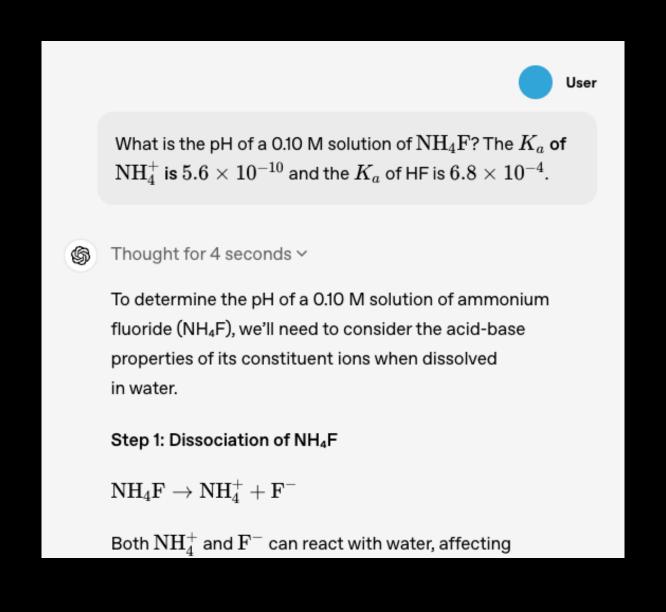
# Selected topics in DL: Equivariance & Dynamics

