Selected topics in DL: Equivariance & Dynamics

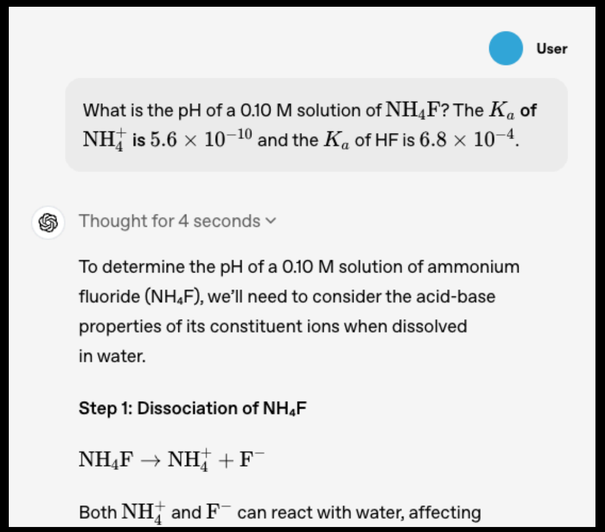
First meeting

CVG, 29.04.2025

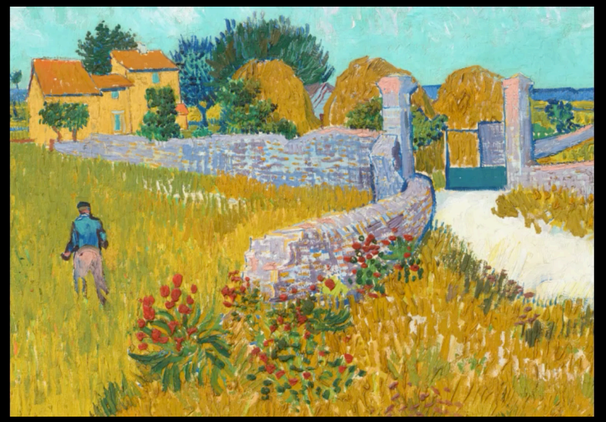
About me

- 2nd year PhD student in the computer vision group
- Research focus: Machine learning for molecular science
  - Neural free energies for dynamical density functional theory
- Application focus: Material discovery for carbon capture

Unconstrained large-scale learning



Large language models



Segment Anything Model

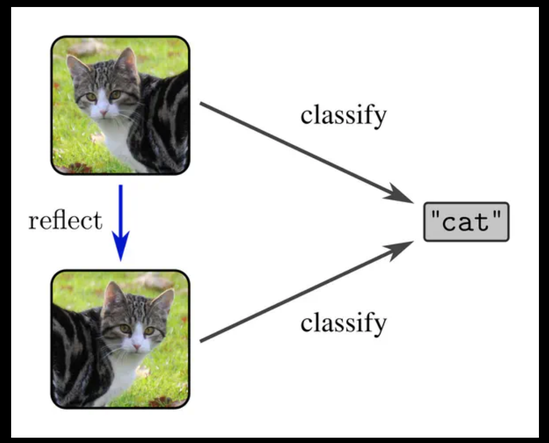
phi-0.5: Vision language action model

Unconstrained large-scale learning

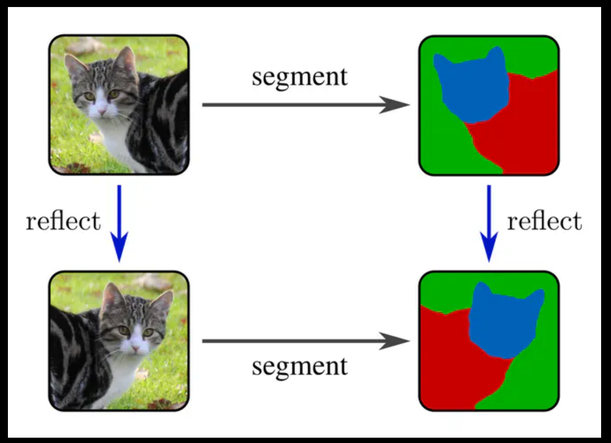
Is attention and scaling all you need?

