Autumn School on Scientific Machine Learning: wrap-up

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CWI

NDNS+

4TU.AMI

MATHEMATICS FOR INNOVATION

AI INSTITUTE IN DYNAMIC SYSTEMS

60 participants, 10 countries

- Netherlands: Delft, Eindhoven, Leiden, Twente, Amsterdam, Utrecht, Groningen
- Germany: Max-Planck, Kassel, München
- Belgium: KU Leuven
- France: INRIA
- Switzerland: EPFL
- Italy: SISSA, Politecnico Milano
- Spain: UPC Barcelona
- Norway: Bergen
- USA: Cornell
- Israel: Tel Aviv


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Day 1: Closure models

- We know the PDE but it is too expensive to solve:

$$\frac{\partial \boldsymbol{u}}{\partial t} = \boldsymbol{f}(\boldsymbol{u})$$

- **Filter** the PDE (remove small scales):

$$\bar{\boldsymbol{u}} = \Phi \boldsymbol{u}$$

- Filtered PDE is **not closed**:

$$\frac{\partial \bar{\boldsymbol{u}}}{\partial t} = \boldsymbol{f}(\bar{\boldsymbol{u}}) + \boldsymbol{c}(\boldsymbol{u}; \bar{\boldsymbol{u}})$$

- **Supervised learning** or **reinforcement learning**

$$\frac{\partial \bar{\boldsymbol{u}}}{\partial t} = \boldsymbol{f}(\bar{\boldsymbol{u}}) + \boldsymbol{m}(\bar{\boldsymbol{u}}; \theta)$$

- **Derivative fitting** vs **trajectory fitting** (automatic differentiation)

Day 2: Reduced order models

- We know the PDE but it is too expensive: $$\frac{\partial \boldsymbol{u}}{\partial t} = \boldsymbol{f}(\boldsymbol{u})$$
- **Approximate** u: $$\boldsymbol{u} \approx \boldsymbol{V}\hat{\boldsymbol{u}}$$
- **Project** (Galerkin): $$\frac{\partial \hat{\boldsymbol{u}}}{\partial t} = \boldsymbol{V}^T \boldsymbol{f}(\boldsymbol{V}\hat{\boldsymbol{u}})$$
- **POD is the workhorse**, but linear approximations are limited
- POD-NN: learn coefficients with a NN
- POD-GP: fit Gaussian process, gives uncertainty bands
- Many deep learning variants

Day 3: SINDy

$$\dot{X} = \Theta(X)\Xi$$

- We don't know the PDE/ODE but we have time-series data and want to derive a (symbolic) form
- We need **interpretability** and **generalizability**: low-dimensional and sparse
- In order to learn the physics, you need to learn the right coordinates
- SINDy **ingredients:** data, library, model selection, sensitivity to noise, ensemble methods

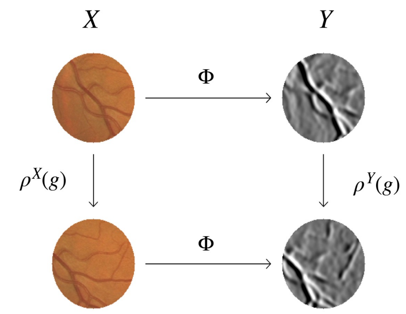
Day 4: Operator learning

- We know the PDE and want to develop a cheap surrogate

- Physics applications: need **neural operators** that map functions to functions

- **Manifold hypothesis**
- Linear decoders suffer from a “fundamental lower bound”, need **nonlinear manifold decoders**
- **Neural fields** provide a unifying viewpoint, which encapsulates existing methods (FNO, DeepONet, …) and gives ideas for new ones

Day 4: Equivariant learning



- We have image data and want efficient classification
- Don't do data augmentation
- Group theory describes translation, rotation, scaling as **group operations**
- Two important concepts: **invariance** vs **equivariance**

