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

Use

What is the pH of a 0.10 M solution of NH_4F ? The K_a of NH_4^+ is $5.6 imes10^{-10}$ and the K_a of HF is $6.8 imes10^{-4}$.

S Thought for 4 seconds ~

To determine the pH of a 0.10 M solution of ammonium fluoride (NH₄F), we'll need to consider the acid-base properties of its constituent ions when dissolved in water.

Step 1: Dissociation of NH₄F

 $m NH_4F
ightarrow
m NH_4^+ + F^-$

Both ${
m NH}_4^+$ and ${
m F}^-$ can react with water, affecting

Large language models



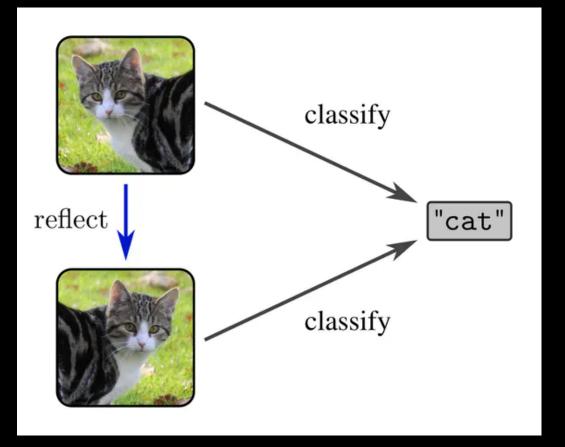
Segment Anything Model



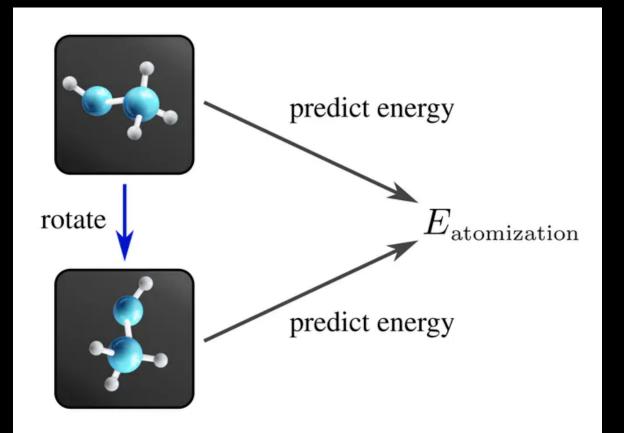
phi-0.5: Vision language action model

Unconstrained large-scale learning Is attention and scaling all you need?

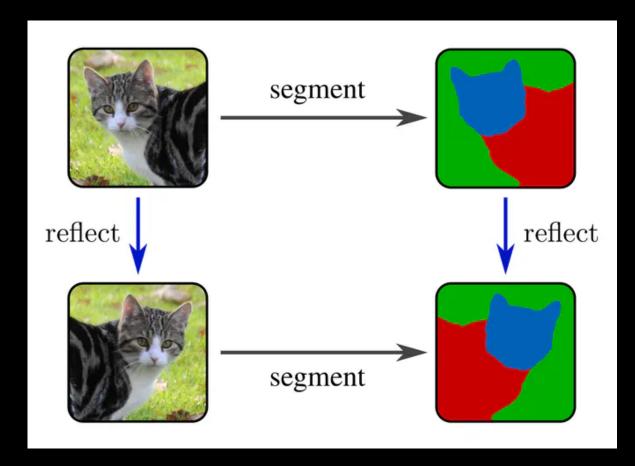
Structure-preserving learning Symmetries



