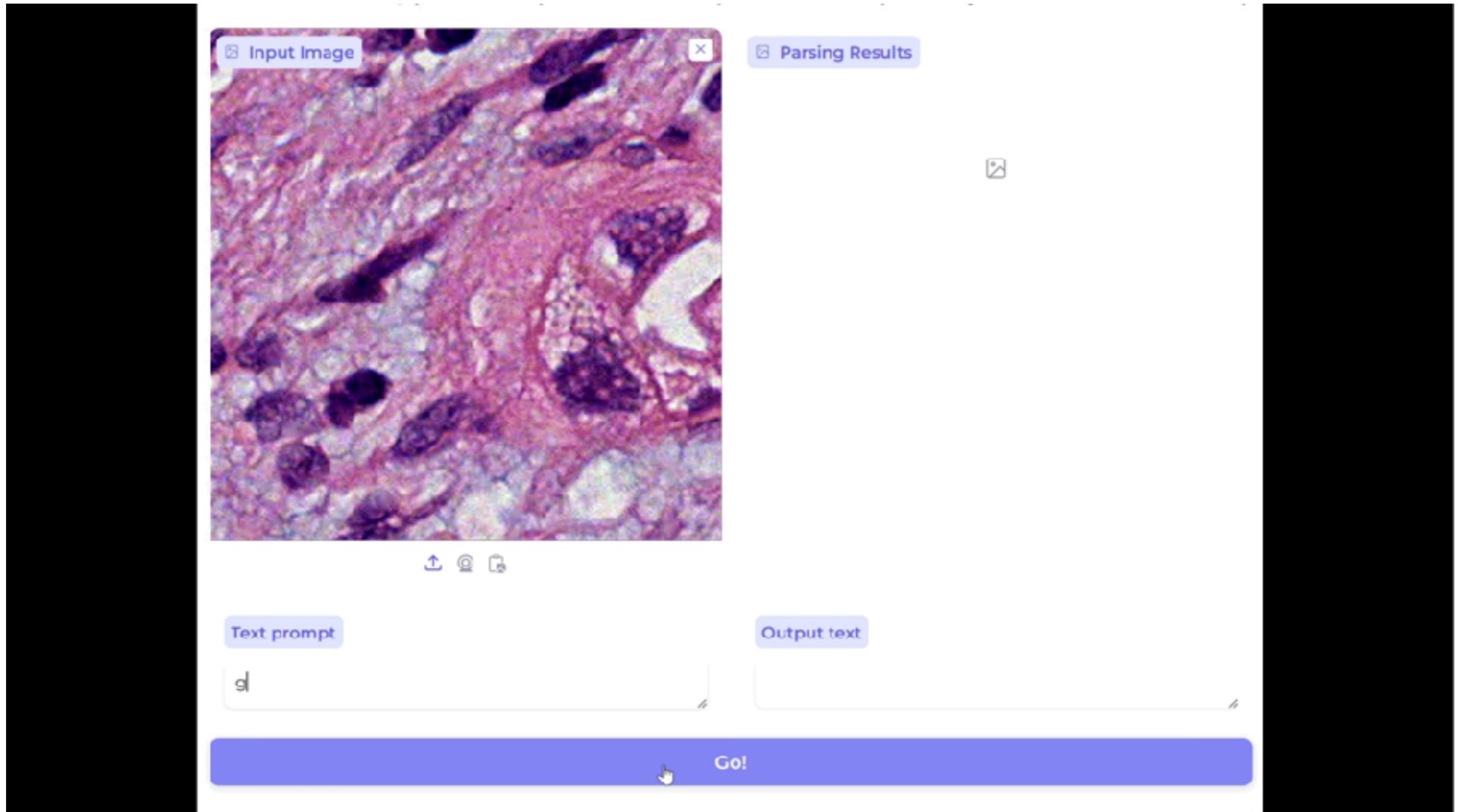
Demol: talk to the AI model to find lung nodule



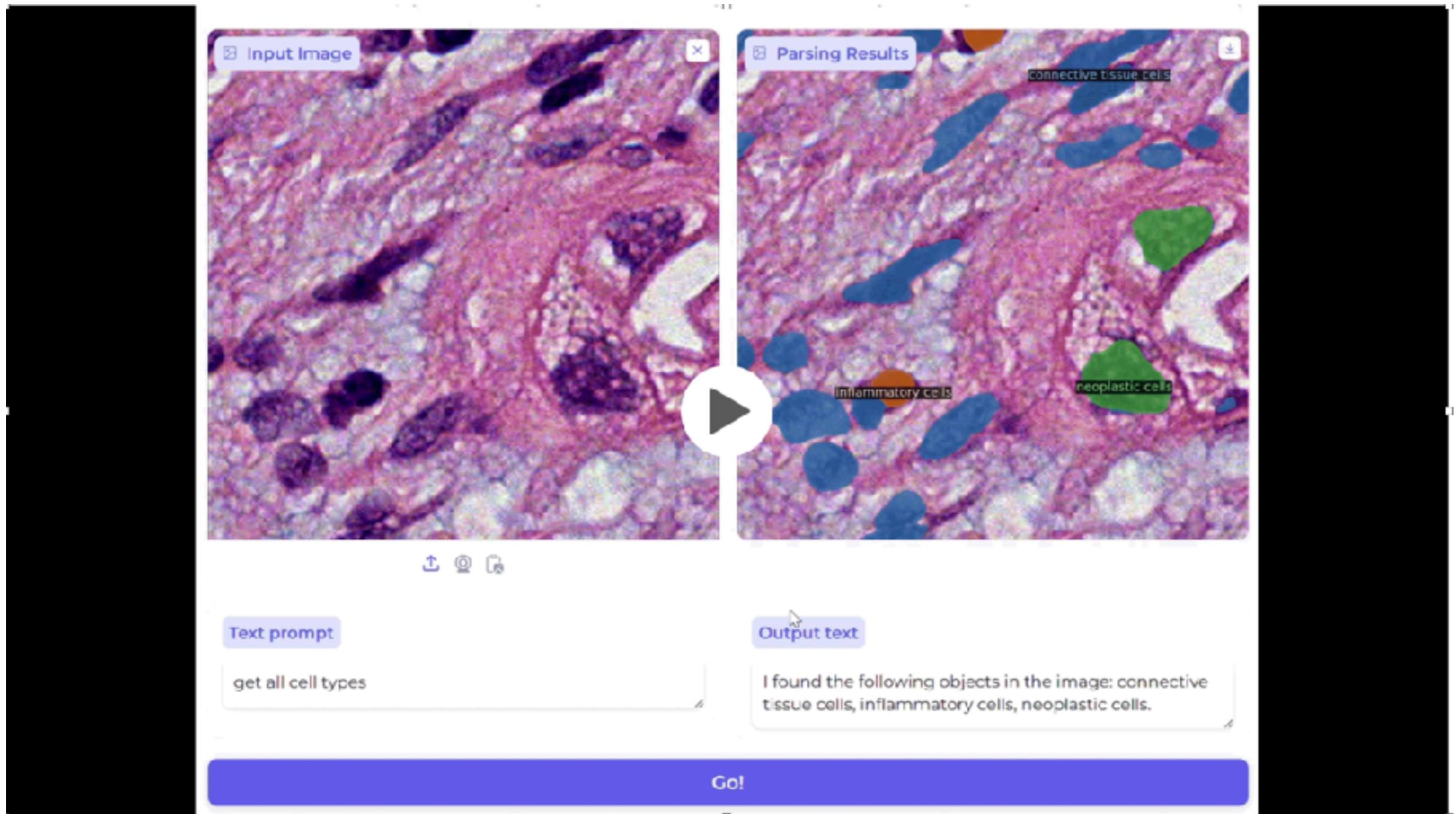
Demol: talk to the AI model to find lung nodule