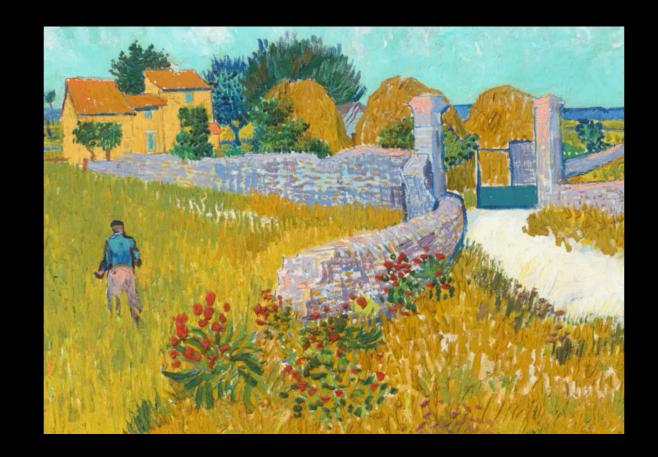
First meeting

# 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







Large language models

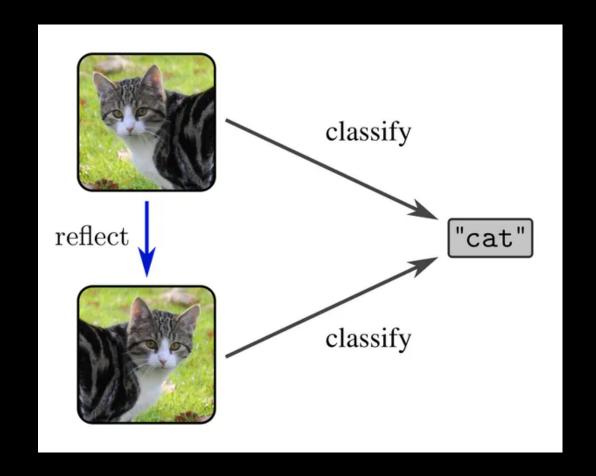
Segment Anything Model

phi-0.5: Vision language action model

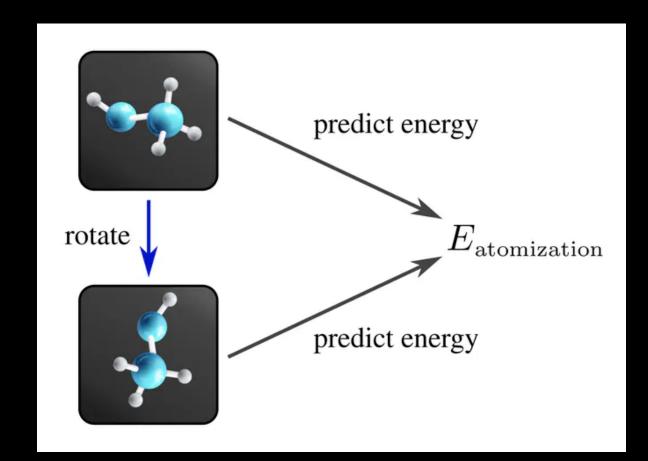
# Unconstrained large-scale learning

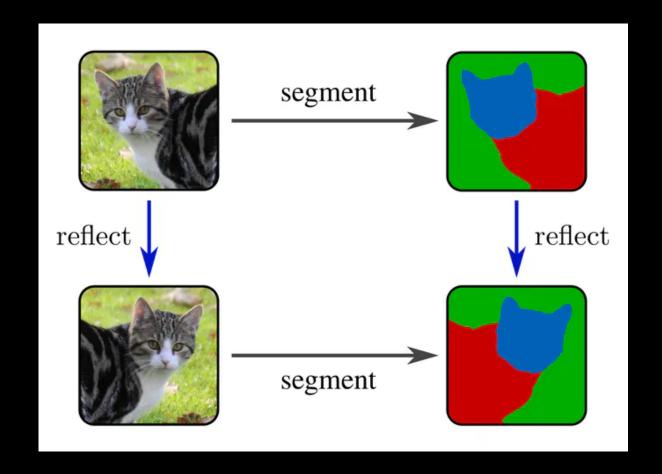
Is attention and scaling all you need?

