

Selected topics in DL: Equivariance & Dynamics

First meeting

14.10.2025

About me

- 2nd year PhD student in the Computer Vision Group & (ELLIS student) in AMLab
- Research focus: Machine learning for molecular science
 - Scaling molecular dynamics simulations

Unconstrained large-scale learning

User

What is the pH of a 0.10 M solution of NH_4F ? The K_a of NH_4^+ is 5.6×10^{-10} and the K_a of HF is 6.8×10^{-4} .

Thought for 4 seconds ▾

To determine the pH of a 0.10 M solution of ammonium fluoride (NH_4F), we'll need to consider the acid-base properties of its constituent ions when dissolved in water.

Step 1: Dissociation of NH_4F

$$\text{NH}_4\text{F} \rightarrow \text{NH}_4^+ + \text{F}^-$$

Both NH_4^+ and F^- can react with water, affecting

Large language models



Segment Anything Model



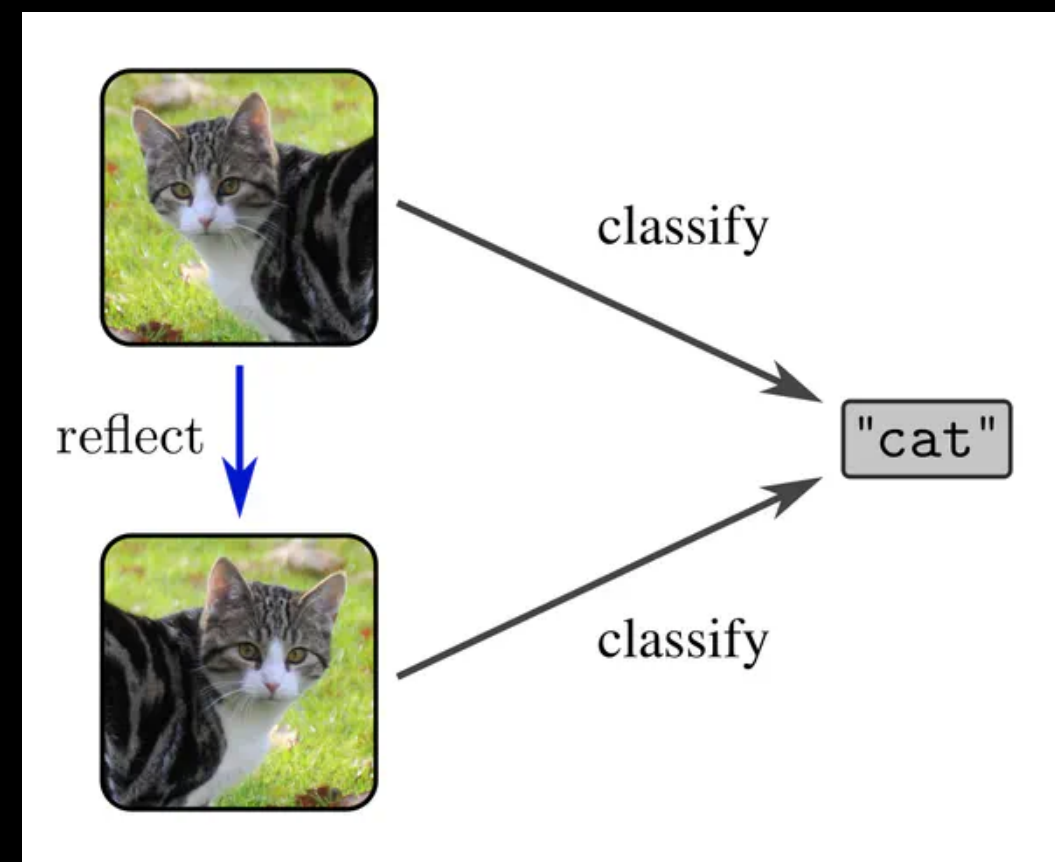
phi-0.5: Vision language action model

Unconstrained large-scale learning

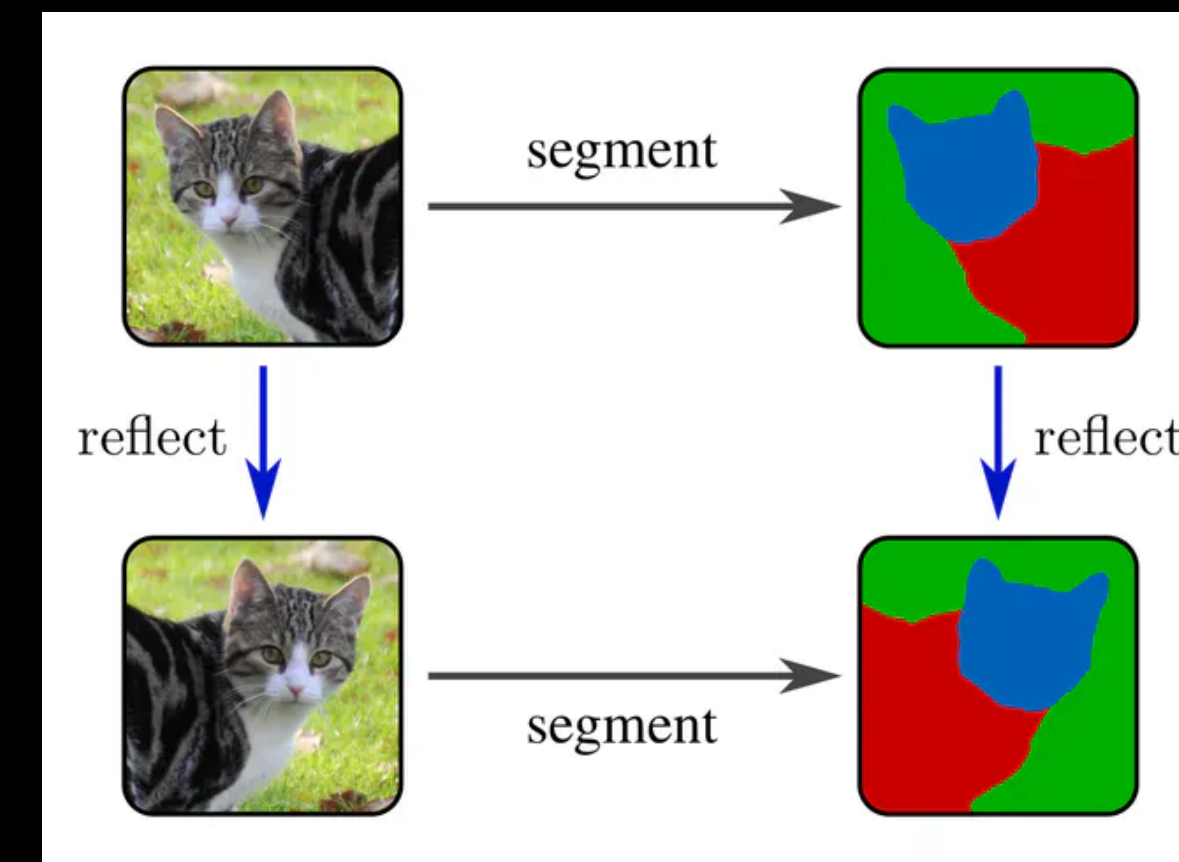
Is attention and scaling all you need?

