Constraining Neural Operators with Conservation Laws Discovered from Data

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Neural Operators

- Neural operators have demonstrated advances in methods for solving parameter-dependent PDE
  - Serve as trainable approximations for mappings between infinite-dimensional function spaces
  - Discretization-invariant universal approximators that are queryable at all input and output points
  - Architecture is of the form

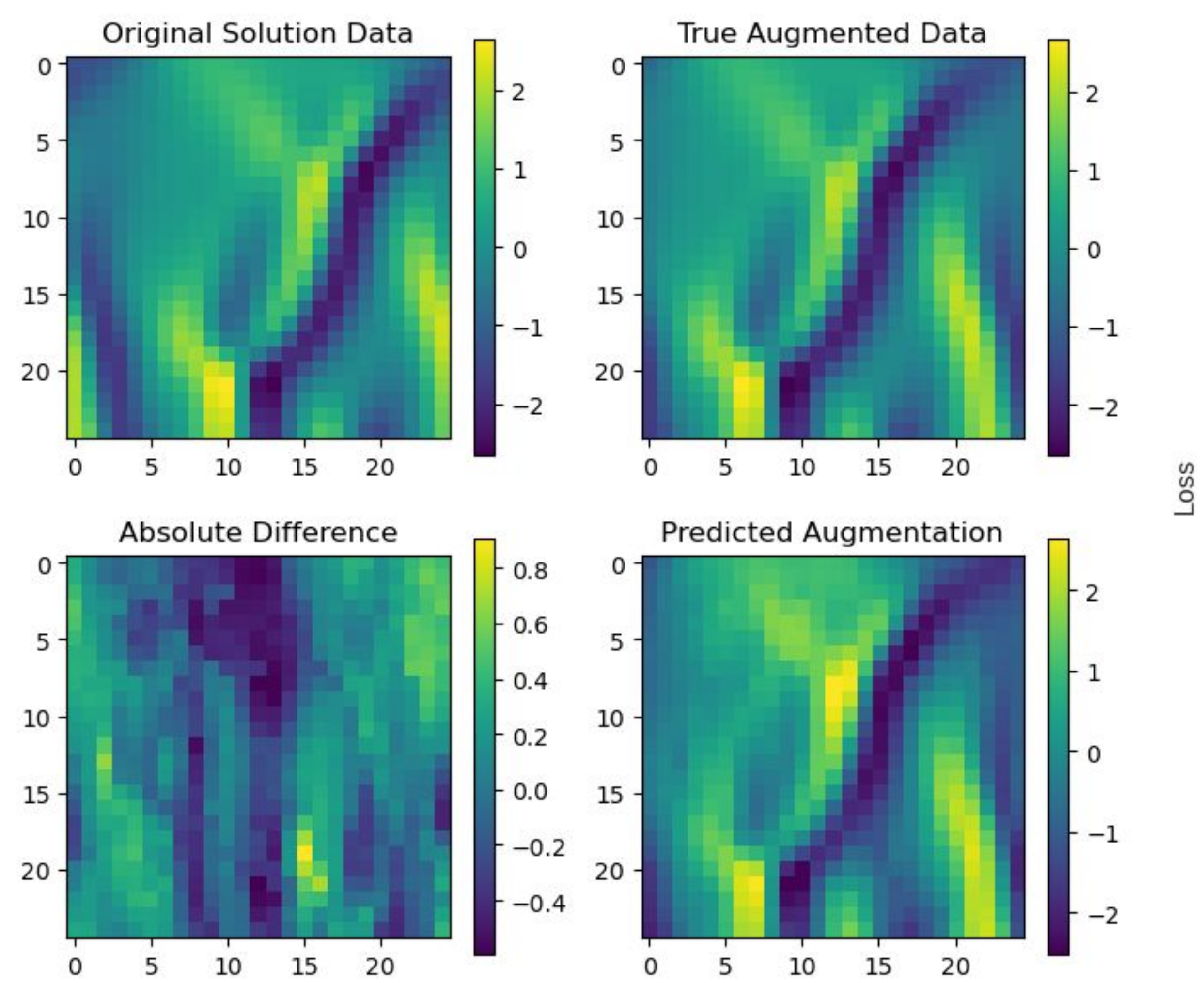
$$\mathcal{G}_\theta := \mathcal{Q} \circ \sigma_T(W_{T-1} + \mathcal{K}_{T-1} + b_{T-1}) \circ \cdots \circ \sigma_1(W_0 + \mathcal{K}_0 + b_0) \circ \mathcal{P}$$