Structure-preserving learning

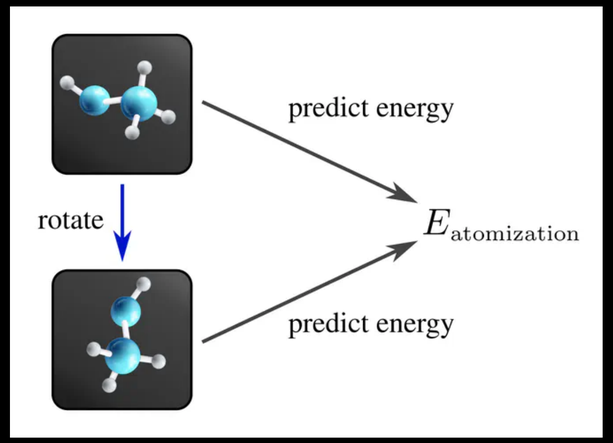
Symmetries

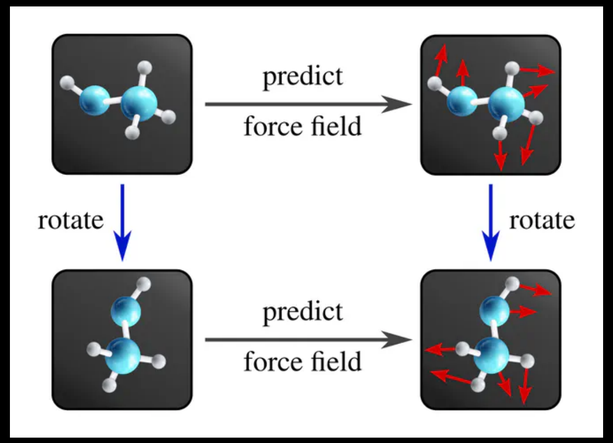


Invariance



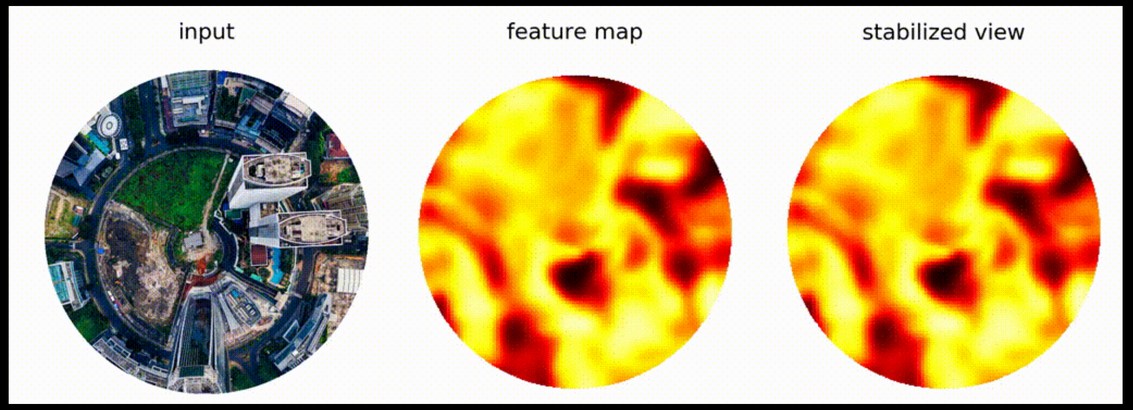
Equivariance



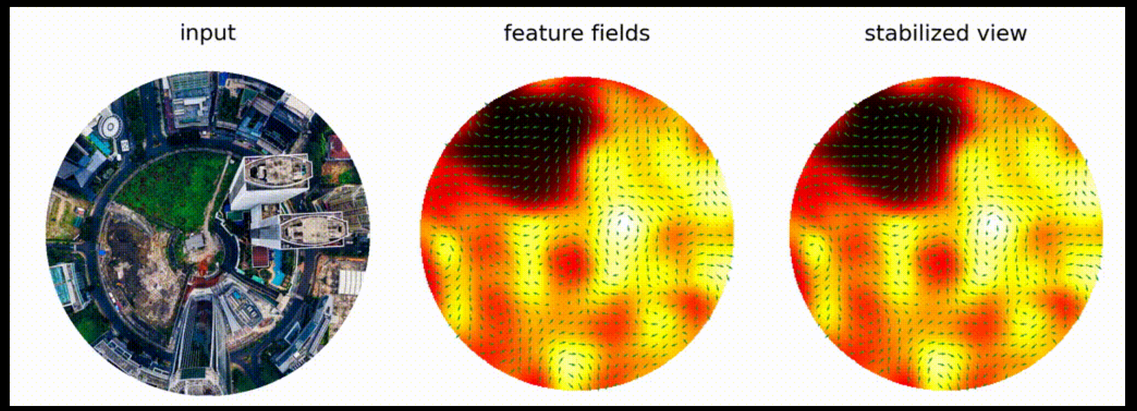


Structure-preserving learning