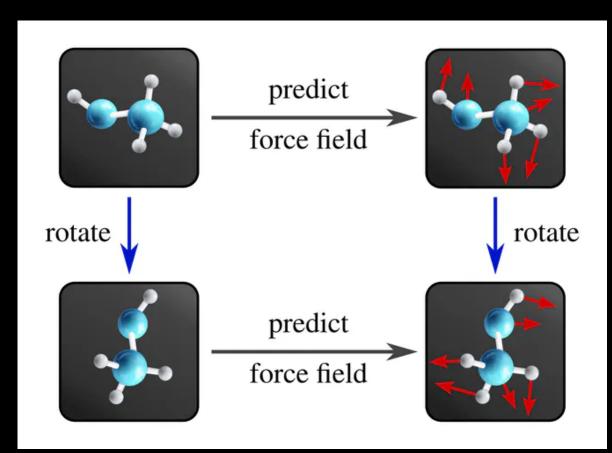
Invariance



Maurice Weiler

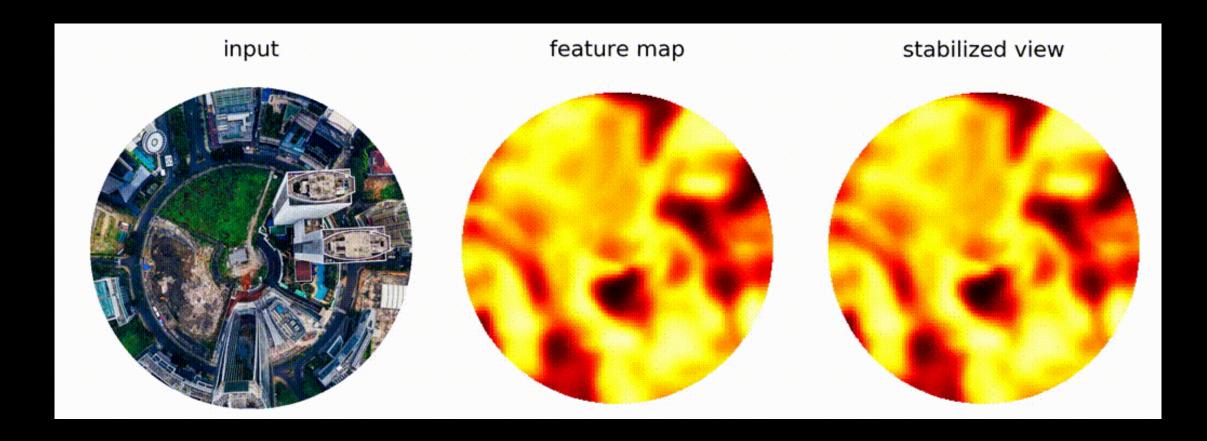


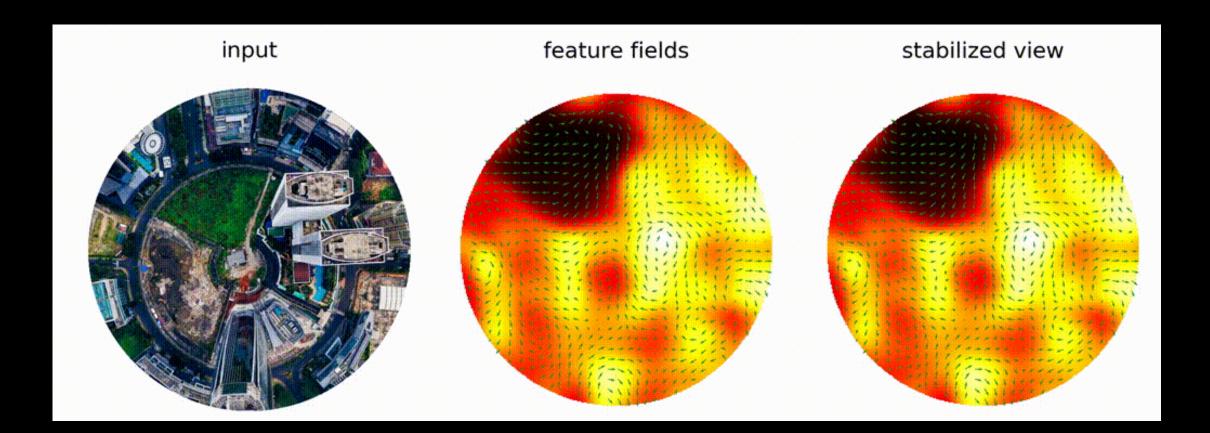
Equivariance





Symmetries