Demo2: talk to the model to find all cell types

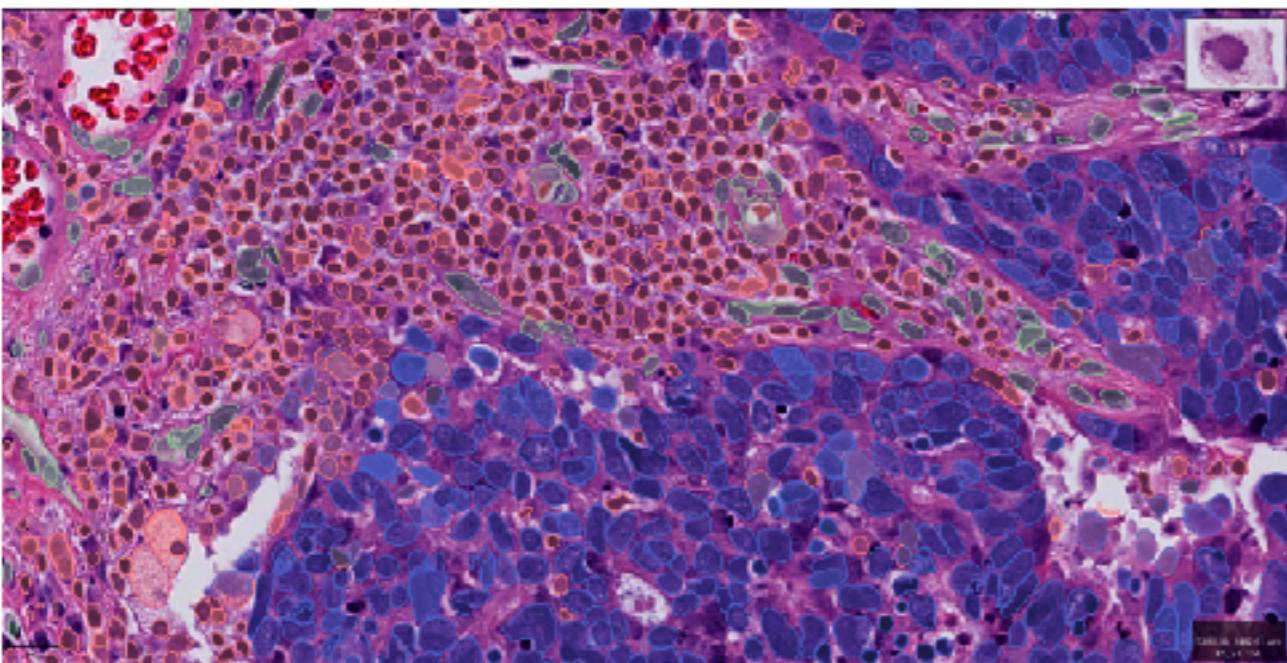


Demo2: talk to the model to find all cell types



0.2 second to segment and label all cells with > 90% consistency

Pathologist annotation

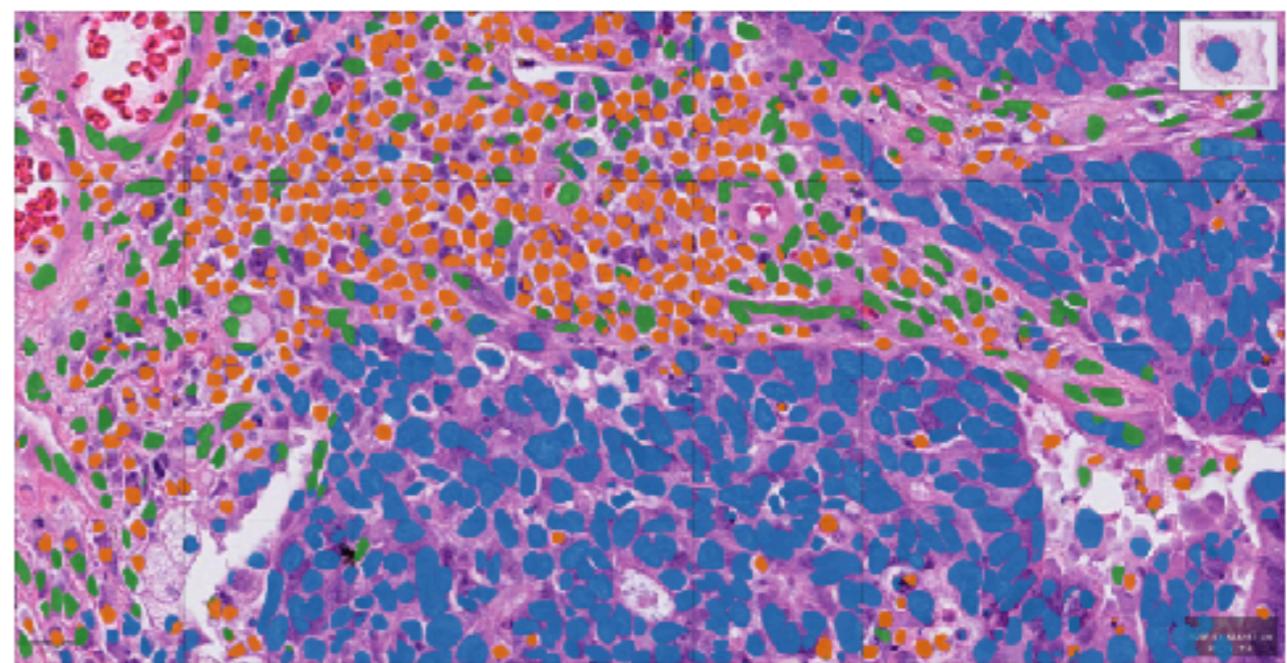


Tumor region

Lymphocyte

Stroma

BiomedParse prediction



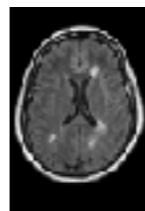
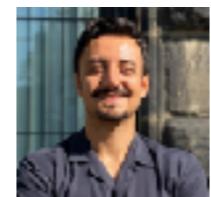
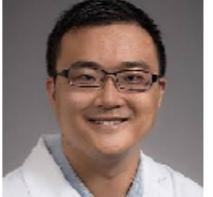
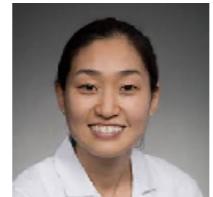
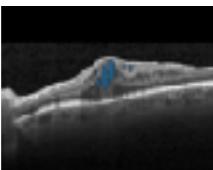
Neoplastic cells

Inflammatory cells

Connective tissue cells

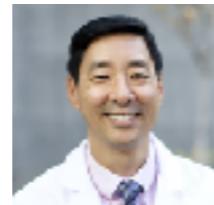
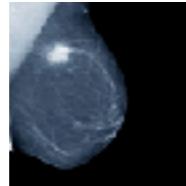
Data-raising from Collaborators at UW School of Medicine

27k OCT
images for
retinal diseases



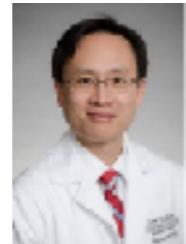
100k brain MRI for stroke, Parkinson, brain cancer

50k Mammogram
for breast cancer



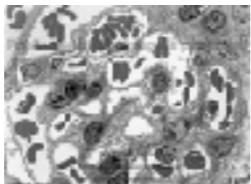
Dr. Christopher Lee (Radiology)

100k CT for
heart
transplant



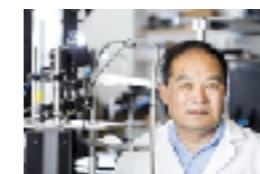
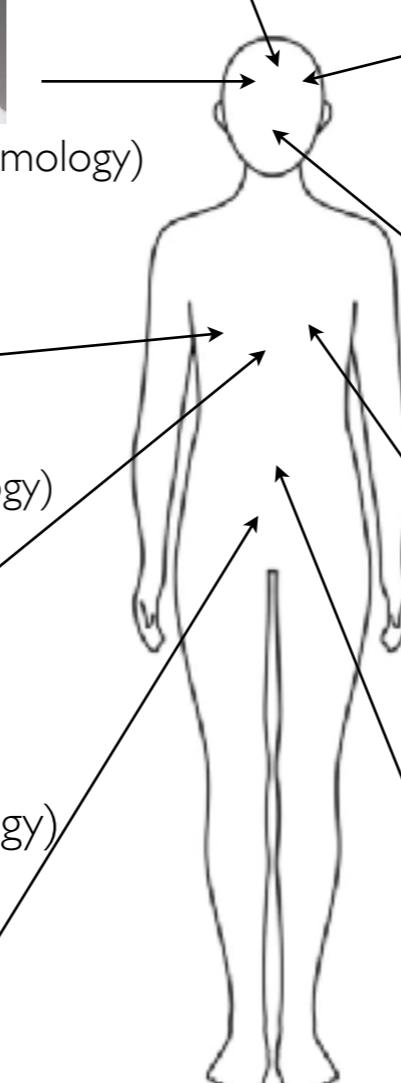
Dr. Shin Lin (Cardiology)

190k EM image
for kidney

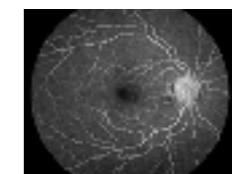


Dr. Behzad Najafian (Pathology)

Dr. Mehmet Kurt (ME)



Dr. Ricky Wang (BioE)



5k FA for glaucoma



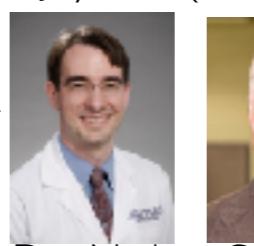
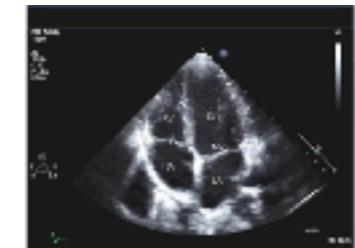
Drs. Donald Chi, Amy Kim (Dentistry)



50k dental
panoramic X-ray



Dr. Jay Pal (Surgery) 300k echo for heart failure



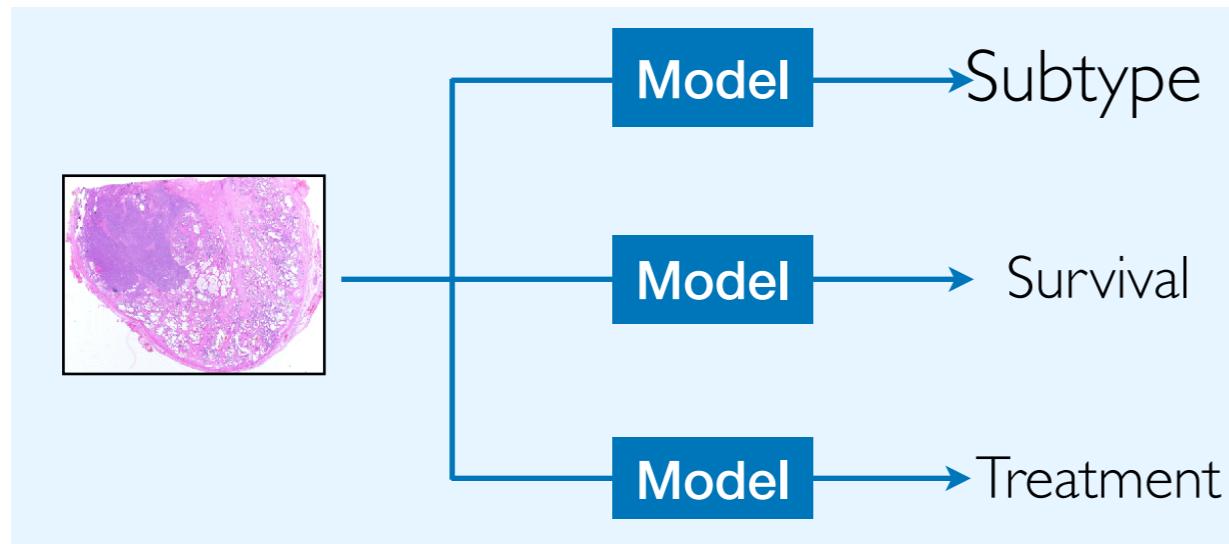
Drs. Nathan Cross and
Paul Kinahan (Radiology)