Structure-preserving learning

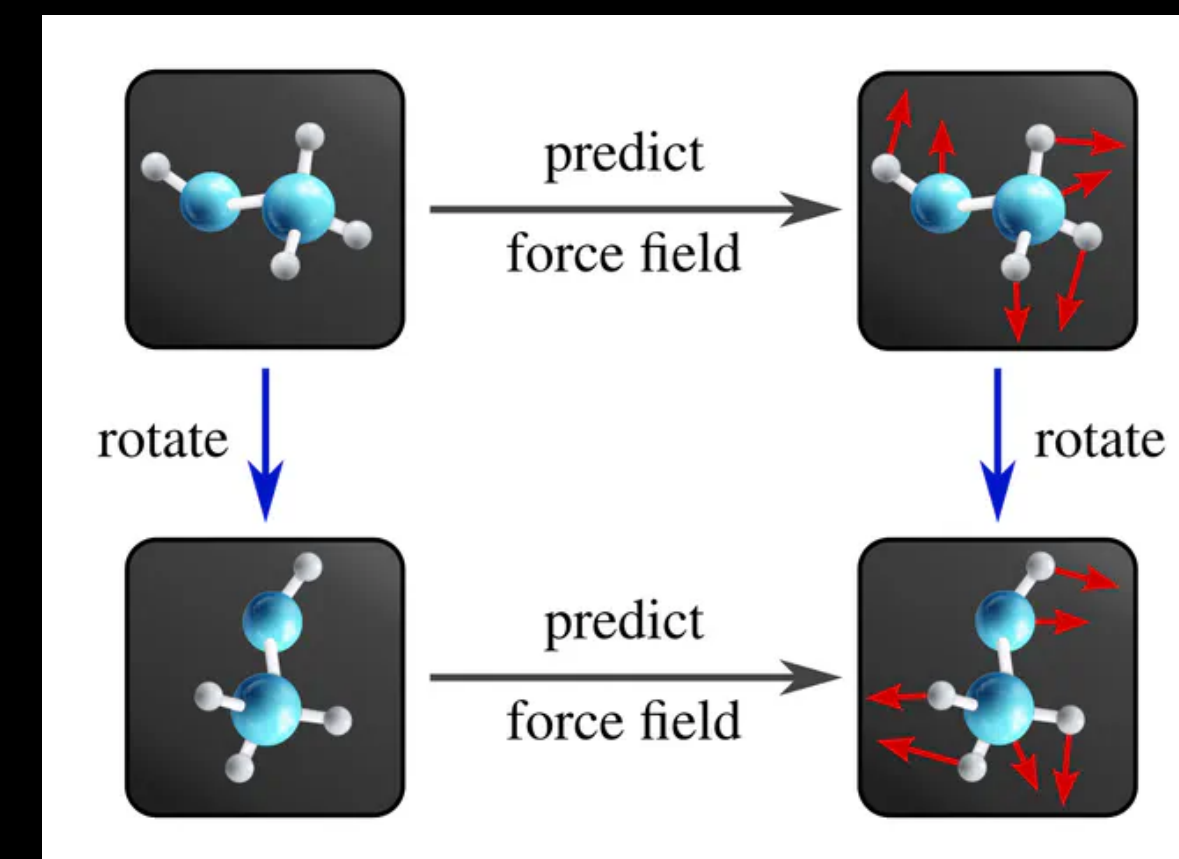
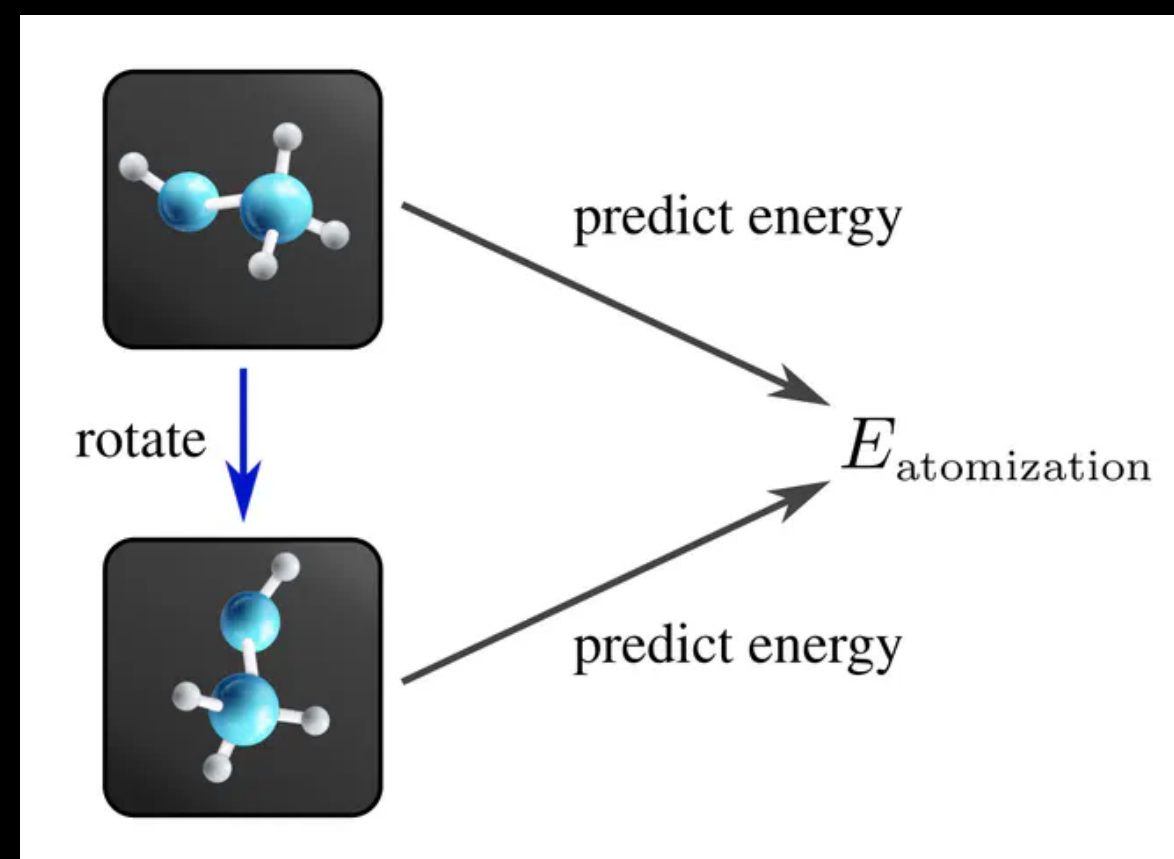
Symmetries