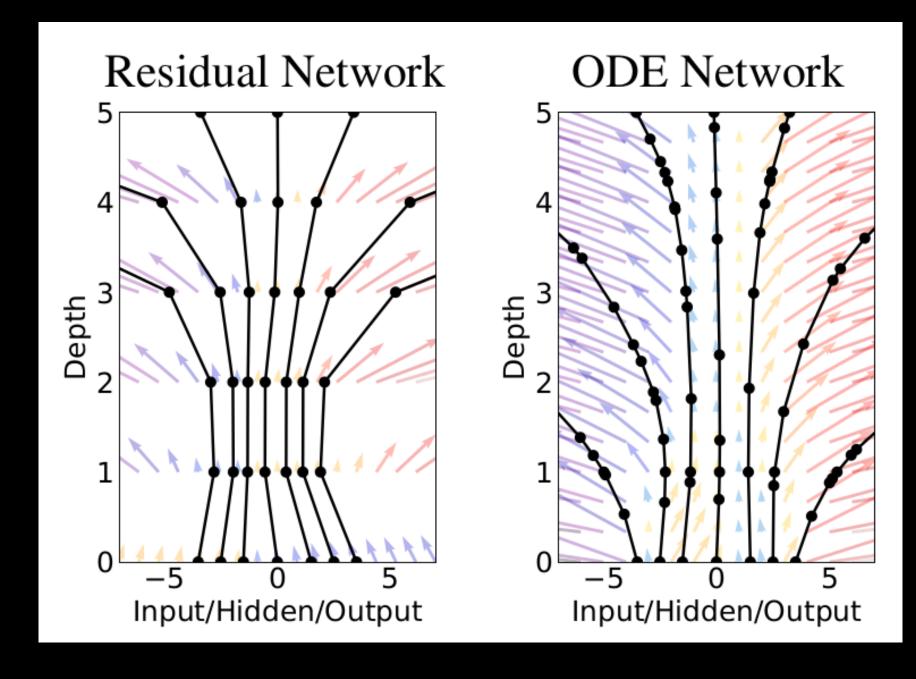


Maurice Weiler & Gabriel Cesa

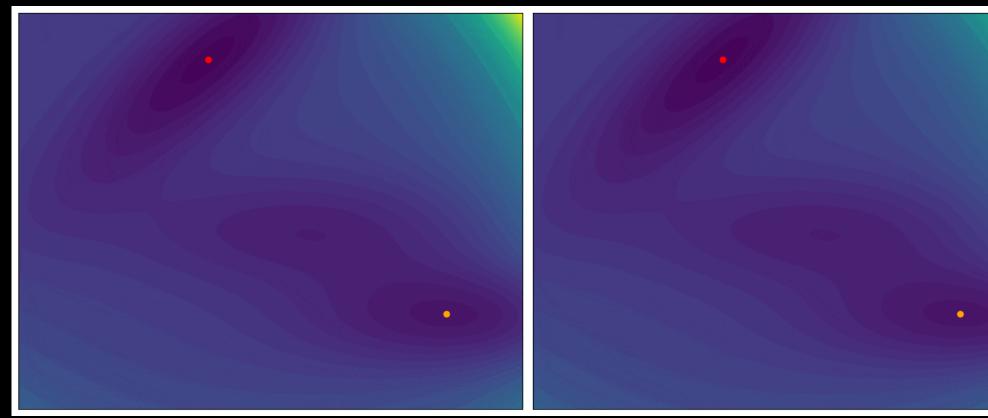


Group-CNN

Structure-preserving learning Dynamics



Neural ODE (Chen et al.)