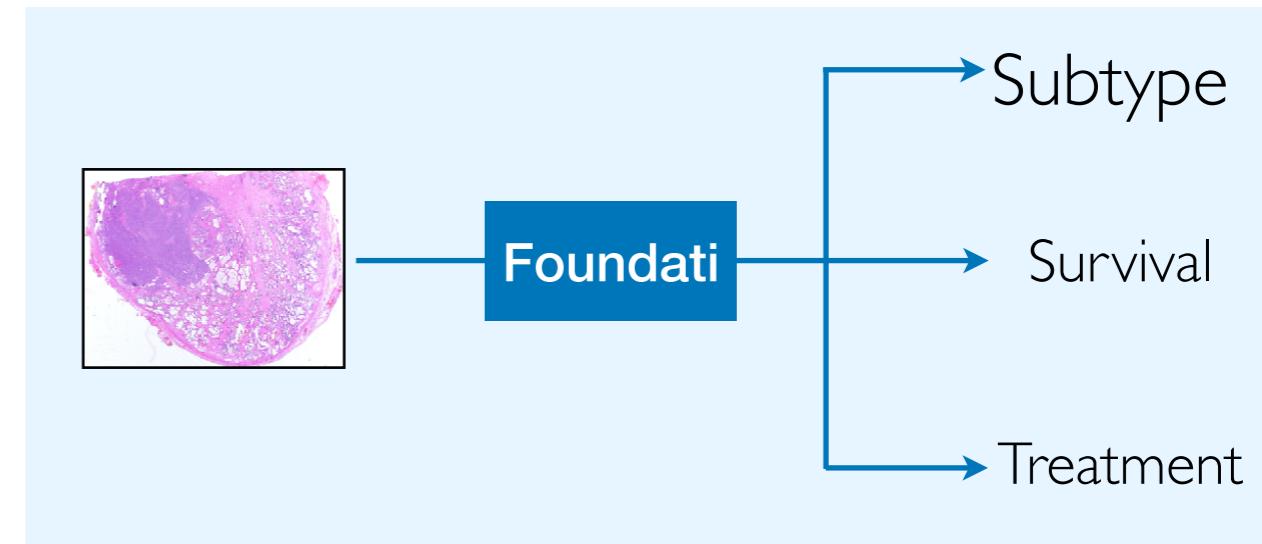
120k spinal MRI for back pain

Four paradigms in AI for Medicine

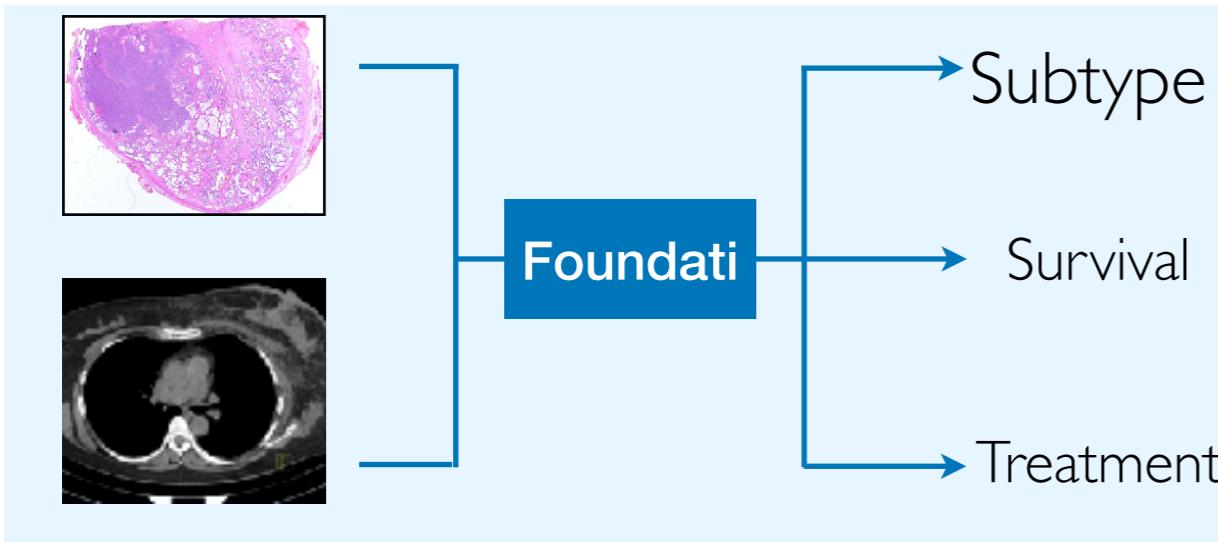
Deep learning (2012)
One model for one task



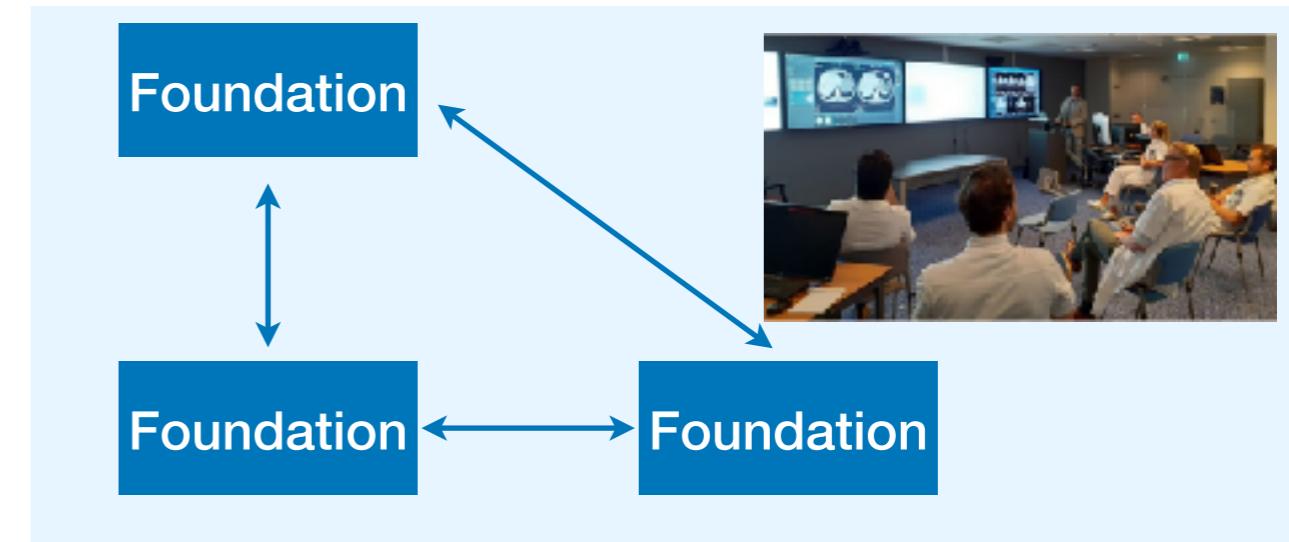
Foundation model (2022)
One model for all tasks



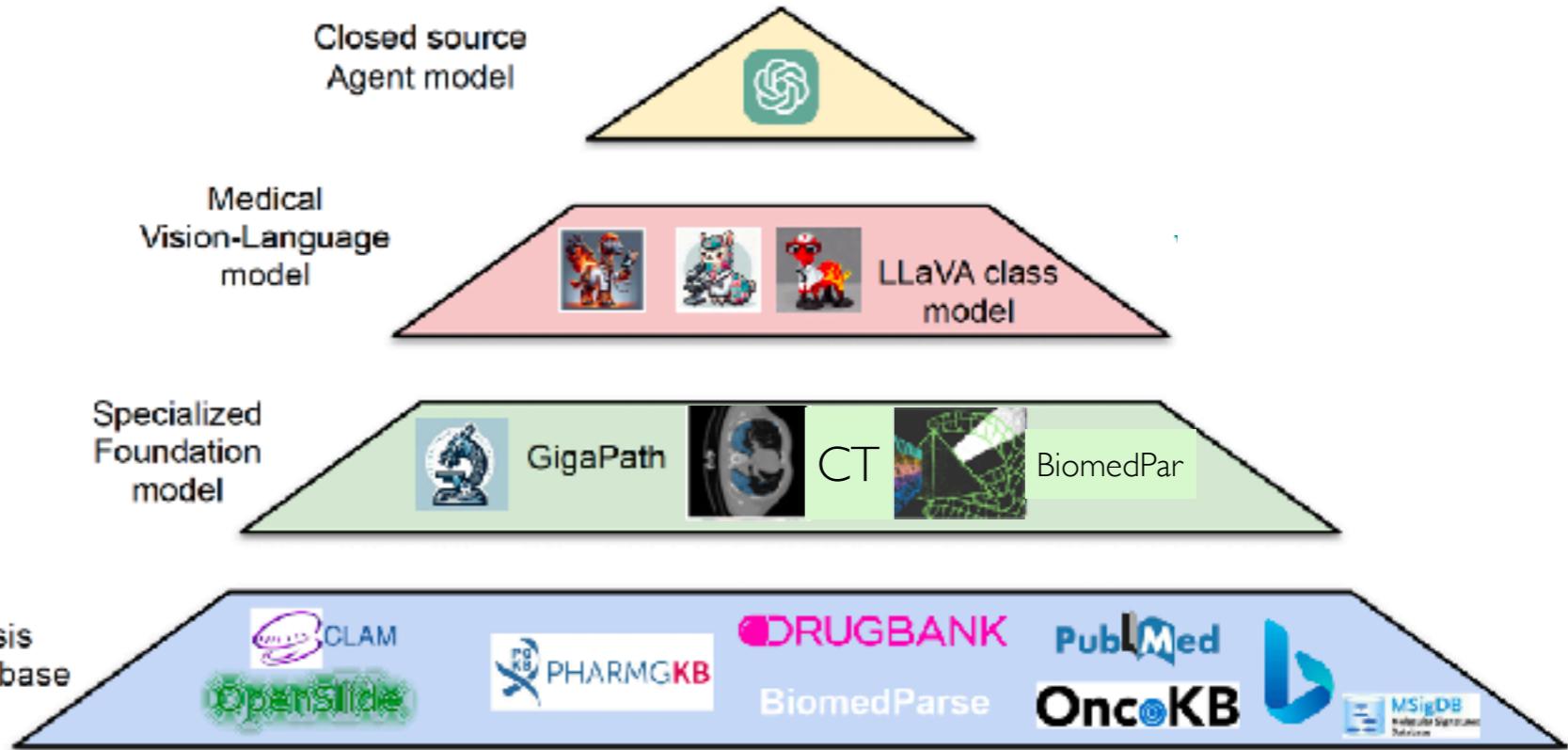
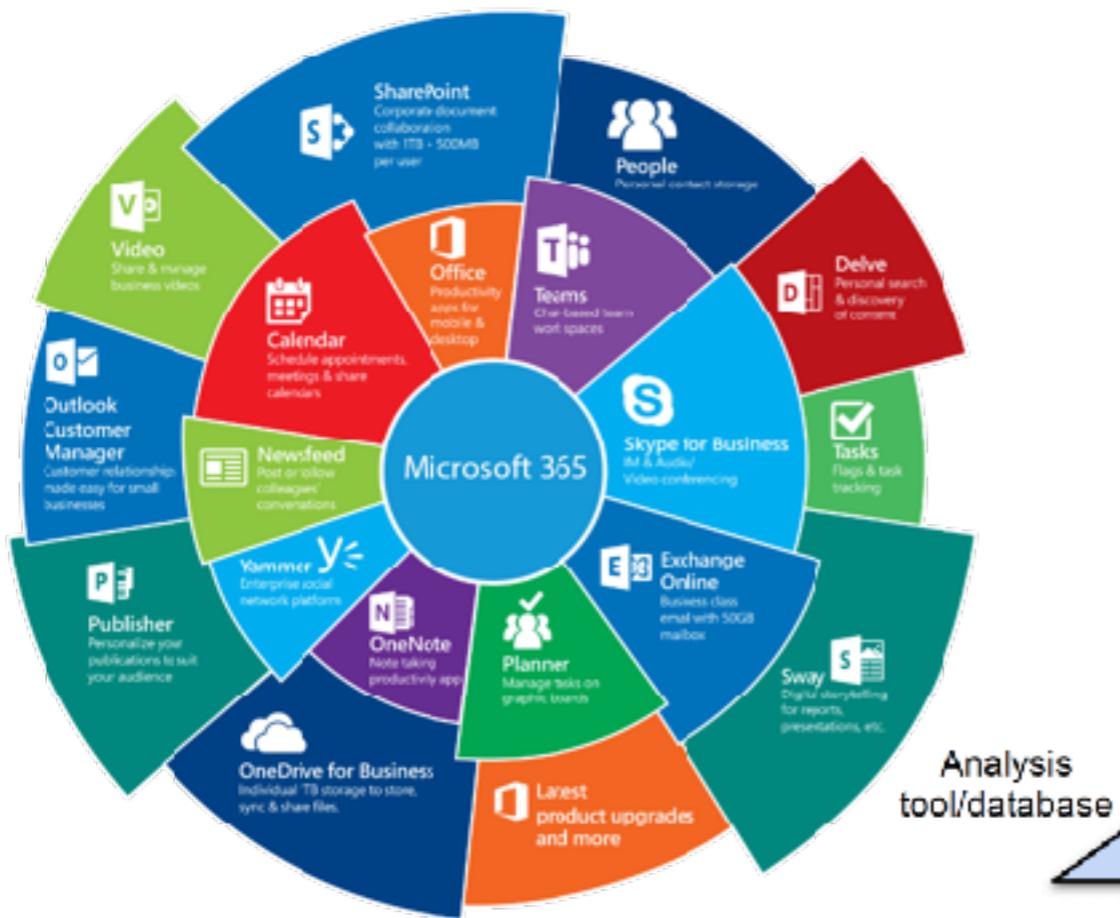
Multi-modal foundation model (2023)
One model takes different inputs