Invariance

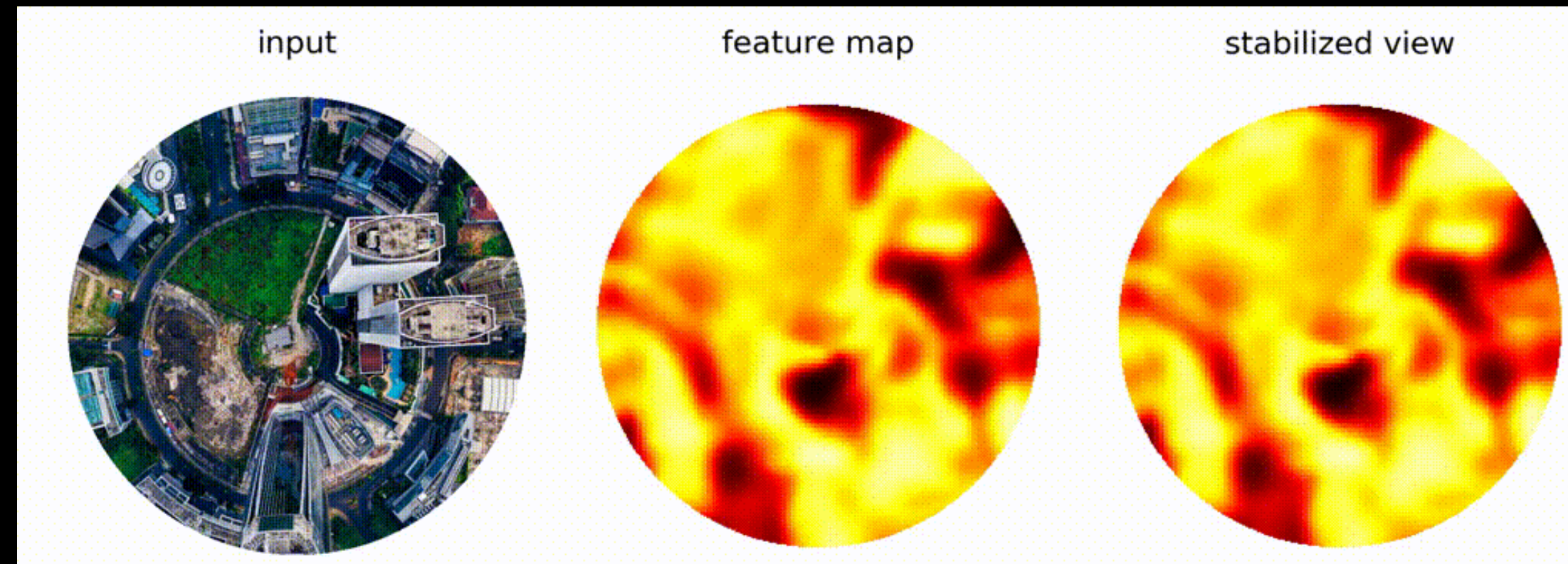


Equivariance

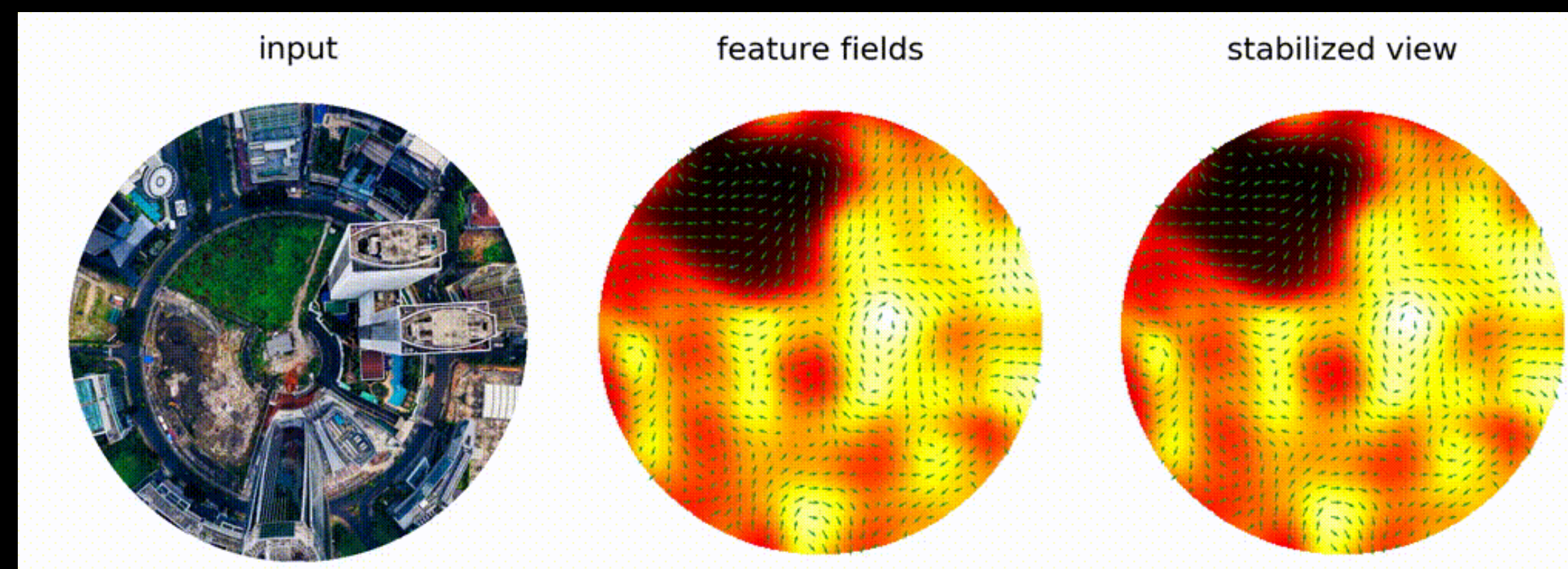


Structure-preserving learning

Symmetries