Symmetries



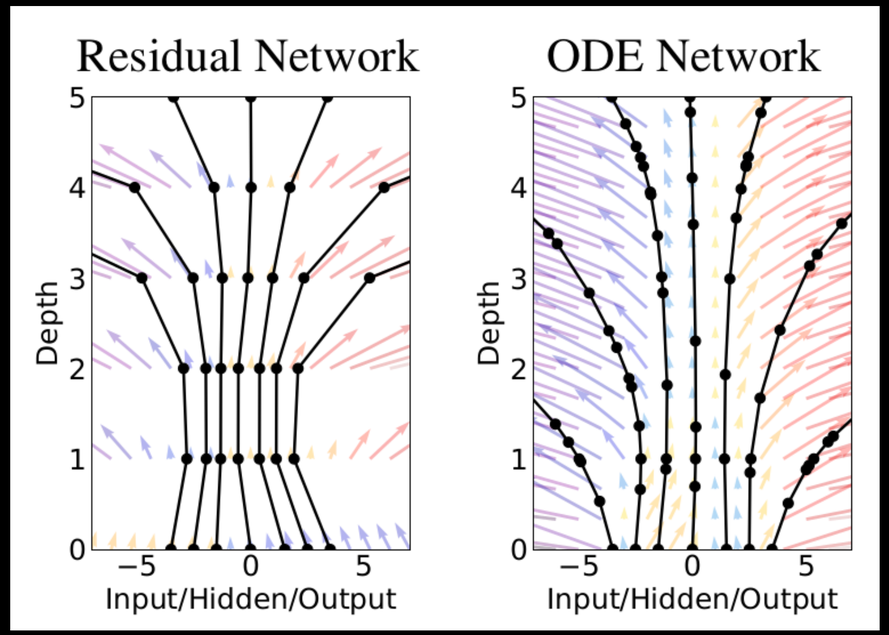
CNN



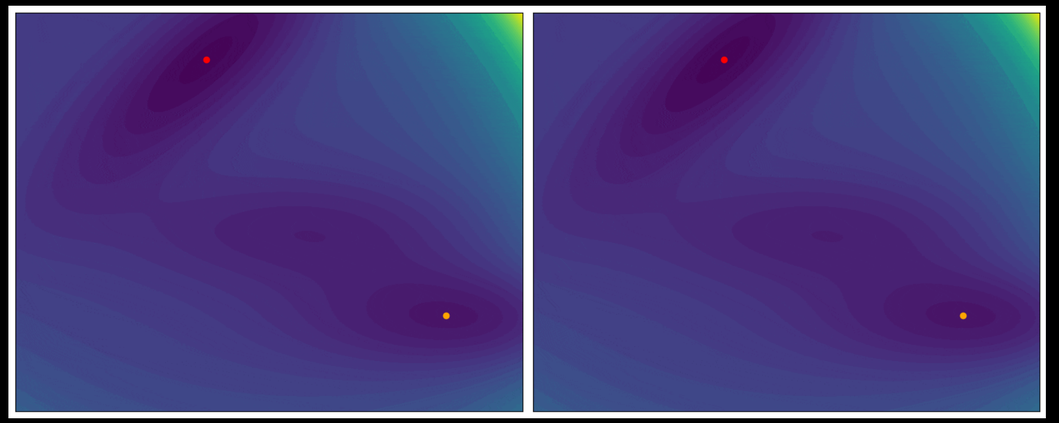
Group-CNN

Structure-preserving learning

Dynamics



Neural ODE
(Chen et al.)

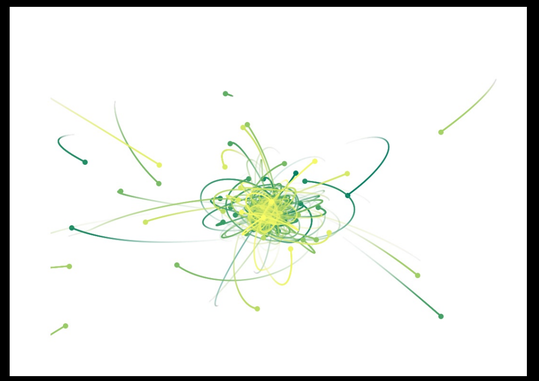


Path Sampling
(Du et al.)