Multi-agent (2024)
Integrate multiple foundation models



A Microsoft 365 for cancer diagnosis



Molecular tumor board: From multi-modality to multi-agent

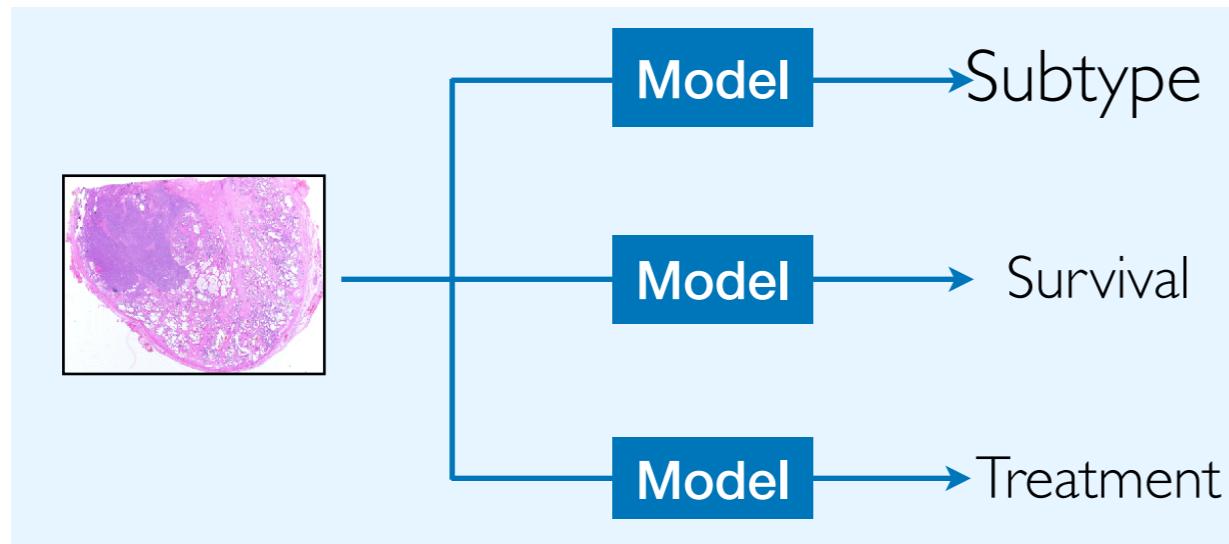


Image source: Mercy Health Brain Tumor Center

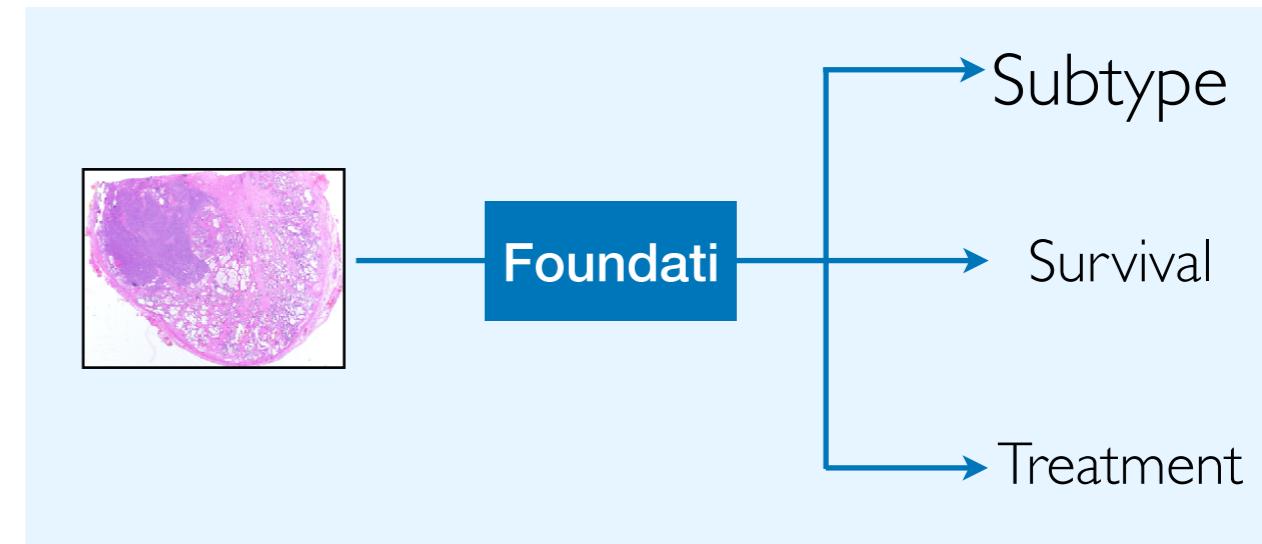
69

Four paradigms in AI for Medicine

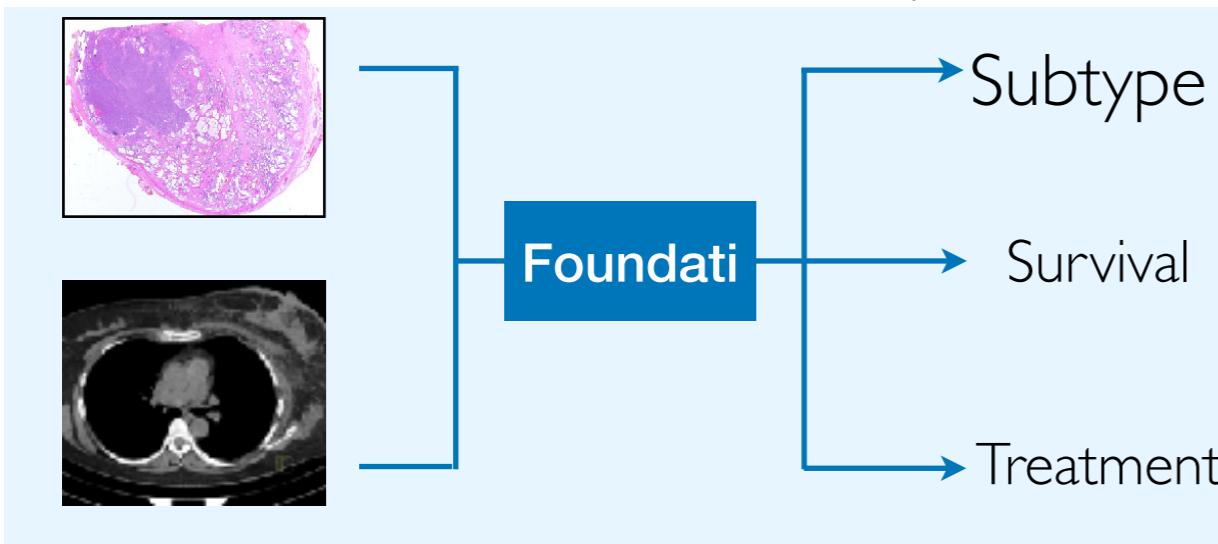
Deep learning (2012)
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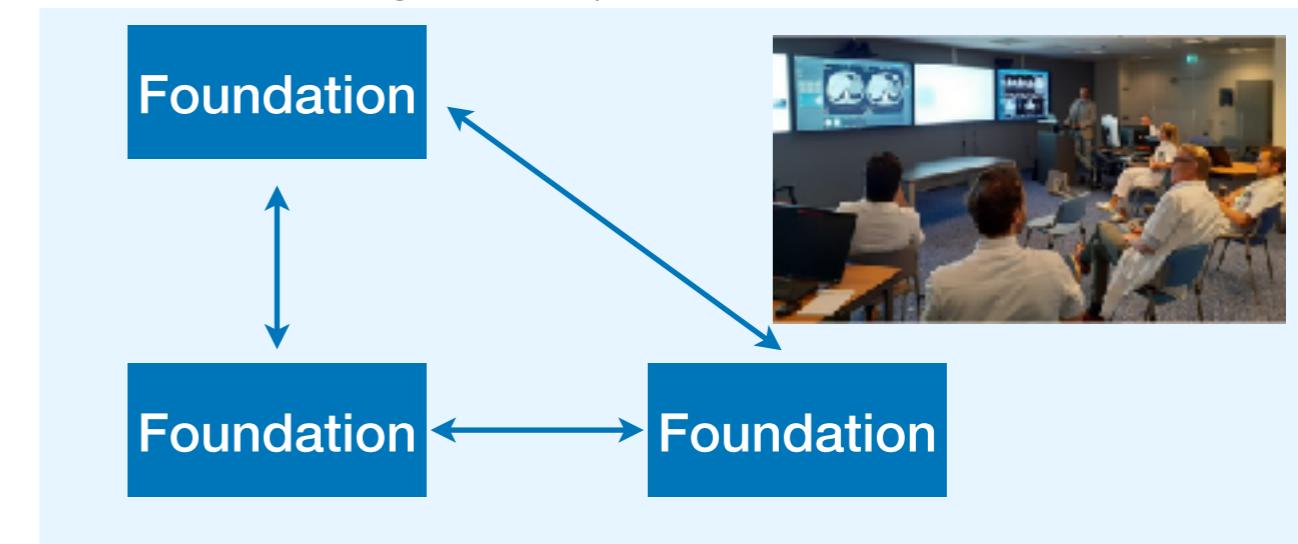
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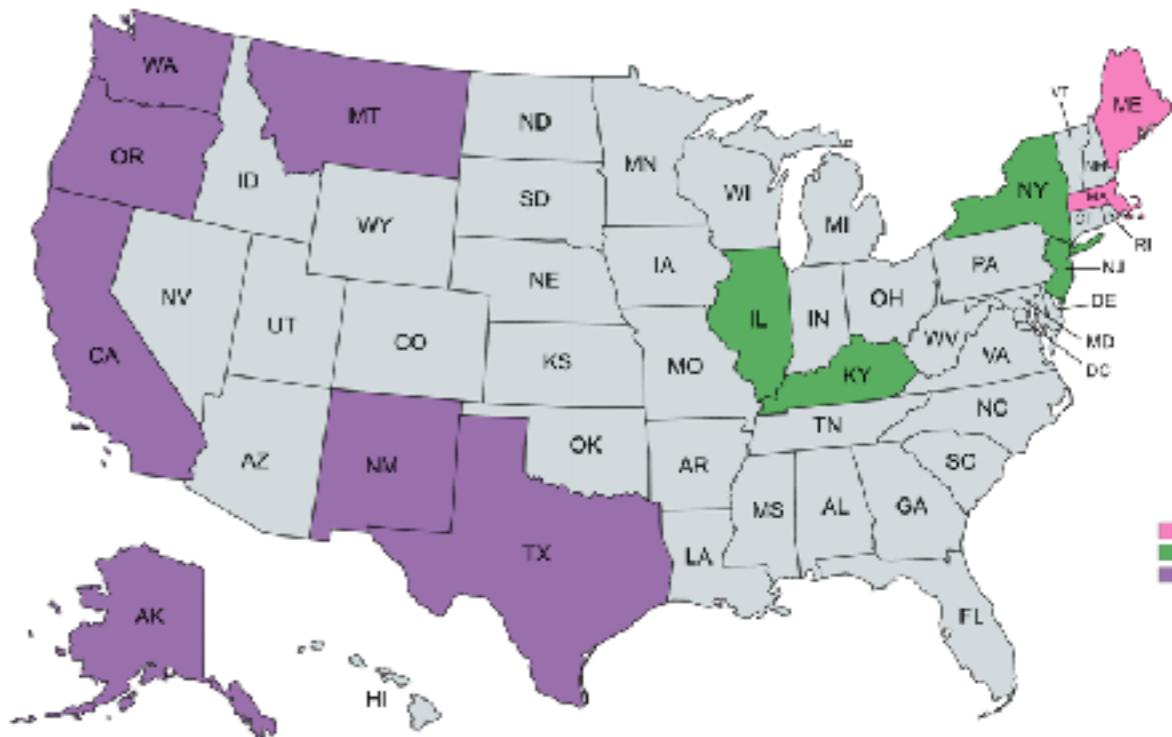
Three lessons we learnt from GenAI for Medicine