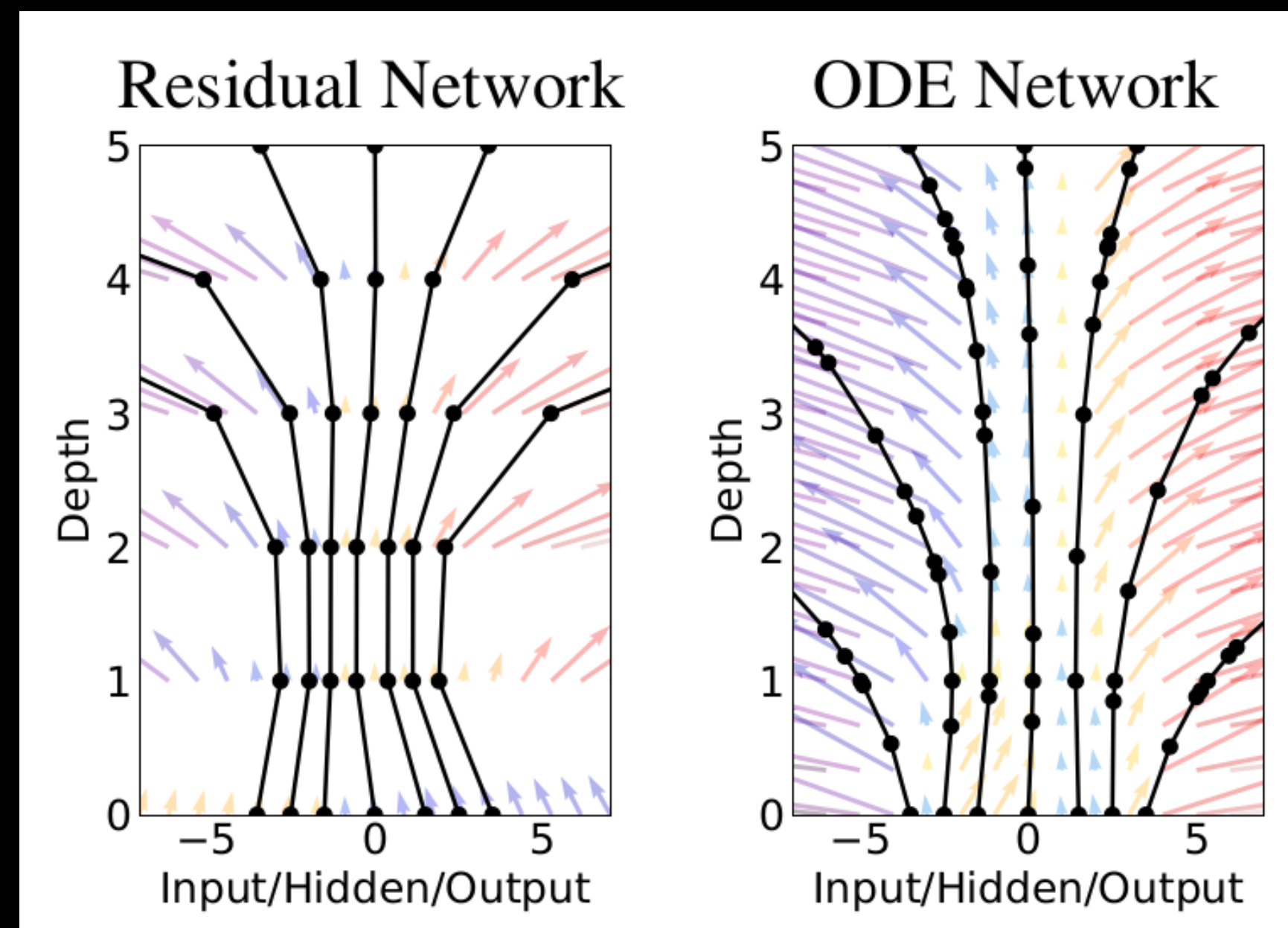
CNN



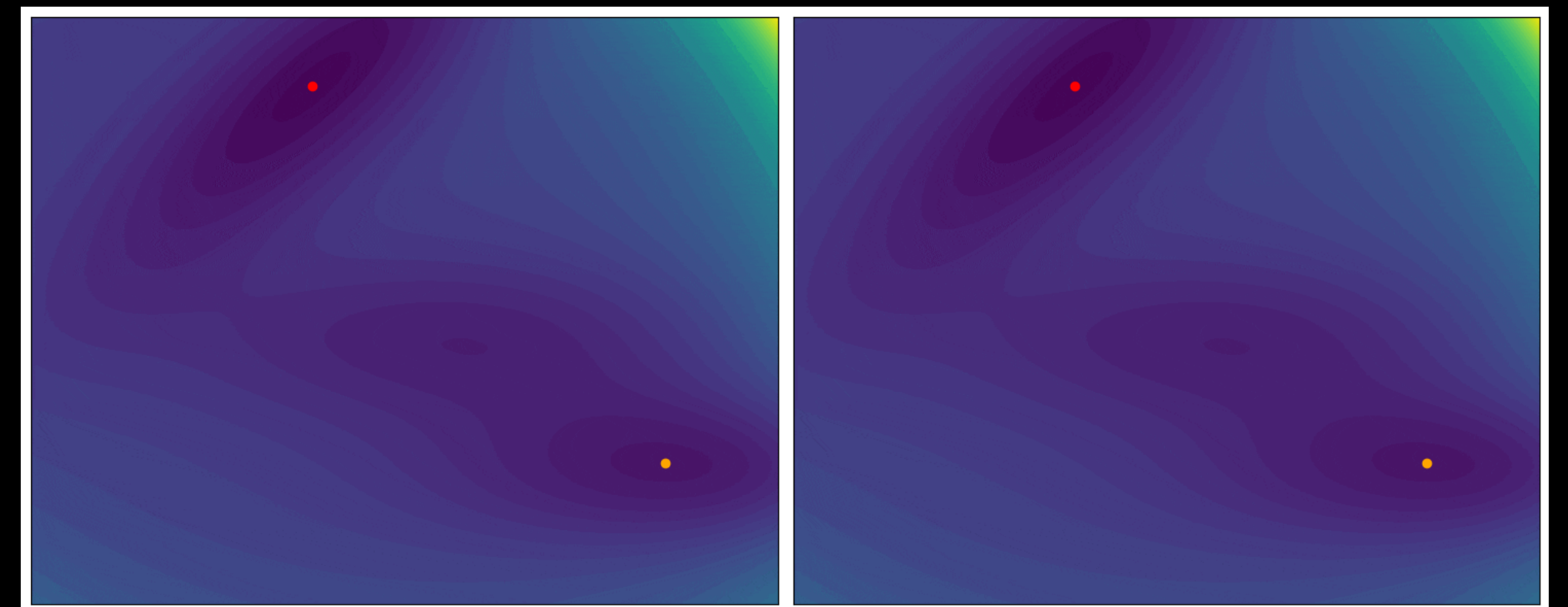
Group-CNN

Structure-preserving learning

Dynamics



Neural ODE
(Chen et al.)