### Symmetries

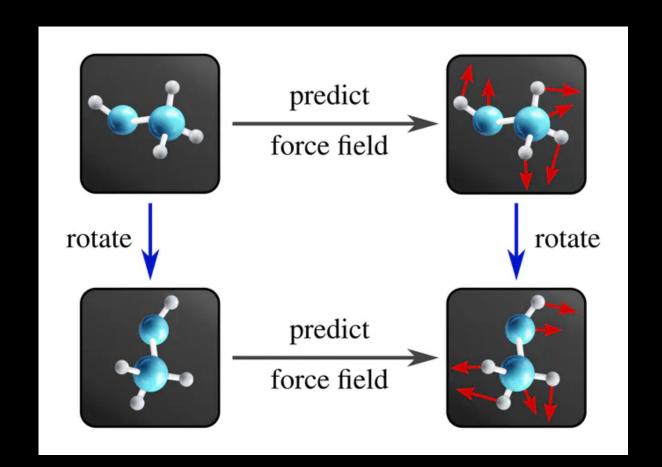


#### Invariance

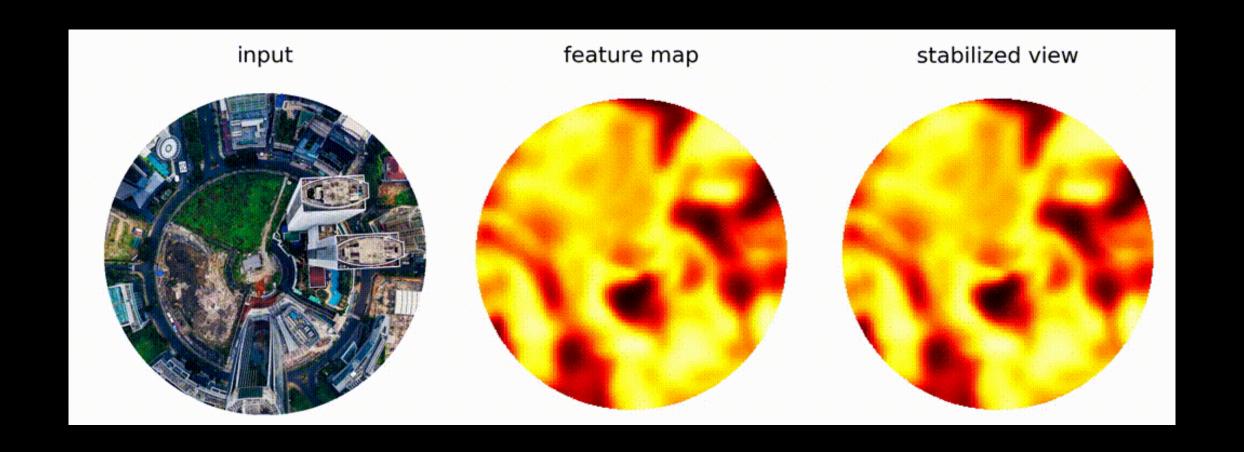




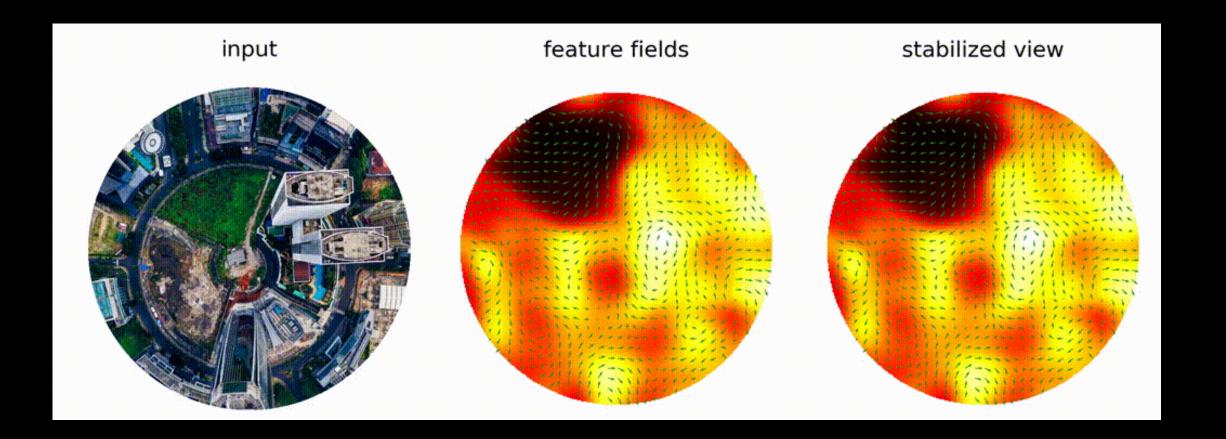
Equivariance



Symmetries