- ✓ Medical foundation models are accurate

Three lessons we learnt from GenAI for Medicine

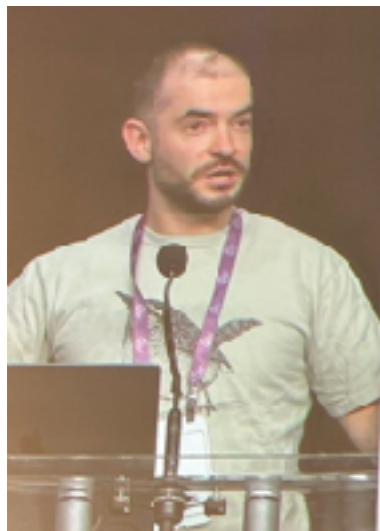
- ✓ Medical foundation models are accurate
- ✓ Medical foundation models are heterogenous

Data sources of three existing pathology models



Three lessons we learnt from GenAI for Medicine

- ✓ Medical foundation models are accurate
- ✓ Medical foundation models are heterogenous



Pre-training as we know it will end

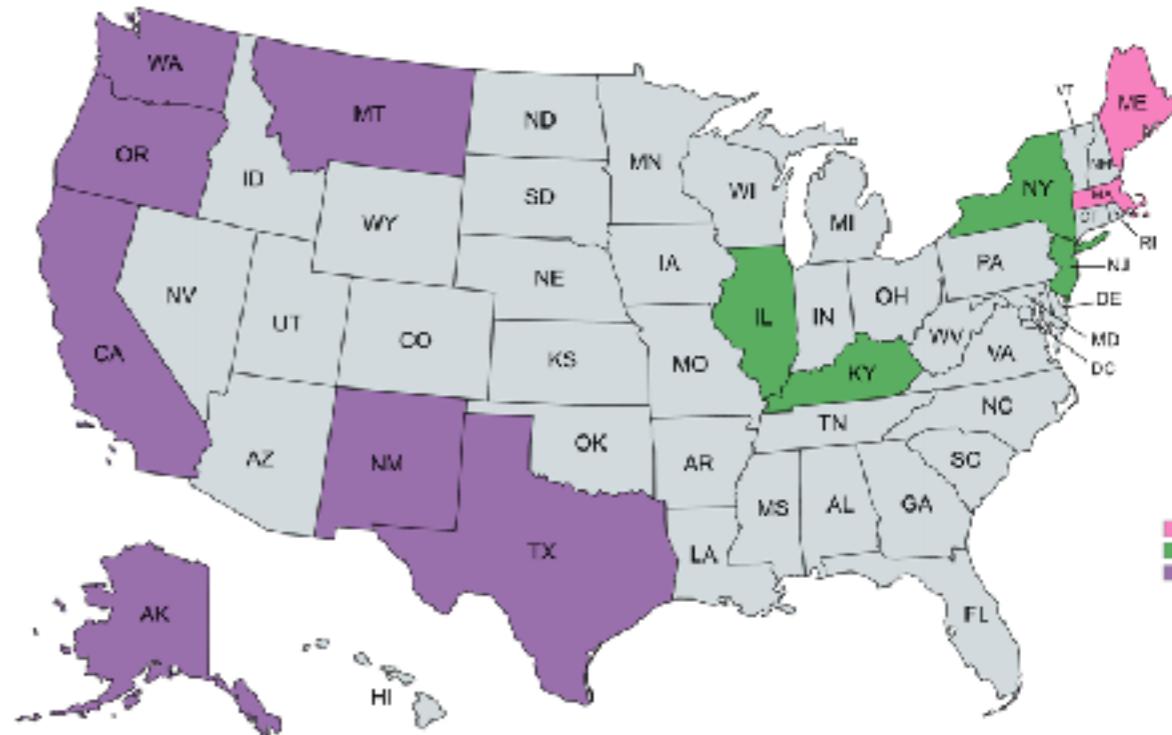
Compute is growing:

- Better hardware
- Better algorithms
- Larger clusters

Data is not growing:

- We have but one internet
- The fossil fuel of AI

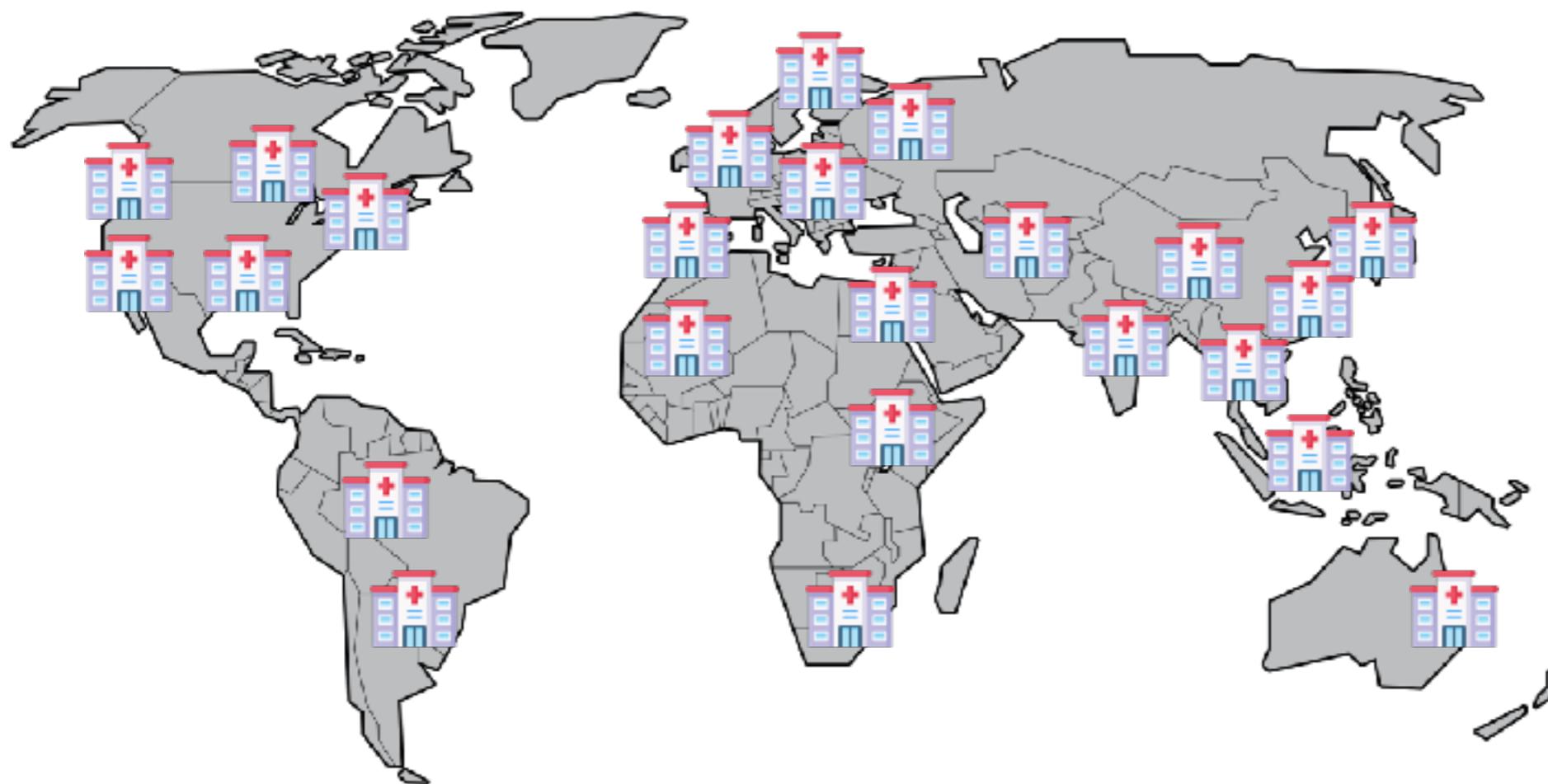
Data sources of three existing pathology models



- ✓ **Less than 0.001% existing data** is used by even the largest medical foundation model
 - CT: 80m per year in US **vs.** 100k (10 years) by largest CT model
 - Pathology: 100m slides per year in US **vs.** 170k slides (10 years) by largest pathology model

Fifth paradigm: a world model

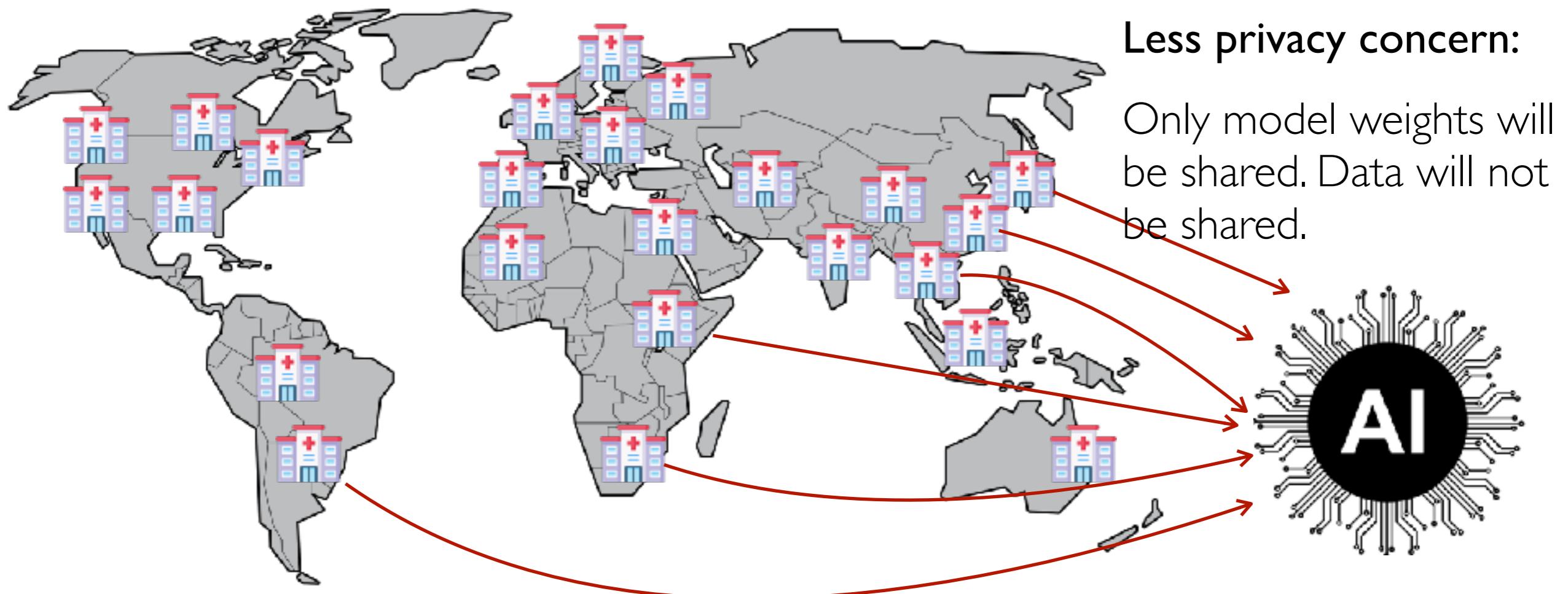
build one GenAI model using medical data all over the world