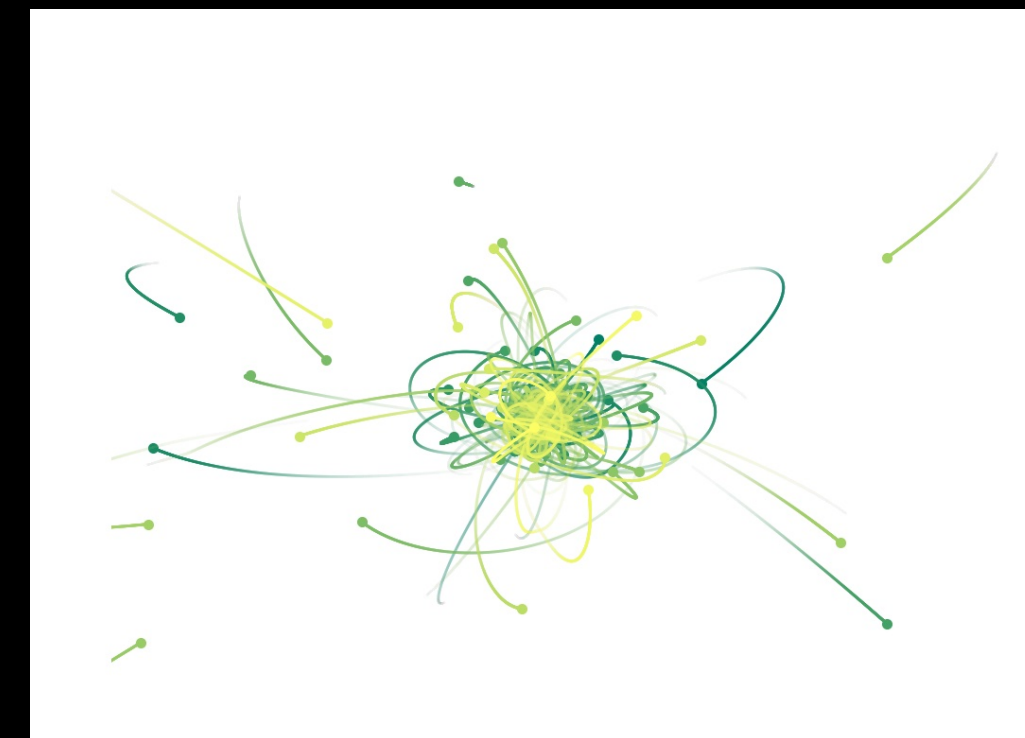


Path Sampling
(Du et al.)

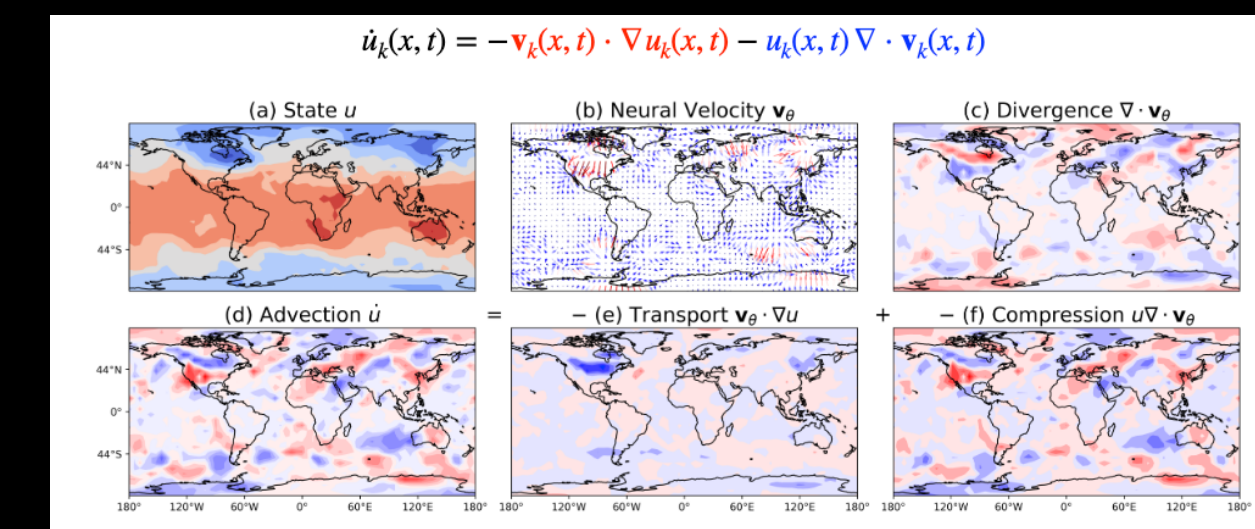
Structure-preserving learning

Applications

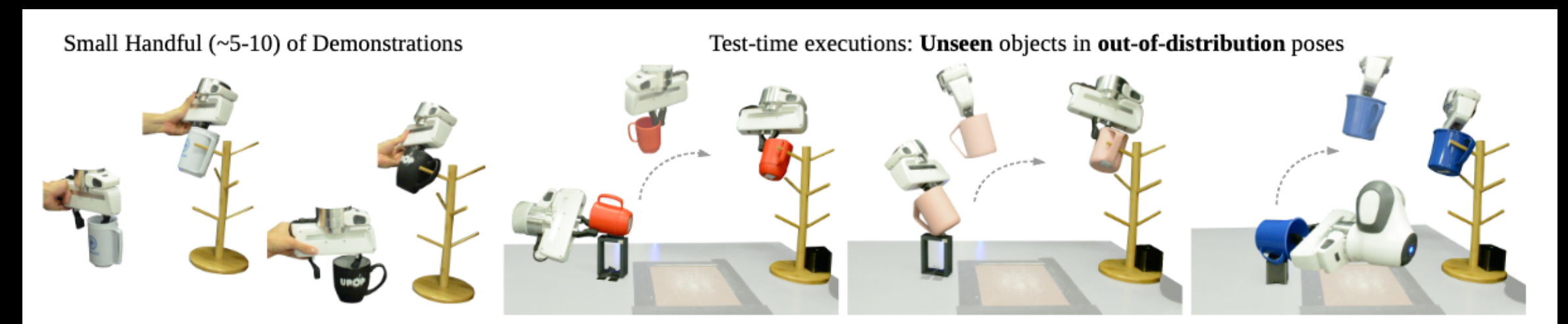
- Architectures with symmetry-preserving guarantees
- Architectures leveraging known dynamics
 - Data efficiency
 - Compute efficiency*



N-body dynamics



ClimODE



Neural Descriptor Fields

* Brehmer et al., Does Equivariance Matter at Scale?

Logistics

- In-person session every other week
 - Tuesdays 14:30 - 16:30. MI 01.13.010
- Two paper presentations in every session
 - 30 - 35 minutes presentation + 10 minutes discussion

Date	Paper	Presenter	Slides
14.10	Introduction & Review (Online)	Karnik	
11.11	Neural Ordinary Differential Equations	Aniket	
	Action Matching: Learning Stochastic Dynamics from Samples	Billy	
25.11	Doob's Lagrangian: A Sample-Efficient Variational Approach to Transition Path Sampling	Sergine	
	Consistent Sampling and Simulation: Molecular Dynamics with Energy-Based Diffusion Models	Hannes	
09.12	Artificial Kuramoto Oscillatory Neurons	Dima	
	Space-Time Continuous PDE Forecasting using Equivariant Neural Fields	Ale	
20.01	3D Steerable CNNs: Learning Rotationally Equivariant Features in Volumetric Data	Perasolo	
	SE(3)-Stochastic Flow Matching for Protein Backbone Generation	Maximilian	
27.01	Probing Equivariance and Symmetry Breaking in Convolutional Networks	Mykhailo	
	Neural Isometries: Taming Transformations for Equivariant ML	Tingwei	
03.02	Flow Equivariant Recurrent Neural Networks	Sander	
	Equivariant Adaptation of Large Pretrained Models	Giacomo	

Evaluation*

- Major component (75%)
 - Paper presentation (40%)
 - Technical review (35%)
- Minor components (25%)
 - Class participation (15%)
 - One paragraph paper summaries before every session (10%)