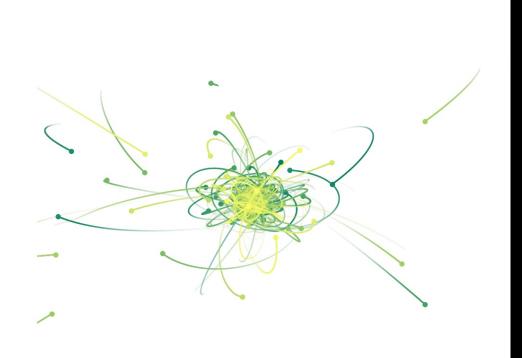
Path Sampling (Du et al.)

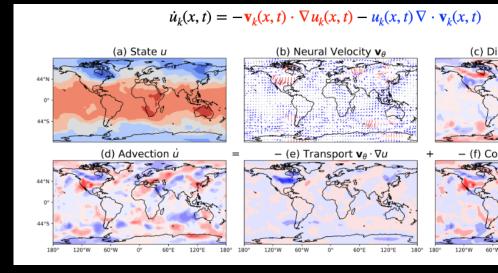


Structure-preserving learning Applications

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

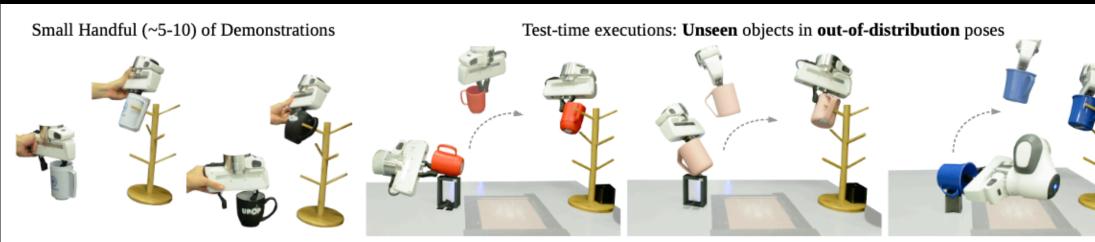
* Brehmer et al., Does Equivariance Matter at Scale?





ClimODE

N-body dynamics



Neural Descriptor Fields

vergence $\nabla \cdot \mathbf{v}_{\theta}$ The second second

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	lñaky	
	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 ightarrow
- If you have questions: ightarrowArrange 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
- 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!

(Optionally) meet with you the week before your talk to discuss the paper and answer your

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 ullet

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 \bullet
- 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! \bullet
- Depends a lot on topic/paper
- Example:
 - Motivation: Why should the audience care about the paper? ullet
 - Method: Which method is used? How does it work? Are there similar other methods? ullet
 - Experiments/Results: How do they evaluate their method? ightarrow
 - Strengths & Limitations: Are there advantages/drawbacks? ightarrow
 - 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 ullet
 - No visualizations / images ullet
- What we want to see:
 - Visualizations of concepts, illustrative plots and figures ullet
 - ullet
 - References to papers, images, and plots ightarrow

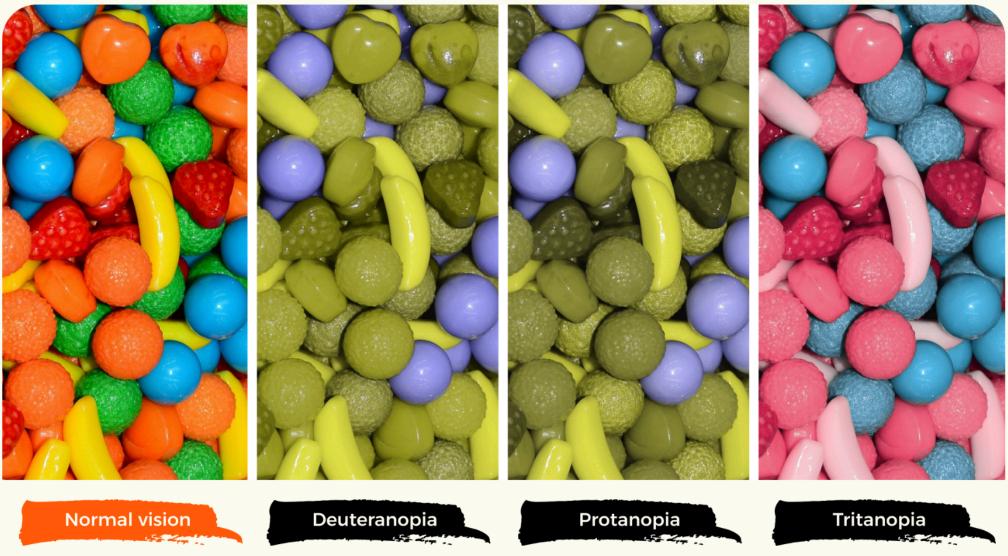
Making the (few!) equations easier to read, e.g. highlighting important terms with colors