  $$f(g \cdot x) = f(x) \qquad\qquad f(g \cdot x) = g \cdot f(x)$$

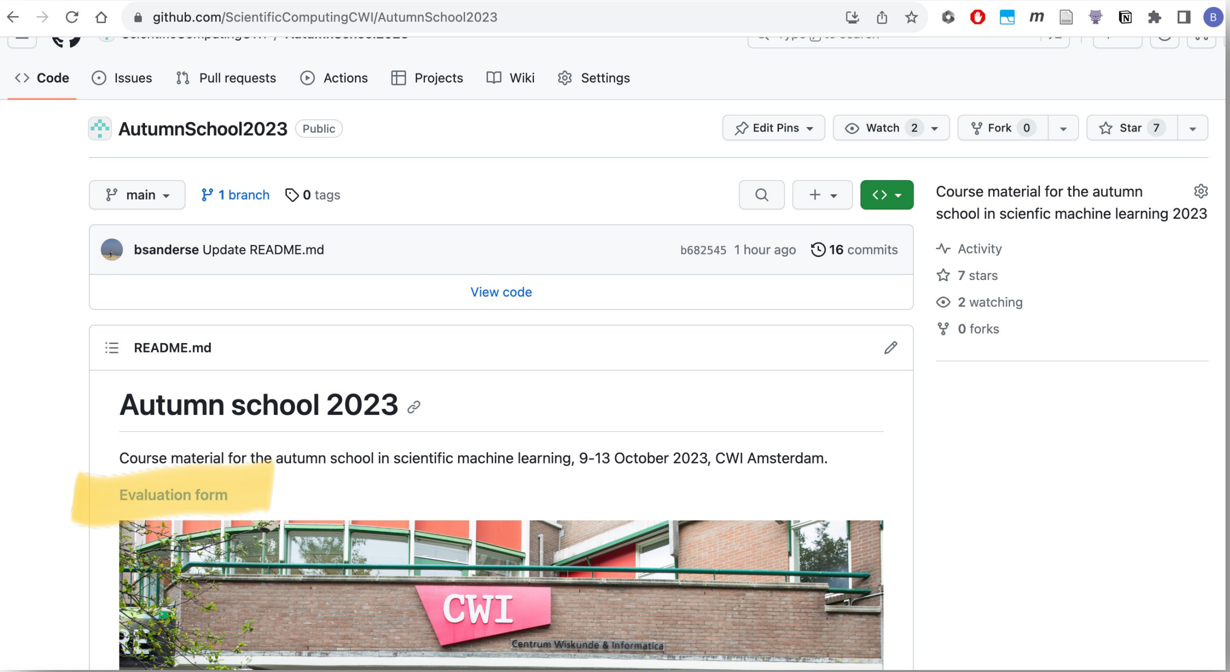
- Group-equivariant CNNs generalize CNNs to be roto-translational invariant

Day 5: Differentiable physics

- We have a PDE/ODE or data and want derive a simplified ODE.

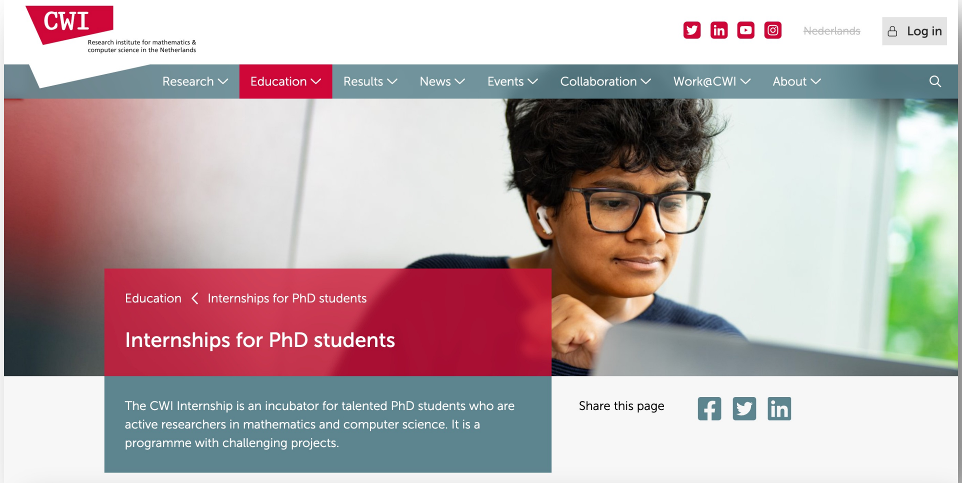
- Universal differential equations. Symbolic regression on NN output gives interpretability.
- Fitting derivatives versus fitting integrals (trajectories).
- Derivative of loss function -> derivation of adjoint system.
- Automatic differentiation (dual numbers!): powerful but with caveats.
    - Computing the gradient is itself an ODE solver process
    - Chaos
- Fitting ODEs is not trivial.

Questionnaire



https://github.com/ScientificComputingCWI/AutumnSchool2023/

PhD internship at CWI



- Open for PhD students **outside of the Netherlands**
- Stay at CWI for 3 months
- Fully funded: flight ticket, housing, stipend
- 1 A4 research proposal
- https://www.cwi.nl/en/education/internships/