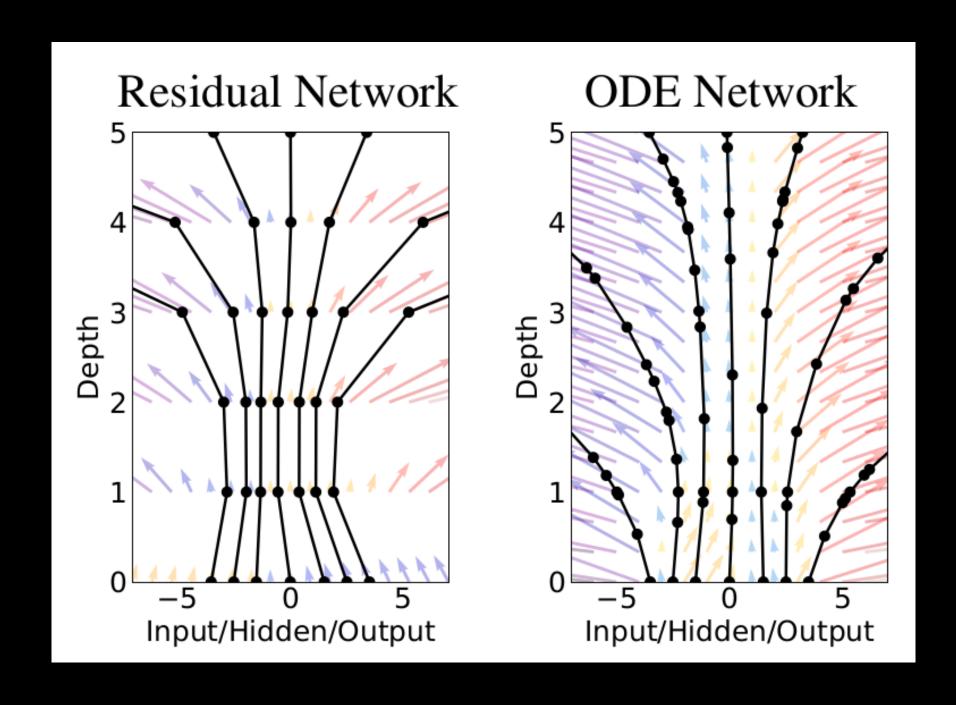


CNN

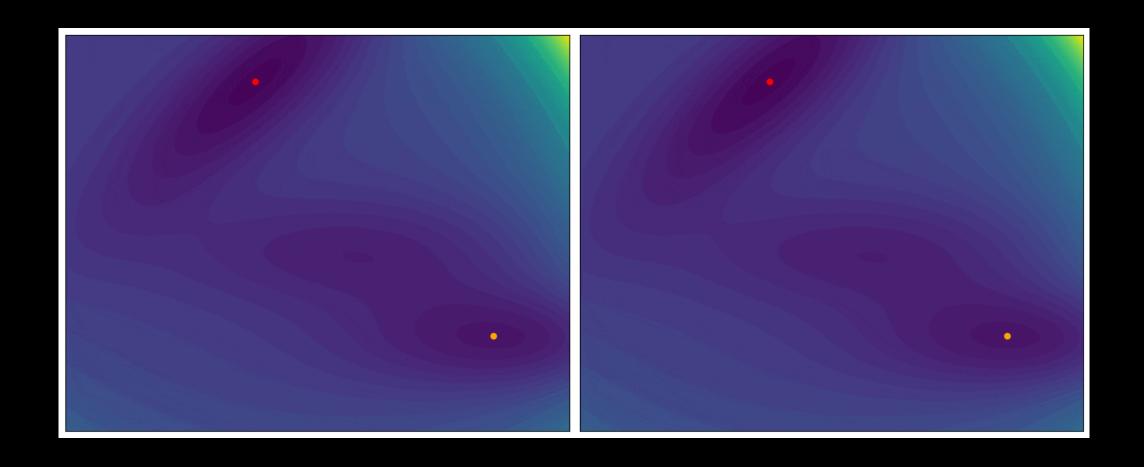


Group-CNN

### Dynamics



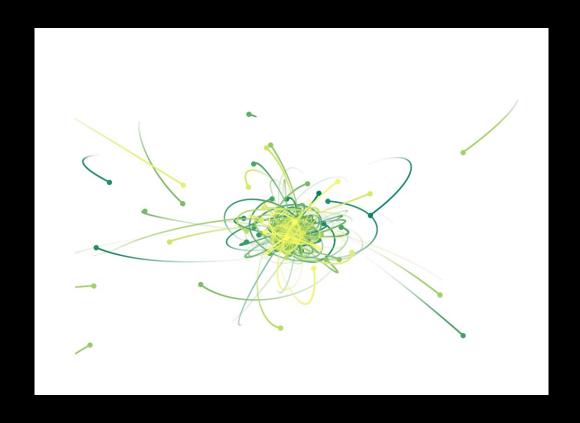
Neural ODE (Chen et al.)