What you have to do

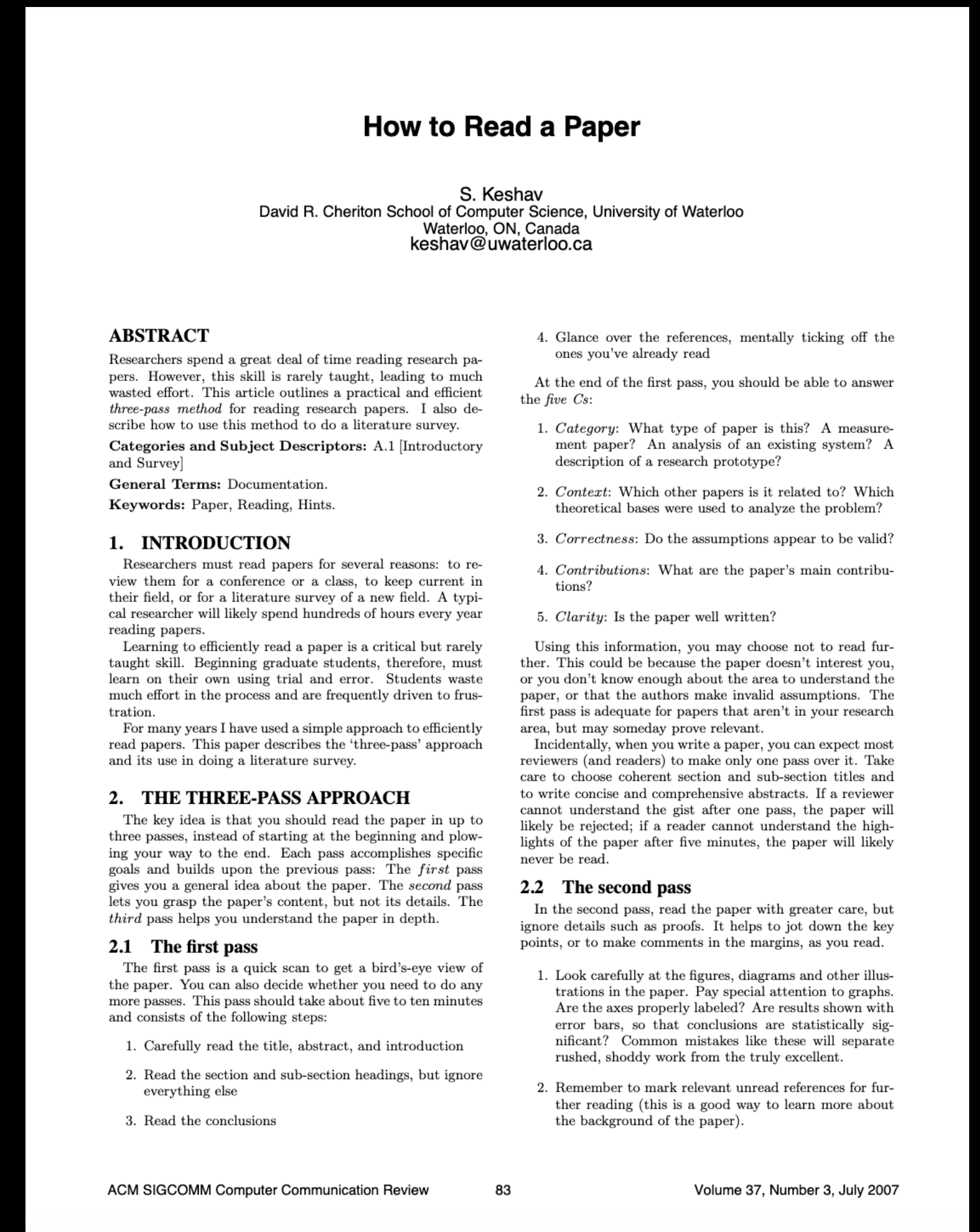
Your Presentation

- Research your assigned paper & read related literature
- If you have paper related questions:
Arrange meeting with me in the week before your presentation.
- Prepare presentation
- Send me your preliminary slides by the Monday before the presentation
(for a quick quality check)
- Give presentation
- Upload your final slides after the session

Reading your paper

The three-pass method

- First pass
 - Carefully read the abstract, introduction, and conclusions
 - Understand the context and contributions
- Second pass
 - Read the full content
 - Understand enough to explain the main idea and results
- Third pass
 - Understand deeply to virtually reimplement the work



[Link](#)

Structure of the talk

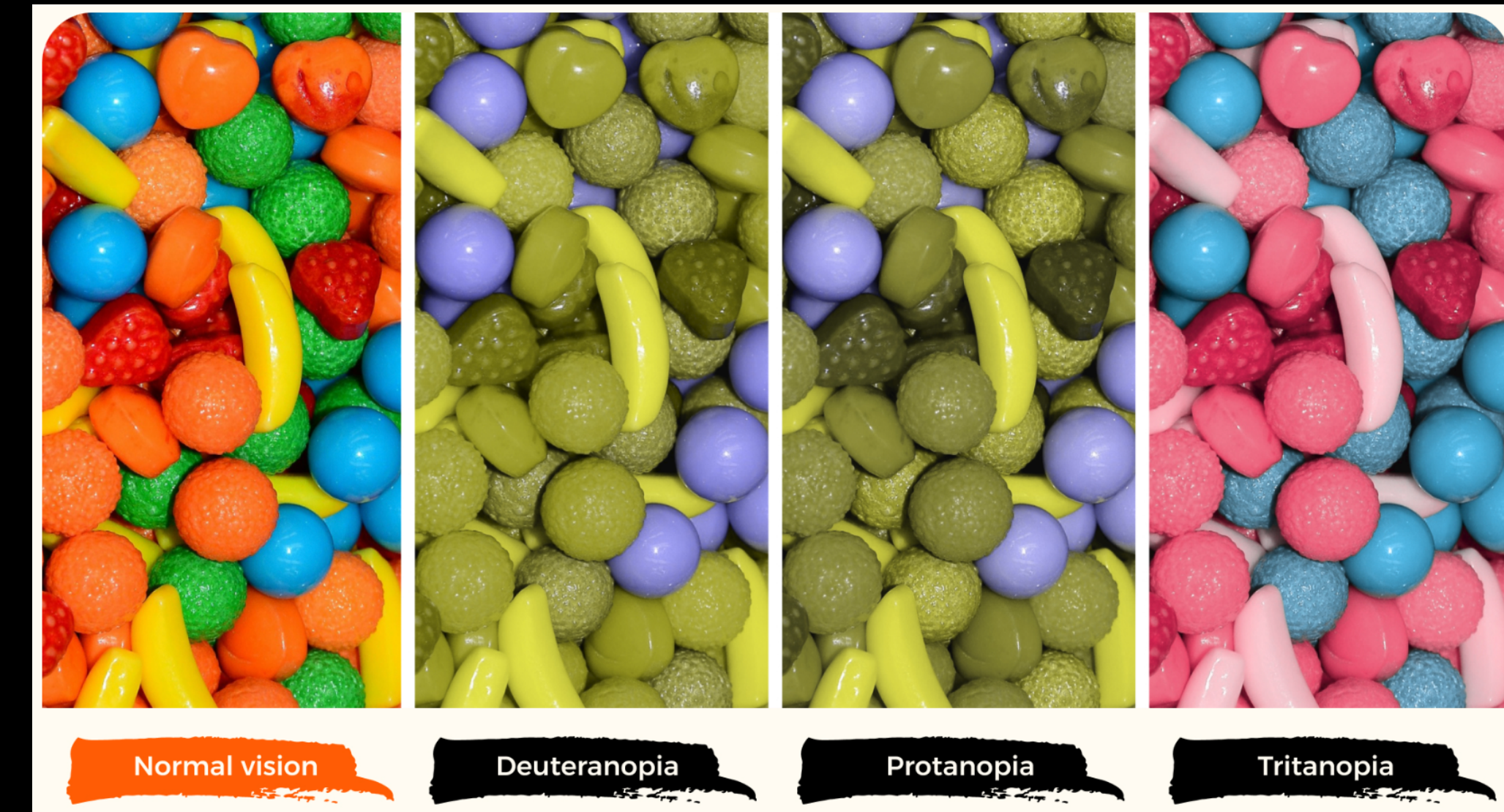
- Up to you!
- Depends a lot on topic/paper
- Example:
 - Motivation: Why should the audience care about the paper?
 - Method: Which method is used? How does it work? Are there similar other methods?
 - Experiments/Results: How do they evaluate their method?
 - Strengths & Limitations: Are there advantages/drawbacks?
 - Conclusion: What are the three main take-aways from this talk?