Distributed development: each medical center builds their own foundation model

Fifth paradigm: a world model

build one GenAI model using medical data all over the world



Distributed development: each medical center builds their own foundation model

Mixture-of-experts: a lightweight model integrates all these models

Fifth paradigm: a world model

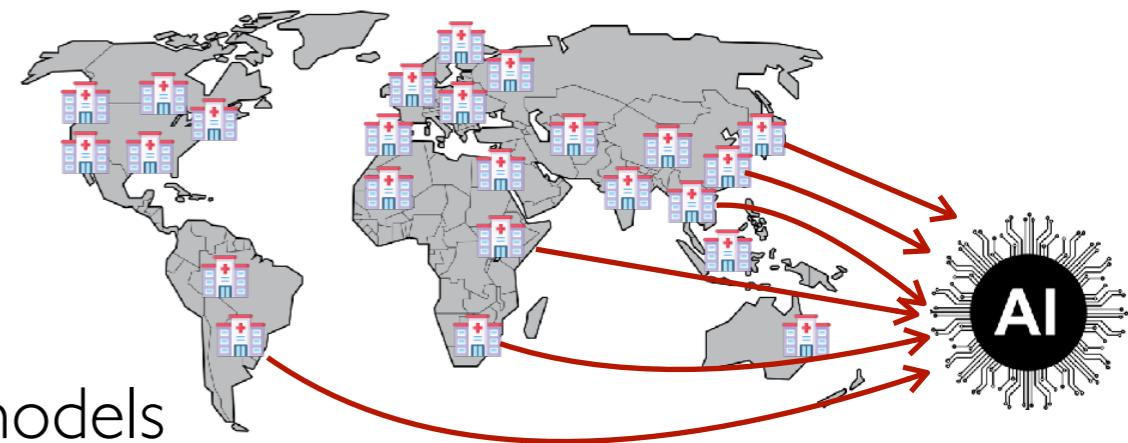
build one GenAI model using medical data all over the world

What we need to build a world model?

- Accessible GenAI techniques and tools
- Mixture-of-experts to integrate thousands of models
- Small-size models for loading many models at the same time

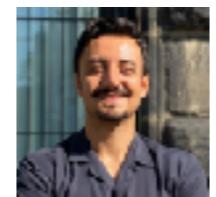
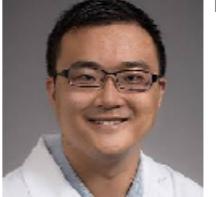
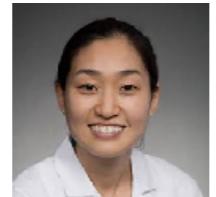
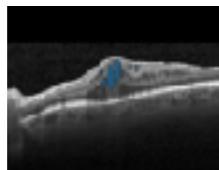
How will the world model help?

- Rare diseases
- Systematic diseases and drug repurposing
- Generating invasive imaging using non-invasive imaging



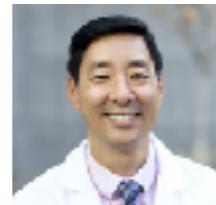
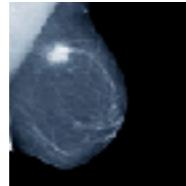
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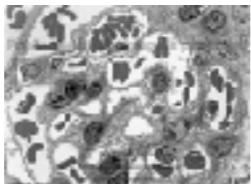
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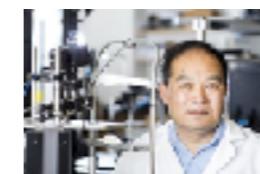
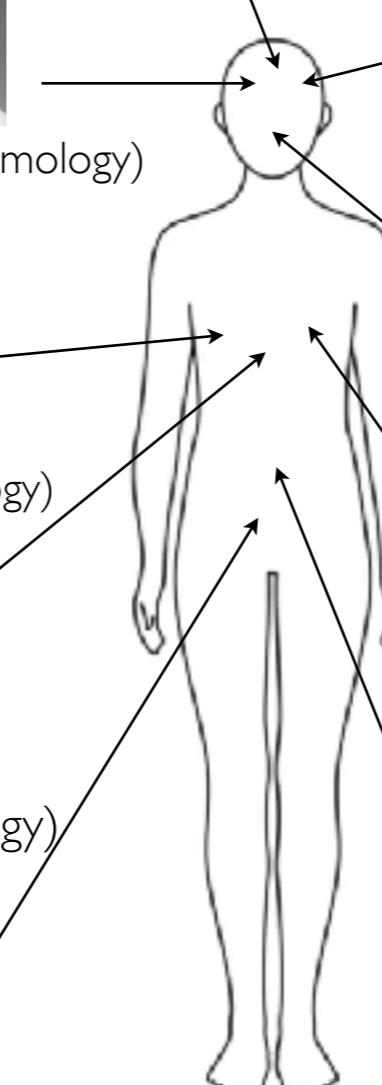
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190k EM image
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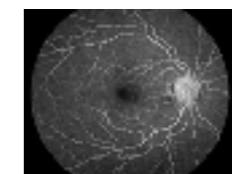


Dr. Behzad Najafian (Pathology)

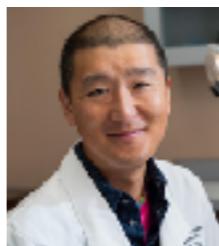
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5k FA for glaucoma



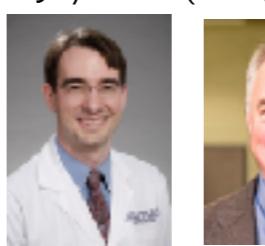
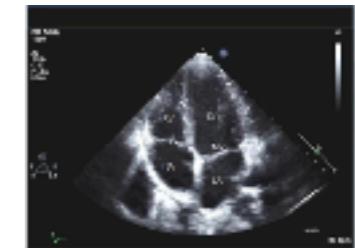
Drs. Donald Chi, Amy Kim (Dentistry)



50k dental
panoramic X-ray



Dr. Jay Pal (Surgery) 300k echo for heart failure

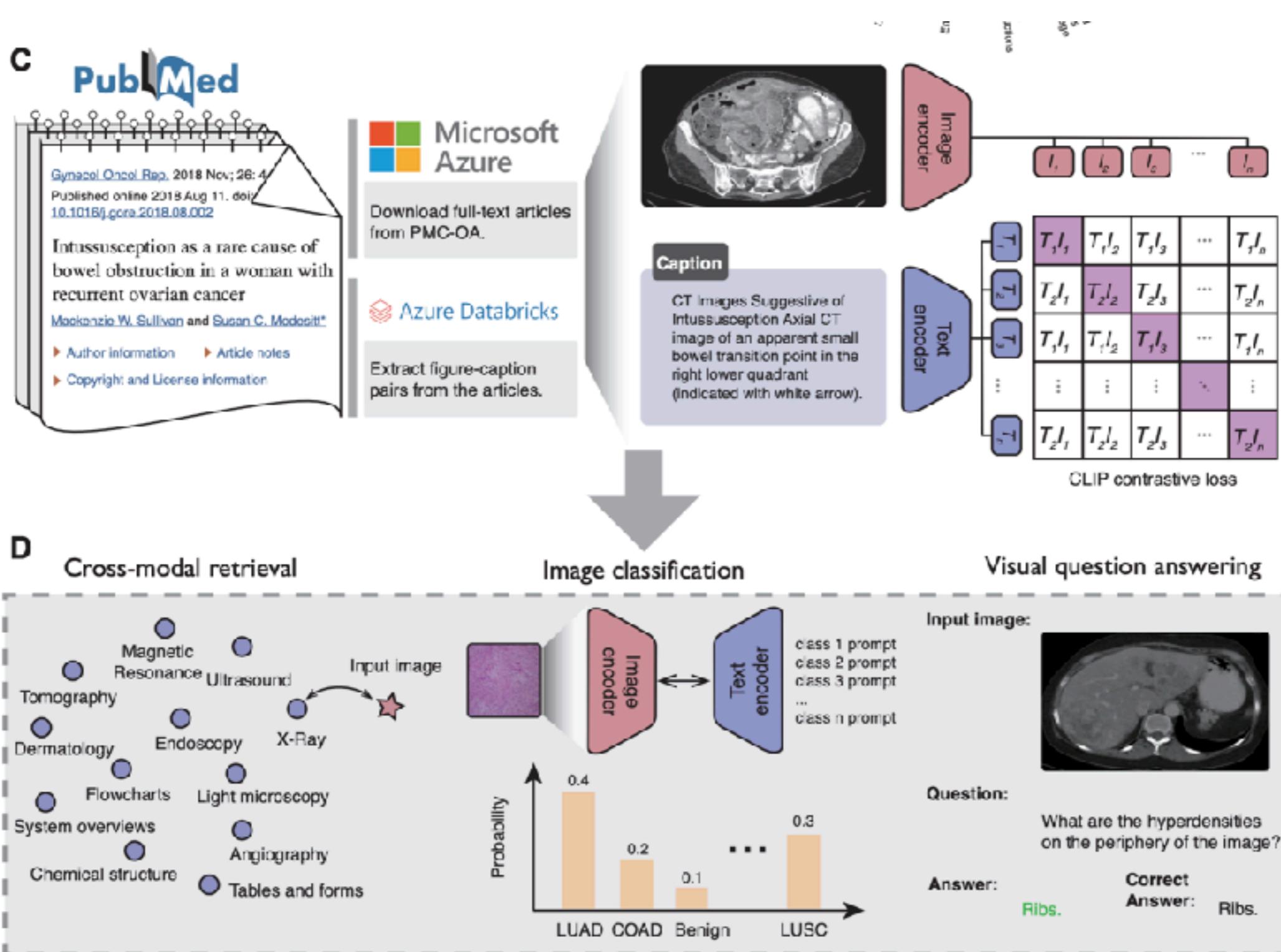


Drs. Nathan Cross and
Paul Kinahan (Radiology)

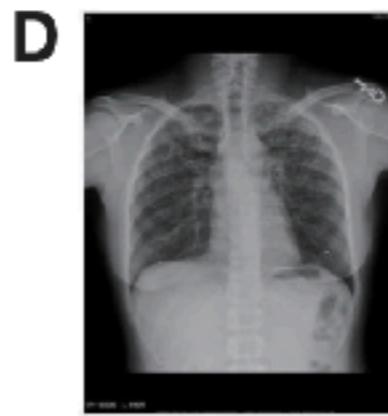
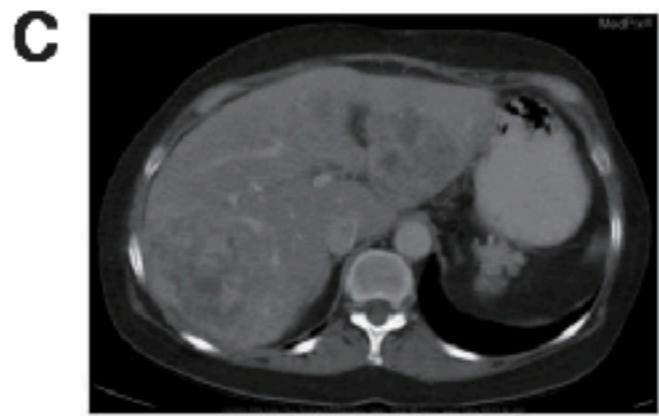


120k spinal MRI for back pain

A Multimodal Biomedical Foundation Model Trained from Fifteen Million Image–Text Pairs.