Resources

- Ted Talks:
 - How to avoid death by PowerPoint
 - <u>The secret structure of great talks</u>
 - How to speak so that people want to listen
 - Articles
 - How to make a good presentation great
 - Storytelling in presentations ightarrow
 - 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 ightarrow \rightarrow Choose suitable colors
 - Difficulty seeing the slides (including people at the back of the room!) \bullet \rightarrow Use large fonts and high contrast colors \rightarrow Describe in words what you see in figures and plots e.g. axis labeling, trends in the graph, ...
 - Difficulty concentrating or hearing \rightarrow 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

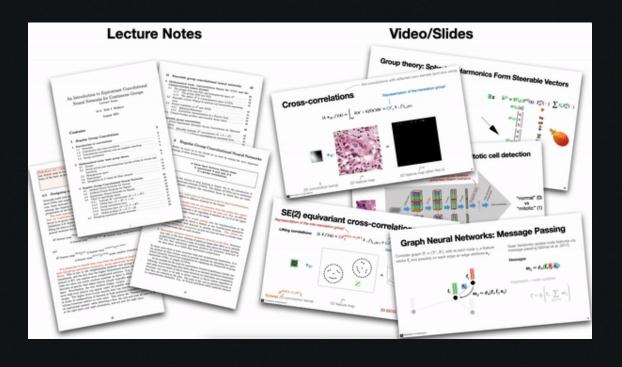
via email and we will do what we can!

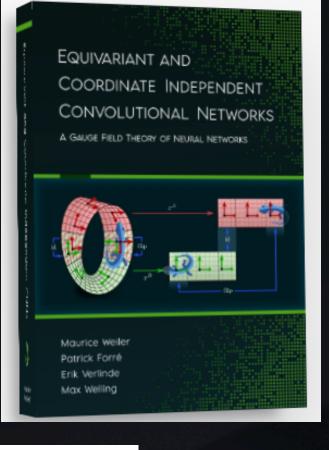
If you need specific adjustments in order to participate in this seminar, please reach out to us

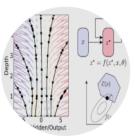
Warning

- 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







Deep Implicit Layers - Neural ODEs, Deep Equilibirum Models, and Beyond

Online courses & Books

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

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



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

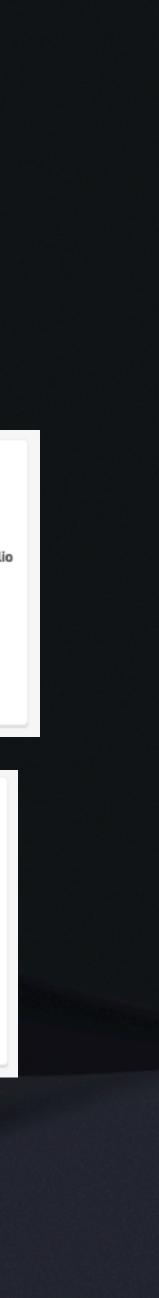
Anna Korba · Aram-Alexandre Pooladian · Charlotte Bunne · David Alvarez-Melis · Marco Cuturi · Ziv Goldfeld

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!
- <u>karnik.ram@tum.de</u>
- CIT, 02.08.038
- https://cvg.cit.tum.de/teaching/ss2025/dl-equi-dynamic