Slides

- What we do not want to see:
 - Too much text/equations/tables/images on one slide
 - Text with very small font
 - No visualizations / images
- What we want to see:
 - Visualizations of concepts, illustrative plots and figures
 - Making the (few!) equations easier to read, e.g. highlighting important terms with colors
 - References to papers, images, and plots

Accessibility

- Please be aware that people in your audience might have disabilities!
- Examples:
 - Colorblindness, Red-Green Weakness
 - Choose suitable colors
 - Difficulty seeing the slides (including people at the back of the room!)
 - Use large fonts and high contrast colors
 - Describe in words what you see in figures and plots
e.g. axis labeling, trends in the graph, ...
 - Difficulty concentrating or hearing
 - Option to annotate slides and provide them before the talk



1 in 12 men, 1 in 200 women!

Accessibility

- Resources:
 - Contrast Checker
 - Color Blind Vision Simulator
 - Microsoft Office Accessibility Checker
 - Many more webpages, e.g. Guide to Accessible Presentation Design
- If you need specific adjustments in order to participate in this seminar, please reach out to us via email and we will do what we can!

Resources

- Ted Talks:
 - [How to avoid death by PowerPoint](#)
 - [The secret structure of great talks](#)
 - [How to speak so that people want to listen](#)
- Articles
 - [How to make a good presentation great](#)
 - [Storytelling in presentations](#)
- Ask ChatGPT, e.g. to get an idea about the structure of your talk

What you have to do

When others present

- We expect you ...
 - To be interested in the presentations of others
 - To read one (of the two) papers before each meeting
 - To write a summary of the one paper and upload it before the meeting
 - To ask questions and actively participate in the discussion session

What you have to do

Final Report

- Research your assigned paper & read related literature
- Write report (critical review) in ICML template
 - Do not copy the paper! Short summary of method and results.
 - What are the limitations/weaknesses of the paper?
 - How has it been adopted? How would you extend the paper?
- Hand in the report until 27 Feb 2026 EOD

How we will help you

- Answer your questions
- (Optionally) meet with you the week before your talk to discuss the paper and answer your questions
- (Optionally) provide you with feedback before the presentation about the slides
- (Optionally) give you feedback after the presentation

You have to tell us whether you want a meeting & feedback! Be proactive!

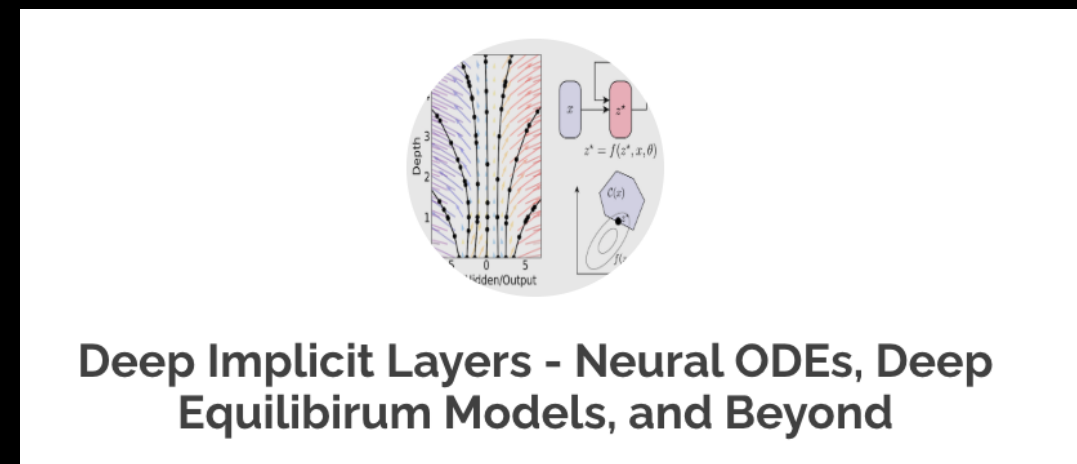
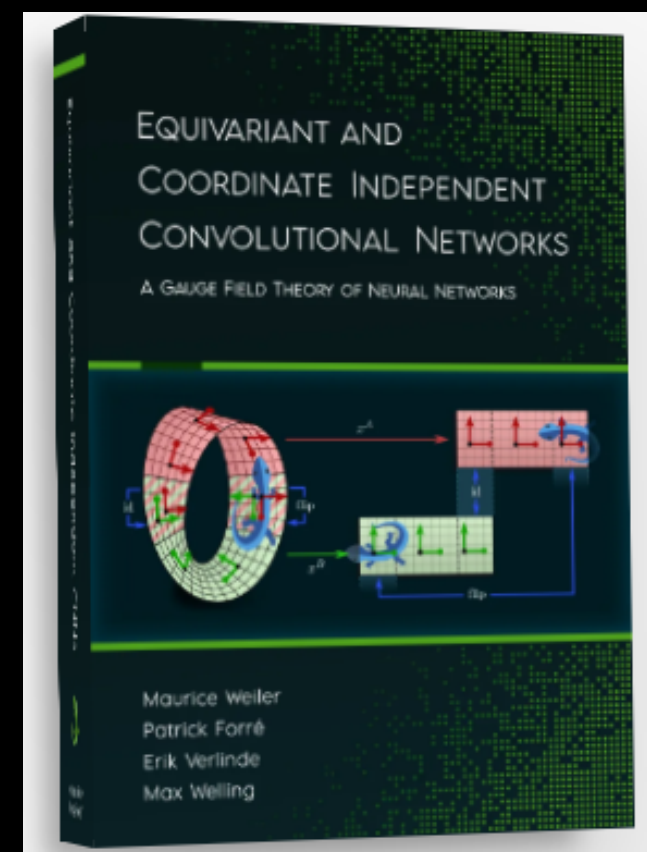
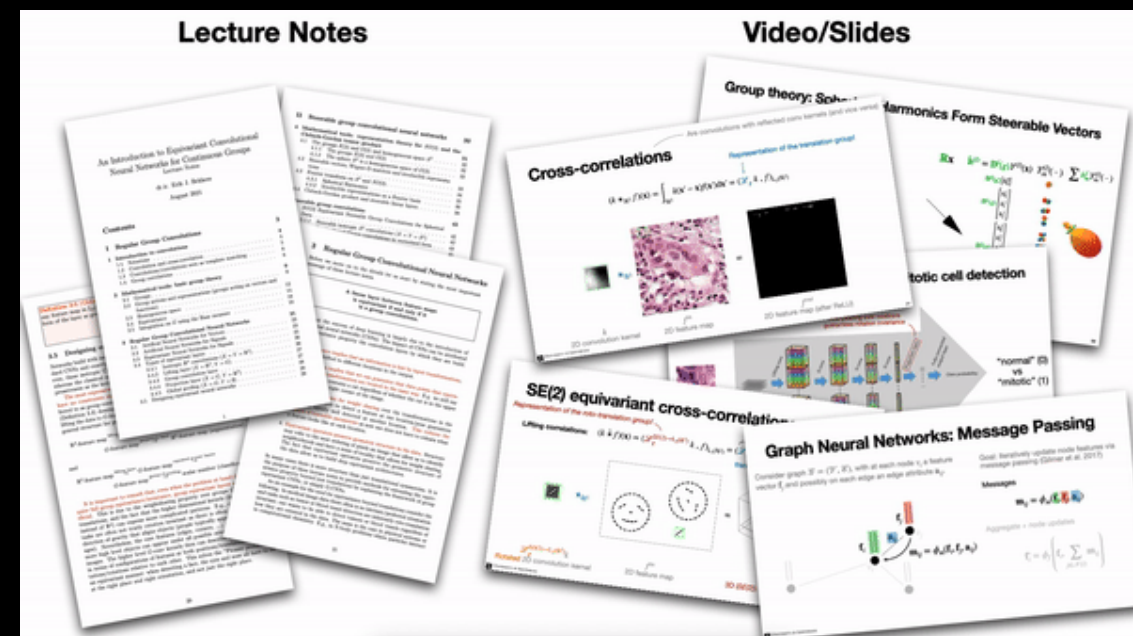
Outcomes