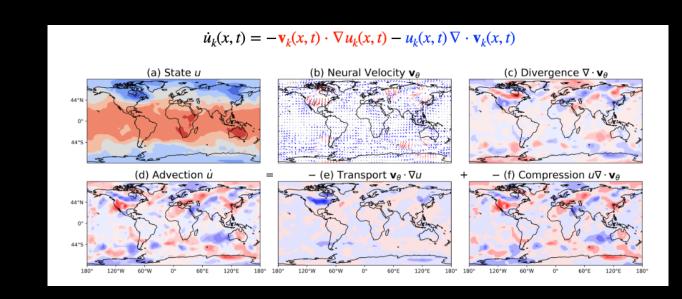
Path Sampling (Du et al.)

### Applications

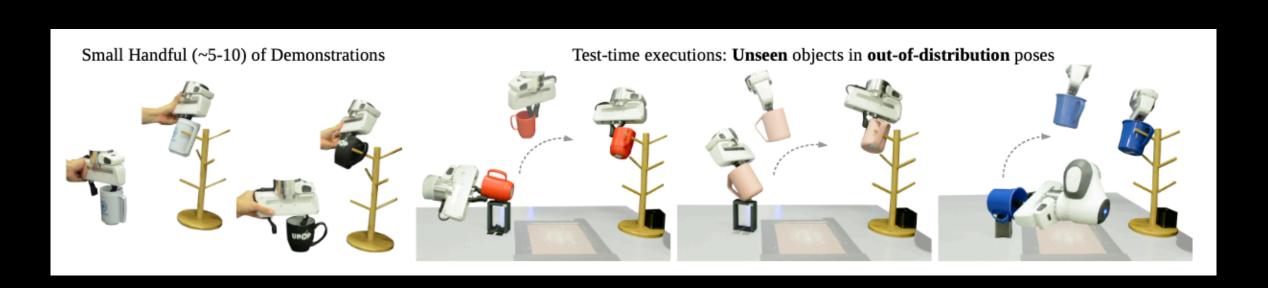
- Architectures with symmetry-preserving guarantees
- Architectures leveraging known dynamics
- Efficient representation learning
  - Data efficiency
  - Compute efficiency\*



N-body dynamics



ClimODE



Neural Descriptor Fields

# 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

#### How to Read a Paper

S. Keshav
David R. Cheriton School of Computer Science, University of Waterloo
Waterloo, ON, Canada
keshav@uwaterloo.ca

#### ABSTRACT

Researchers spend a great deal of time reading research papers. However, this skill is rarely taught, leading to much wasted effort. This article outlines a practical and efficient three-pass method for reading research papers. I also describe how to use this method to do a literature survey.

Categories and Subject Descriptors: A.1 [Introductory and Survey]

General Terms: Documentation.

Keywords: Paper, Reading, Hints.

#### 1. INTRODUCTION

Researchers must read papers for several reasons: to review them for a conference or a class, to keep current in their field, or for a literature survey of a new field. A typical researcher will likely spend hundreds of hours every year reading papers.

Learning to efficiently read a paper is a critical but rarely taught skill. Beginning graduate students, therefore, must learn on their own using trial and error. Students waste much effort in the process and are frequently driven to frustration.

For many years I have used a simple approach to efficiently read papers. This paper describes the 'three-pass' approach and its use in doing a literature survey.

#### 2. THE THREE-PASS APPROACH

The key idea is that you should read the paper in up to three passes, instead of starting at the beginning and plowing your way to the end. Each pass accomplishes specific goals and builds upon the previous pass: The *first* pass gives you a general idea about the paper. The *second* pass lets you grasp the paper's content, but not its details. The *third* pass helps you understand the paper in depth.

#### 2.1 The first pass

The first pass is a quick scan to get a bird's-eye view of the paper. You can also decide whether you need to do any more passes. This pass should take about five to ten minutes and consists of the following steps:

- 1. Carefully read the title, abstract, and introduction
- 2. Read the section and sub-section headings, but ignore everything else  $\,$
- 3. Read the conclusions

 Glance over the references, mentally ticking off the ones you've already read

At the end of the first pass, you should be able to answer ae  $five\ Cs$ :

- Category: What type of paper is this? A measurement paper? An analysis of an existing system? A description of a research prototype?
- 2. Context: Which other papers is it related to? Which theoretical bases were used to analyze the problem?
- 3. Correctness: Do the assumptions appear to be valid?
- 4. Contributions: What are the paper's main contributions?
- 5. Clarity: Is the paper well written?