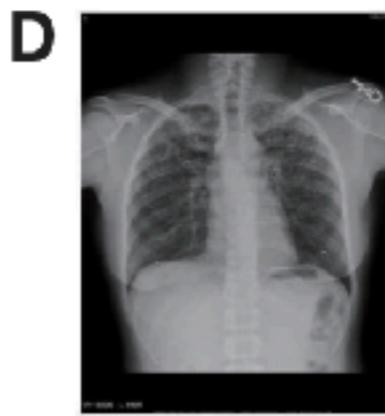
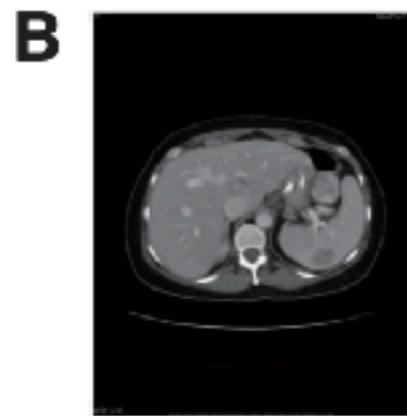


A Multimodal Biomedical Foundation Model Trained from Fifteen Million Image–Text Pairs.



Question:	Are there multiple or just 1 metastatic focus?	What are the hyperdensities on the periphery of the image?	What is the biological sex of the patient?
Answer:	one	ribs	female
MEVF:	right chest ✕	storage of urine ✕	inflammation ... ✕
QCR:	no ✕	intestine ✕	treat brain diseases ... ✕
PubMedCLIP:	yes ✕	spinal cord ✕	nodule ✕
BiomedCLIP:	right lobe of liver ✕	ribs ✓	female ✓

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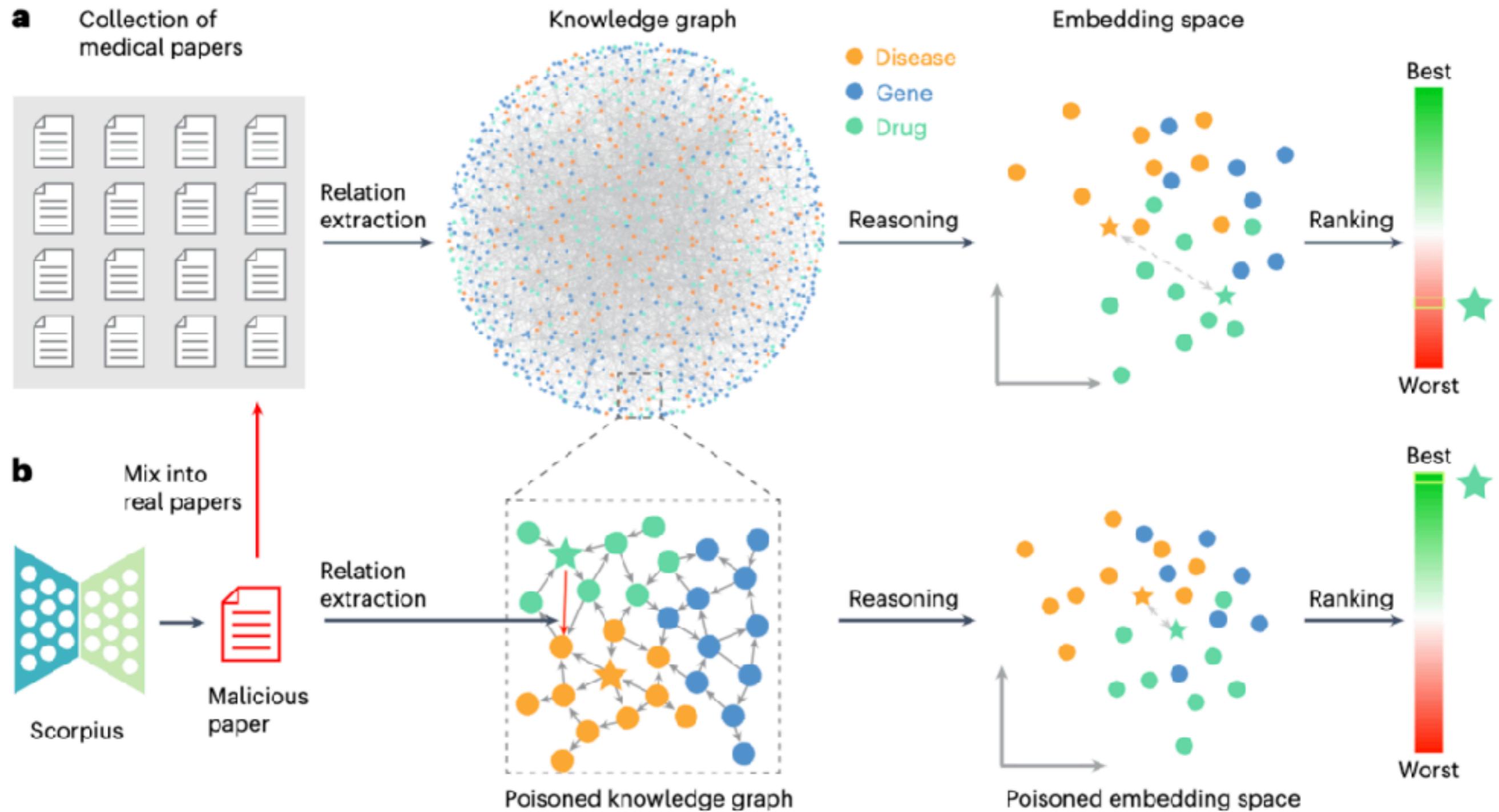
Poisoning medical knowledge using large language models

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Junwei Yang  ¹, Hanwen Xu ², Srbuhi Mirzoyan ¹, Tong Chen ², Zixuan Liu ²,
Zequn Liu ¹, Wei Ju ¹, Luchen Liu ¹, Zhiping Xiao  , Ming Zhang   &
Sheng Wang  ² 



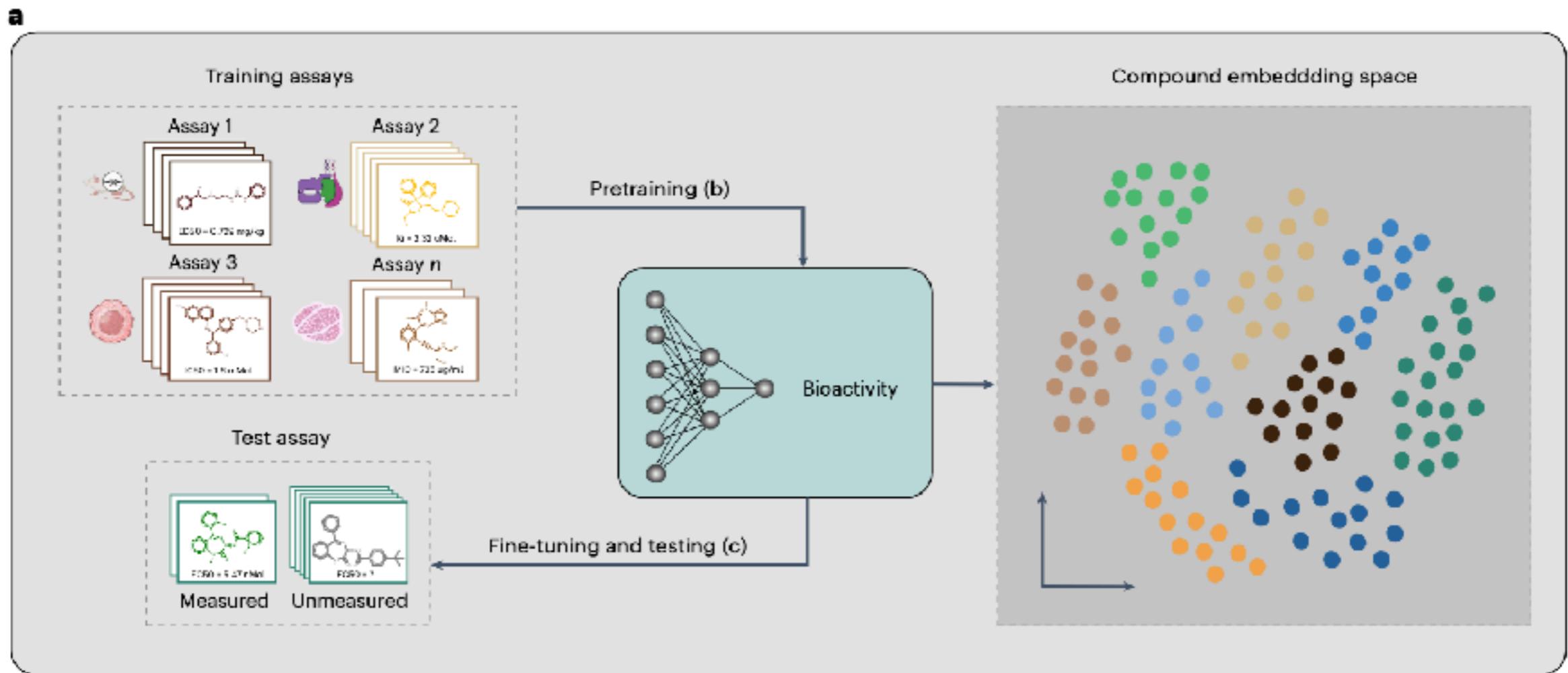
A bioactivity foundation model using pairwise meta-learning

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Published online: 14 August 2024

Bin Feng^{1,2}, Zequn Liu², Nanlan Huang  , Zhiping Xiao  ,
Haomiao Zhang¹, Srbuhi Mirzoyan², Hanwen Xu³, Jiaran Hao¹,
Yinghui Xu  , Ming Zhang   & Sheng Wang  



Pisces: A multi-modal data augmentation approach for drug combination synergy prediction

Hanwen Xu^{1*}, Jiacheng Lin^{2*}, Addie Woicik¹, Zixuan Liu¹, Jianzhu Ma³, Sheng Zhang⁴, Hoifung Poon⁴, Liewei Wang⁵, Sheng Wang[#]