- Deep understanding of your chosen paper
- Good familiarity with the latest and important papers in the area
- Practice for scientific presentation and writing
 - in the future: more important presentations / reports than this seminar
e.g. Master's thesis presentation, pitch to promote your work project, ...
- Inspiration / toolkit for your future projects

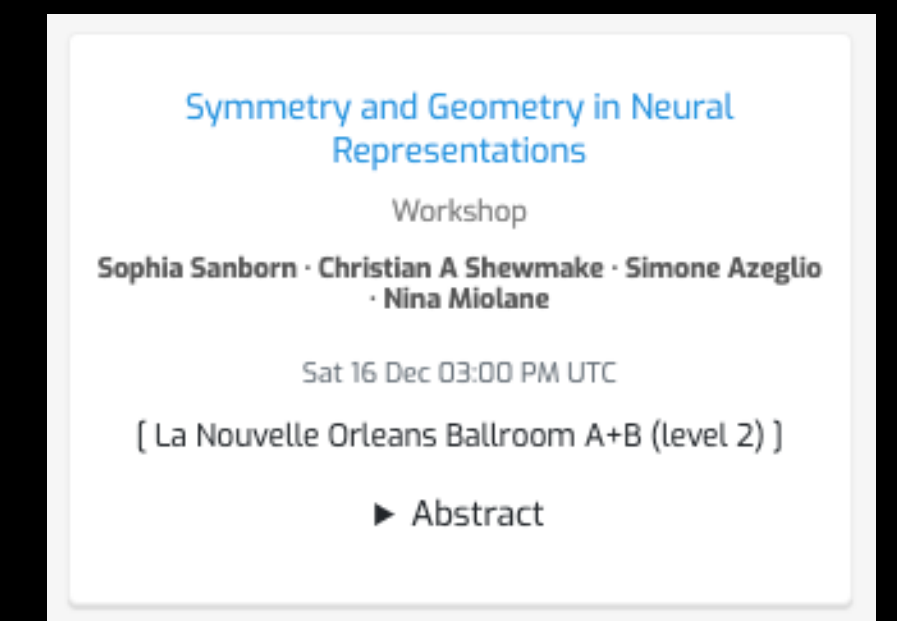
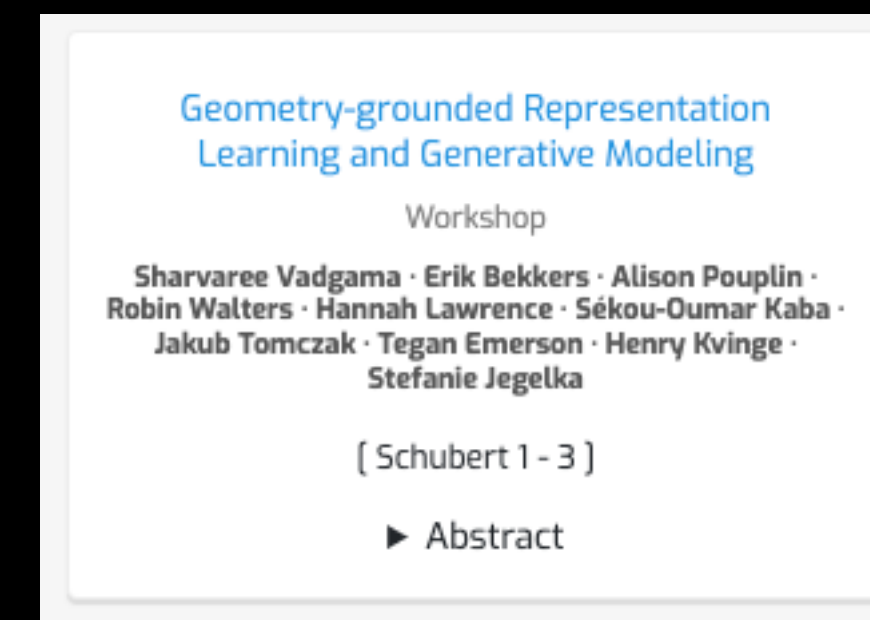
Warning

- Papers are dense in theory
 - ..which also makes it interesting
- I'm not an expert on these topics

Further resources



Online courses & Books



Workshops

<https://cvg.cit.tum.de/teaching/ws2024/dl4science>

Contact

- Mainly through the Discord Server.
Feel free to ask questions to everyone and share interesting events/papers!
- karnik.ram@tum.de
- CIT, 02.08.039
- <https://cvg.cit.tum.de/teaching/ws2025/dl-equi-dynam>