  - Learn via integral kernel operators in high-dimensional spaces to which data are lifted
  - Kernels include Fourier, multiwavelet transforms and low-rank approximations/multi-scale decompositions
- L_2 Data-driven loss even in combination with PDE loss may yield an insufficiently constrained solution space and resulting solution approximations lose fine-scale features of the true solution

Lie Symmetries

- Several existing SciML frameworks regularize network training by enforcing explicit conservation laws, which are assumed to be known a priori
  - Conservation laws are not always known!
- Noether's theorem guarantees a corresponding conservation law for every symmetry of the system
  - i.e conservation of linear momentum corresponds to spatial translation uniformity
- Lie group acts on space of independent and dependent variables $(\tilde{x}, \tilde{u}) = g \cdot (x, u) = (\Xi(x,u), \Phi(x,u))$
  - The resulting coordinates and graphs under the group action of the symmetry group satisfy the original PDE

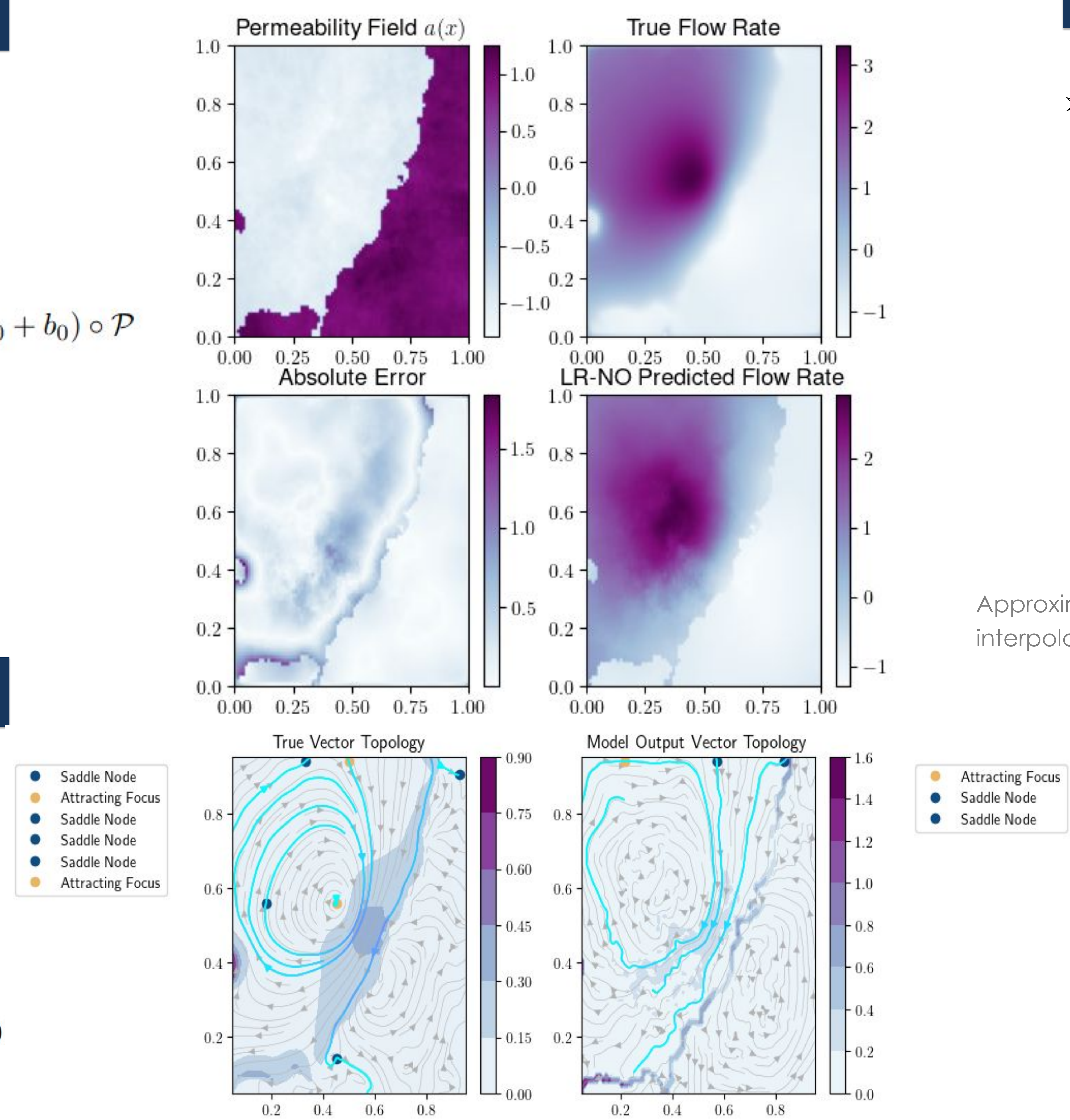
L-Conv RMSE: 0.2445777517930053



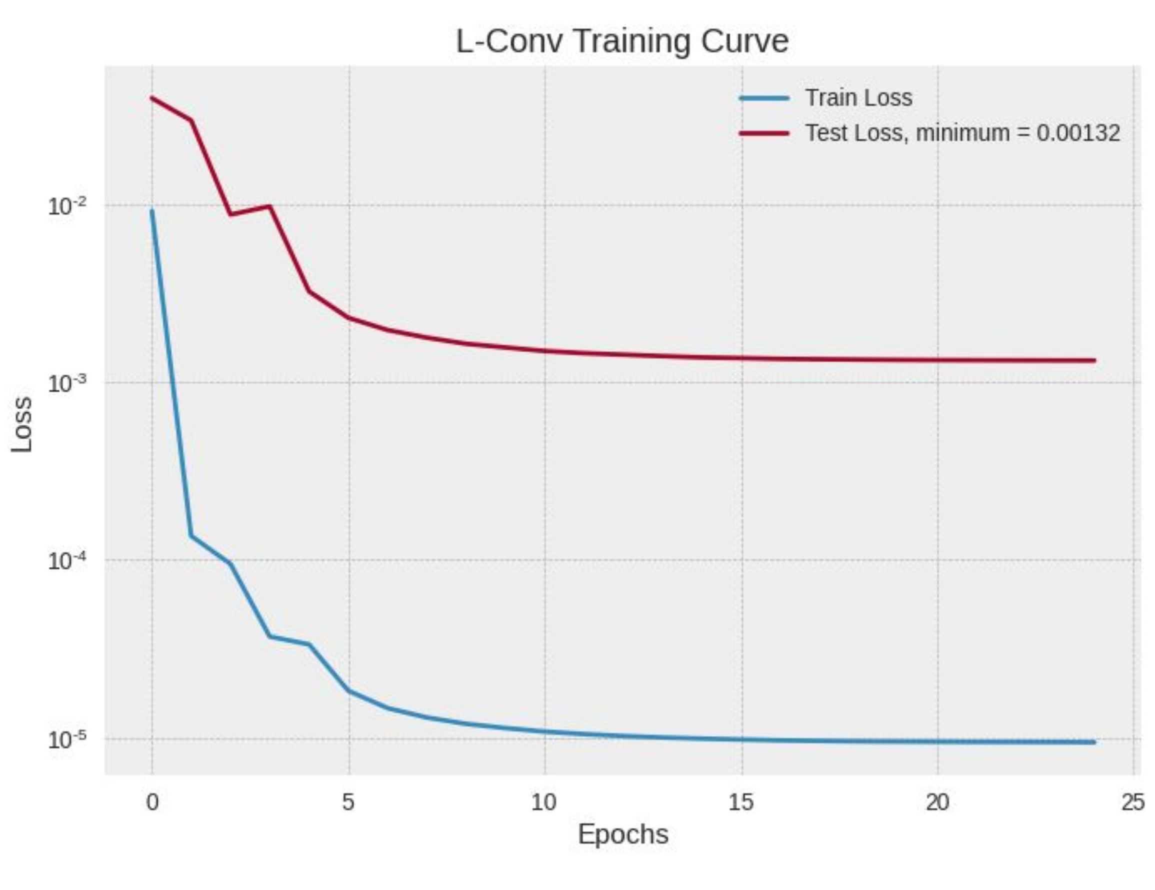
2D Darcy Flow

$$\begin{cases} -\nabla \cdot (a(x)\nabla u(x)) = 1 & x \in (0,1)^2 \\ u(x) = 0 & x \in \partial(0,1)^2 \end{cases}$$

Prediction MSE: 0.0868



Vector topology breaking for 2D Darcy flow by low-rank neural operator; extrema are not upheld, flow field has non-existent features. These features can be a diagnostic tool for identifying regions where conservation is not upheld.