Using this information, you may choose not to read further. This could be because the paper doesn't interest you, or you don't know enough about the area to understand the paper, or that the authors make invalid assumptions. The first pass is adequate for papers that aren't in your research area, but may someday prove relevant.

Incidentally, when you write a paper, you can expect most reviewers (and readers) to make only one pass over it. Take care to choose coherent section and sub-section titles and to write concise and comprehensive abstracts. If a reviewer cannot understand the gist after one pass, the paper will likely be rejected; if a reader cannot understand the highlights of the paper after five minutes, the paper will likely never be read.

#### 2.2 The second pass

In the second pass, read the paper with greater care, but ignore details such as proofs. It helps to jot down the key points, or to make comments in the margins, as you read.

- Look carefully at the figures, diagrams and other illustrations in the paper. Pay special attention to graphs.
   Are the axes properly labeled? Are results shown with error bars, so that conclusions are statistically significant? Common mistakes like these will separate rushed, shoddy work from the truly excellent.
- Remember to mark relevant unread references for further reading (this is a good way to learn more about the background of the paper).

ACM SIGCOMM Computer Communication Review

Volume 37, Number 3, July 2007



### Structure of the talk

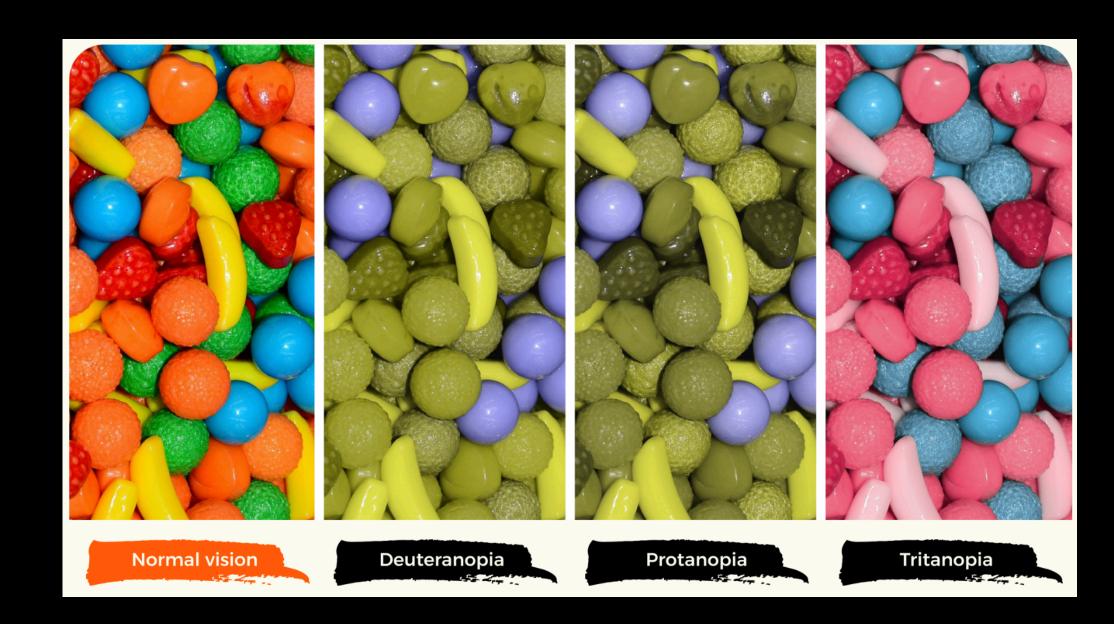
- Up to you!
- Depends a lot on topic/paper
- Example:
  - Motivation: Why should the audience care about the paper?
  - Method: Which method is used? How does it work? Are there similar other methods?
  - Experiments/Results: How do they evaluate their method?
  - Strengths & Limitations: Are there 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!