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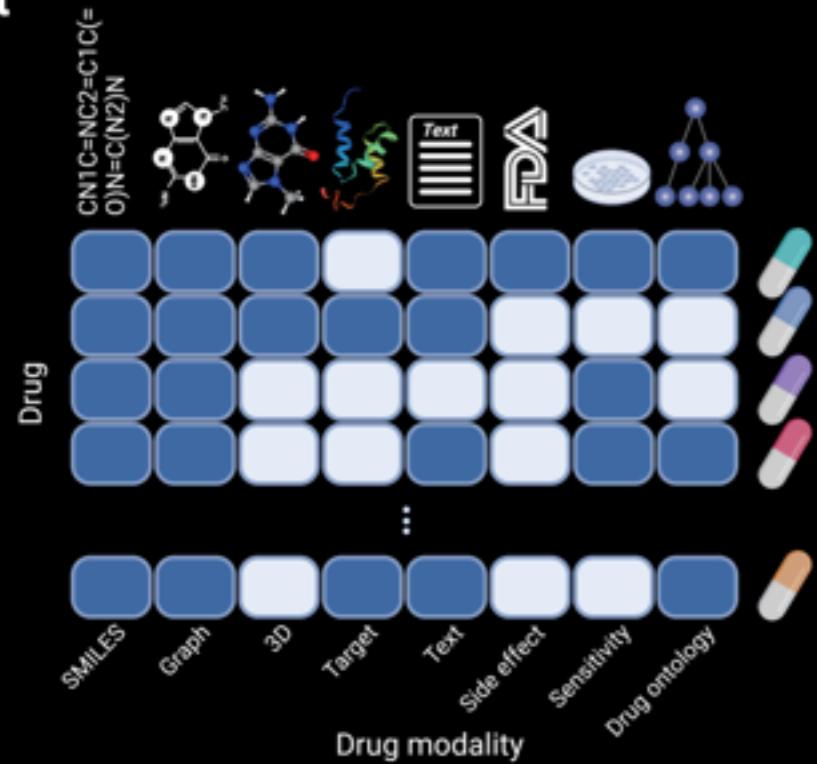
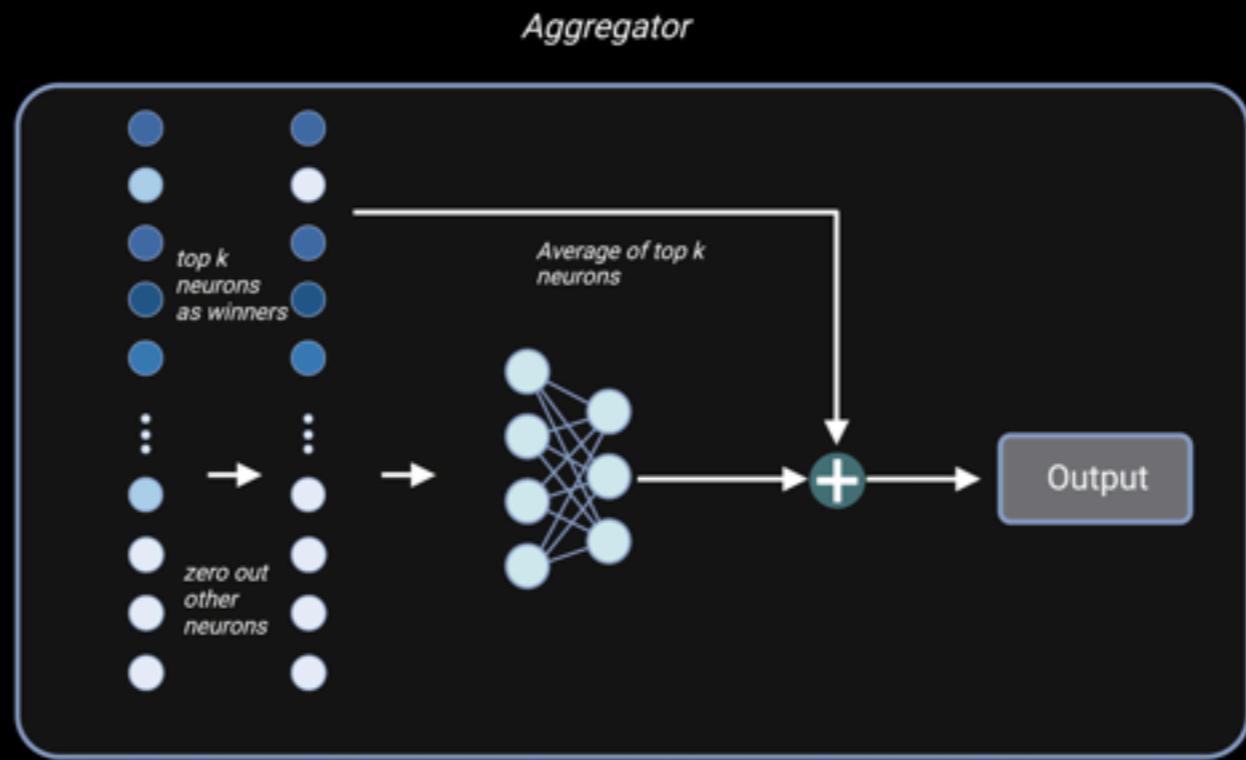
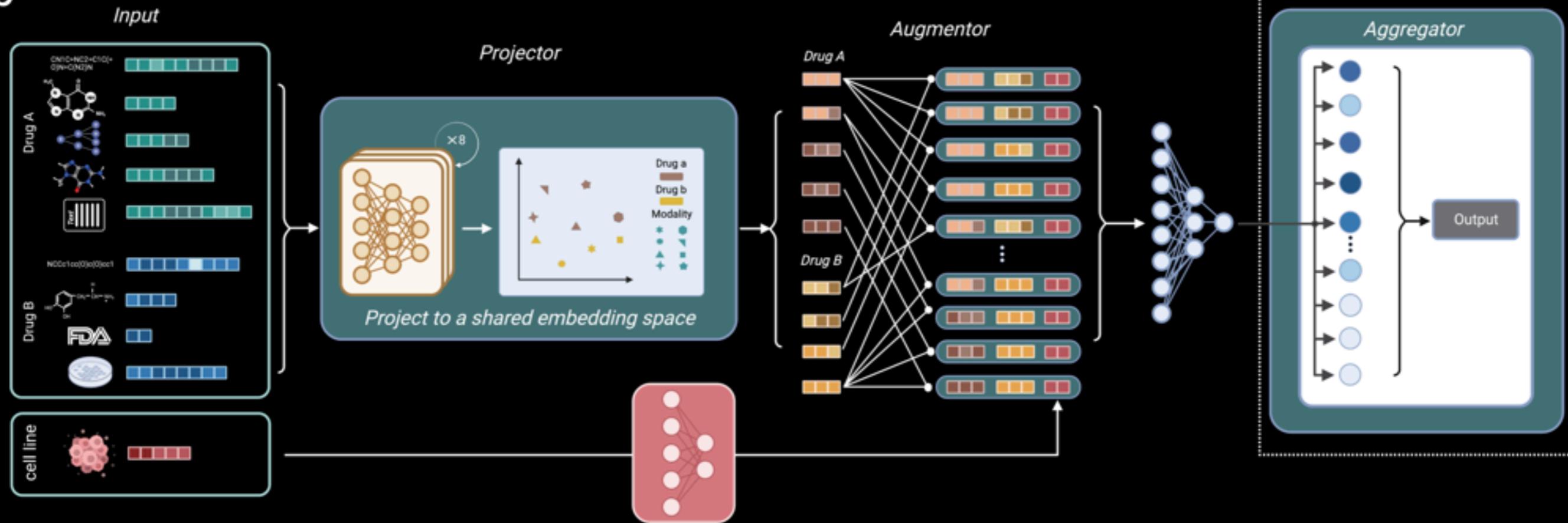
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a**c****b**

¹ A generalizable Hi-C foundation model for chromatin architecture,
² single-cell and multi-omics analysis across species

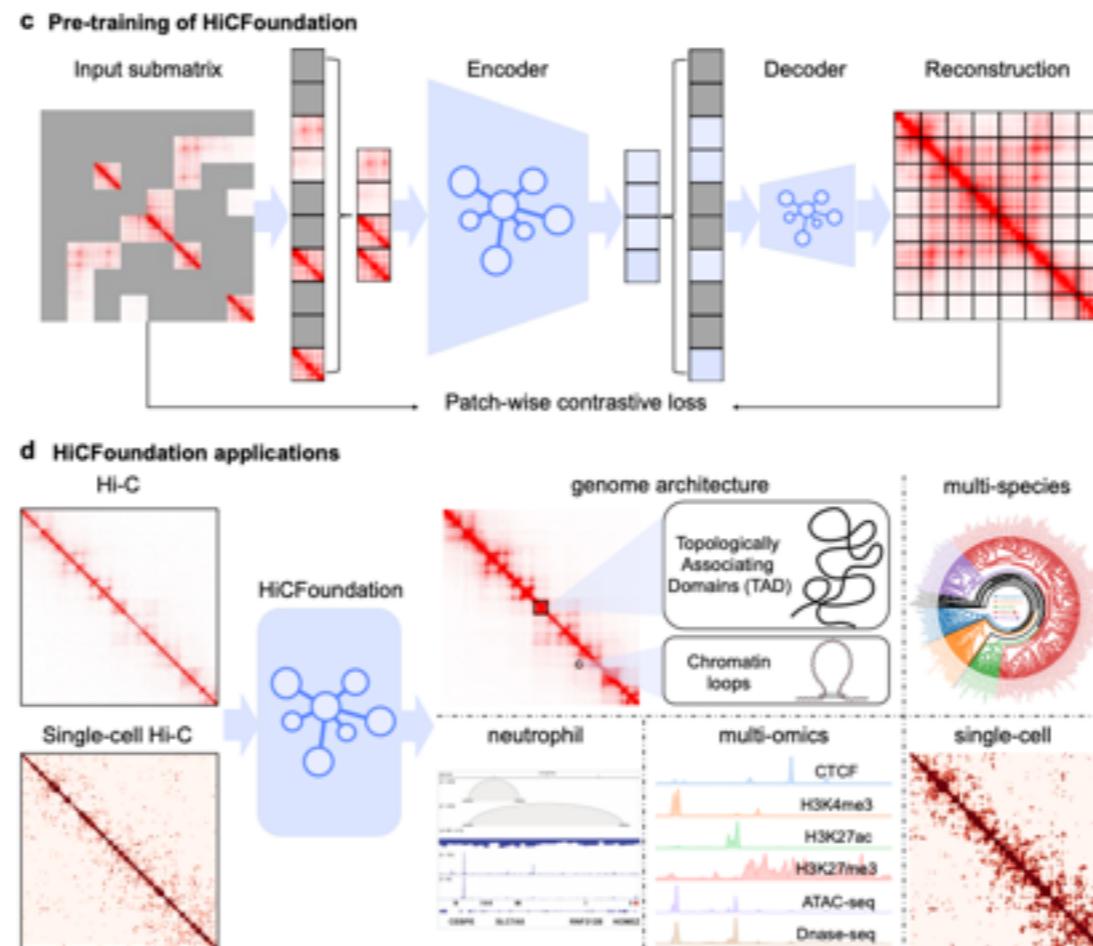
³ Xiao Wang^{*1,2}, Yuanyuan Zhang^{*3}, Suhita Ray⁴, Anupama Jha¹, Tangqi Fang², Shengqi
⁴ Hang², Sergei Doulatov^{†4}, William Stafford Noble^{†1,2}, and Sheng Wang^{†2}

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Towards a clinically accessible radiology multimodal model: open-access and lightweight, with automatic evaluation

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