Demonstration of L-Conv learning translational symmetry for the Kuramoto-Sivashinsky PDE

$$u_t + u_{xx} + u_{xxxx} + uu_x = 0$$

with uniformly random initial conditions

$$u_0(x) = \sum_{k=1}^{K} A_k \sin(2\pi \ell_k x / L + \phi_k)$$

$$A_k \in [-0.5, 0.5], \ell_k \in \{1,2,3\}, \phi_k \in [0, 2\pi]$$

This PDE has infinitesimal Lie symmetry generators given by

$$(x, t+\varepsilon, u), (x+\varepsilon, t, u), (x+\varepsilon t, t, u+\varepsilon)$$

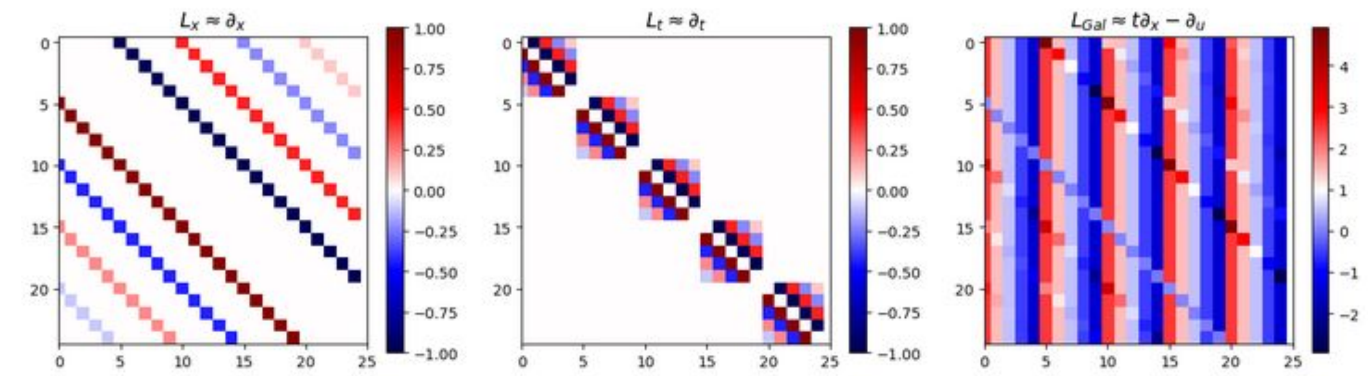
Methods for Symmetry Detection

Several methods have recently been developed to detect Lie symmetries purely from data.

- L-Conv is a Lie algebra convolutional network that generalizes CNNs and GCNs under appropriate groups
  - Learns parameter-dependent infinitesimal generators which characterize the symmetry group
  - Locally approximates Global Convolutions

$$[\kappa \star f](g) = \int_G \kappa(g^{-1}v) f(v) dv = \int_G \kappa(v) f(gv) dv$$

  - With Shannon-Whittaker interpolation on uniform discretization of solution space, yield operator matrices



Approximate operator matrices for symmetries of the Kuramoto-Sivashinsky PDE interpolated from uniform 25x25 spatiotemporal discretization

Discussion

This is still a work in progress.

- Additional diagnostics for assessing neural operator performance across the parameter range have been developed and demonstrated
  - Flow field considerations extend to higher dimensions in tensor fields with index counting on critical points
- Remains to assess the approximation improvement of Conservative Neural Operators from known symmetries as compared to unconstrained
  - A direct construction method that yields conservation laws from symmetries is exactly Noether's 2nd theorem if the Lagrangian is known
  - Next, the results of L-Conv or another automatic symmetry-detection method are used the same way to obtain approximate conservation laws
  - This process constrains global symmetries while a *progressive learning* method may extend this methodology to discovering local symmetries and to adaptively sampling the parameter space

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