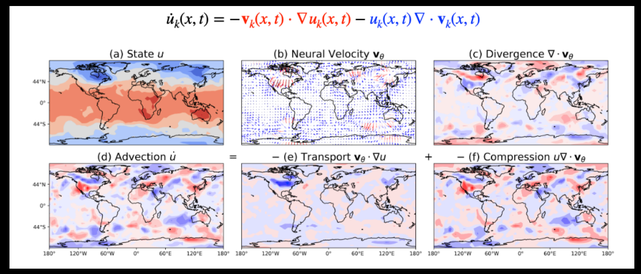
Structure-preserving learning

Applications

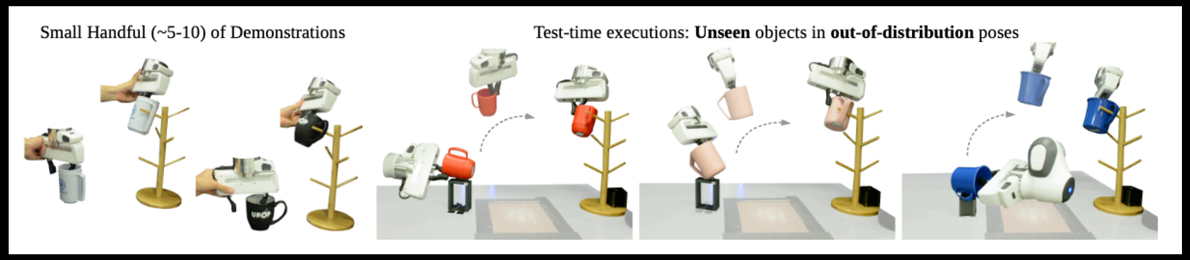
- Architectures with symmetry-preserving guarantees
- Architectures leveraging known dynamics
- Efficient representation learning
  - Data efficiency
  - Compute efficiency*



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. 00.08.055
- Two paper presentations in every session
  - 30 - 35 minutes presentation + 10 minutes discussion

Date	Paper	Presenter	Material
29.04	Introduction		
20.05	Group Equivariant Convolutional Networks	Iñaky	
	SE(3)-Transformers: 3D Roto-Translation Equivariant Attention Networks	Omar	
27.05	Tensor field networks: Rotation- and translation-equivariant neural networks for 3D point clouds	Gleb	
	Equivariance with Learned Canonicalization Functions	Gianluca	
17.06	Geometric Algebra Transfromers	Yung Jhang	
	Spherical Channels for Modeling Atomic Interactions	Jean-Pasqual	
24.06	Neural Ordinary Differential Equations	Yaxuan	
	ClimODE: Climate and Weather Forecasting with Physics-informed Neural ODEs	Aditi	
08.07	Equivariant Spatio-Temporal Attentive Graph Networks to Simulate Physical Dynamics	Celia	
	Continuous PDE Dynamics Forecasting with Implicit Neural Representations	Clemens	

What you have to do
Your Presentation

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

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 paper and hand it in before the meeting
  - To ask questions and 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 08.25 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!

Evaluation*

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

Outcomes

- Deep understanding of your chosen paper
- Good familiarity with the latest and important papers in the area
- Practice for scientific presentation and writing
- Inspiration / toolkit for your future research projects

Presenting

Why should you care?

- in the future: more important presentations than this seminar
  e.g. Master's thesis presentation, pitch to promote your work project, ...
- More will depend on it than a grade, e.g. whether you get a job
- People will listen and enjoy your presentation!

Know your audience

- Why should they care about your presentation?
- What is important for your audience/What are they interested in?
- What is the background of the audience?
- Which concepts might they not know that seem simple to you?
- What should the audience learn from your talk?