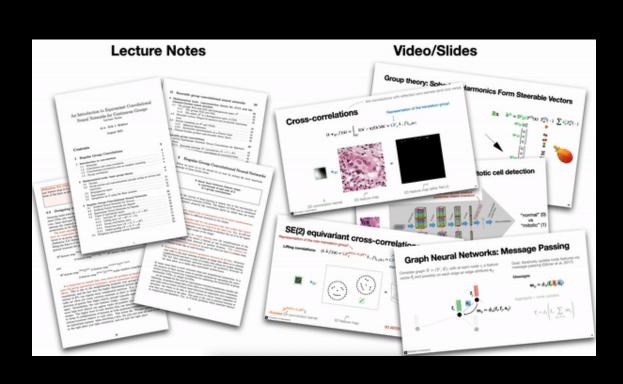
### Outcomes

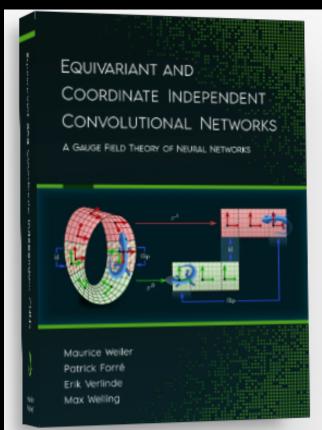
- Deep understanding of your chosen paper
- Good familiarity with the latest and important papers in the area
- Practice for scientific presentation and writing
  - in the future: more important presentations / reports than this seminar e.g. Master's thesis presentation, pitch to promote your work project,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

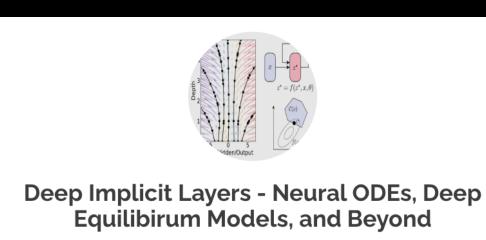
# Warning

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

# Further resources







Online courses & Books

#### Geometry-grounded Representation Learning and Generative Modeling

Workshop

Sharvaree Vadgama · Erik Bekkers · Alison Pouplin · Robin Walters · Hannah Lawrence · Sékou-Oumar Kaba · Jakub Tomczak · Tegan Emerson · Henry Kvinge · Stefanie Jegelka

[Schubert 1-3]

Abstract

#### ML for Life and Material Science: From Theory to Industry Applications

Workshop

Aviv Regev · Andrea Volkamer · Bruno Trentini · Cecilia Clementi · Charles Harris · Charlotte Deane · Christian Dallago · Ellen Zhong · Francesca Grisoni · Jinwoo Leem · Kevin Yang · Marwin Segler · Michael Pieler · Nicholas Sofroniew · Olivia Viessmann · Peter Koo · Pranam Chatterjee · Puck Van Gerwen · Rebecca Lindsay · Umberto Lupo · Ying Wai Li

Fri 26 Jul 07:00 AM UTC

[Stolz 2]

Abstract

#### Symmetry and Geometry in Neural Representations

Workshop

Sophia Sanborn · Christian A Shewmake · Simone Azeglio · Nina Miolane

Sat 16 Dec 03:00 PM UTC

[ La Nouvelle Orleans Ballroom A+B (level 2) ]

Abstract

#### Optimal Transport and Machine Learning

Workshop

Anna Korba · Aram-Alexandre Pooladian · Charlotte Bunne · David Alvarez-Melis · Marco Cuturi · Ziv Goldfeld

Sat 16 Dec 02:30 PM UTC

( Room 220 - 222 )

Abstract

Workshops

## 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