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

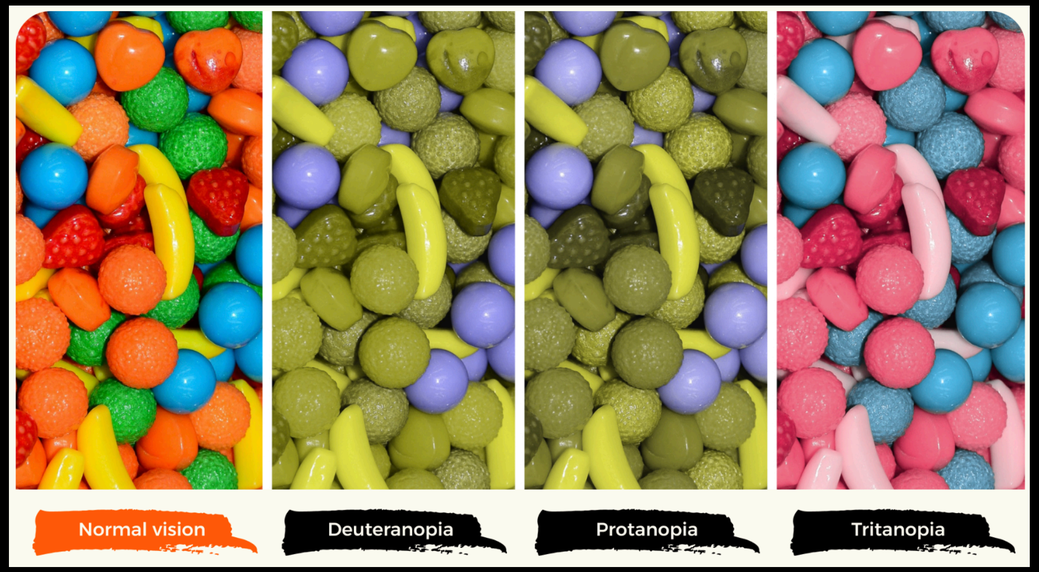
- What we do not want to see:
  - Too much text/equations/tables/images on one slide
  - Text with very small font
  - No visualizations / images
- What we want to see:
  - Visualizations of concepts, illustrative plots and figures
  - Making the (few!) equations easier to read, e.g. highlighting important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

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

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

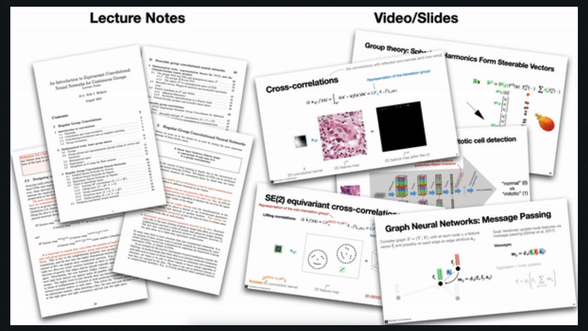
- Resources:
    - Contrast Checker
    - Color Blind Vision Simulator
    - Microsoft Office Accessibility Checker
    - Many more webpages, e.g. Guide to Accessible Presentation Design

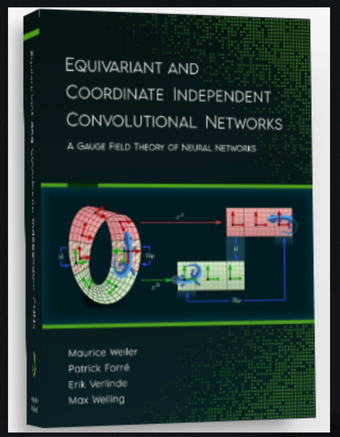
- If you need specific adjustments in order to participate in this seminar, please reach out to us via email and we will do what we can!

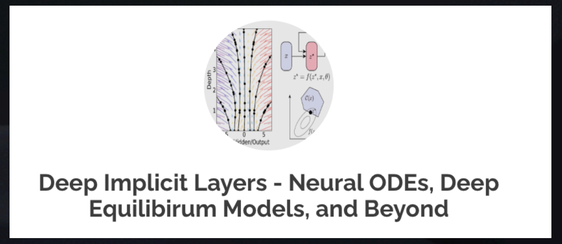
Warning

- First offering of the seminar
  - Expect some rough edges!
- Papers are dense in theory
  - ..which also makes it interesting
- I’m not an expert on these topics

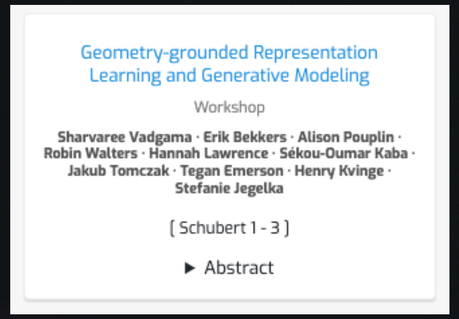
Further resources

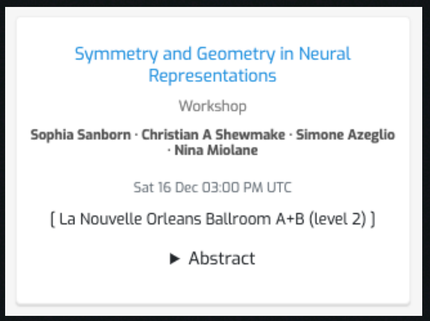






Online courses & Books





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, 02.08.038
- https://cvg.cit.tum.de/teaching/ss2025/dl-equi-dynam