Lie Point Symmetry Data Augmentation for Neural PDE Solvers

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Neural PDE training: a chicken-and-egg problem

Neural PDE solver ‘chicken-and-egg problem’

Neural PDE solvers *accelerate* solution time but require *abundant* training data.
Training data comes from *slow* solvers!

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- Need cheap ways to enlarge our datasets
- **Solution**: Data augmentation! But how?

PDE formulation

PDE $\boldsymbol{\Delta}$ specifies relationship between *solution* $\mathbf{u} : \mathcal{X} \to \mathbb{R}^n$ and its derivatives $\{\mathbf{u_x}, \mathbf{u_{xx}}, \ldots, \mathbf{u}_{n\mathbf{x}}\}$ at all points $\mathbf{x} \in \mathcal{X}$ as

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Example

1 + 1 dimensional Heat equation in space and time:

$$\Delta(\mathbf{x}, u^{(2)}\Big|_{\mathbf{x}}) = u_t - \alpha u_{xx} = 0$$

- Pointwise transformation:

$$(\mathbf{x}, \mathbf{u}|_{\mathbf{x}}) \overset{g}{\mapsto} (g\mathbf{x}, g\mathbf{u}|_{\mathbf{x}}) \ , \qquad \text{for all } g \text{ and } (\mathbf{x}, \mathbf{u})$$

Lie point symmetries

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Lie point symmetry

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Cauchy-Kovalevskaya theorem

$\{g_1, ..., g_d\}$ exhaustive if PDE analytic in its arguments

Example: Korteweg-de Vries equation

$$\Delta((x,t),u^{(3)}) = u_t + uu_x + u_{xxx} = 0\ .$$

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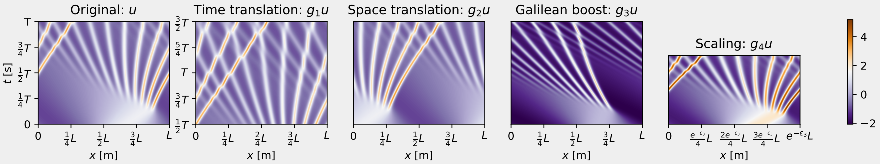
One-parameter symmetries:



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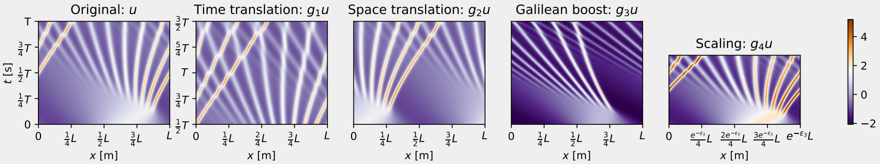
One-parameter symmetries:

$$g_1(\epsilon)(x,t,u) = (x, t+\epsilon, u) \qquad \text{time shift,}$$



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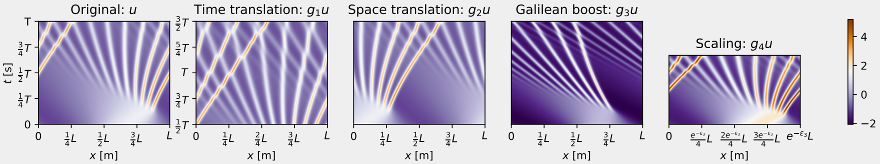

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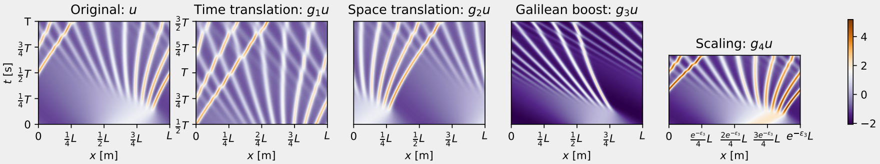

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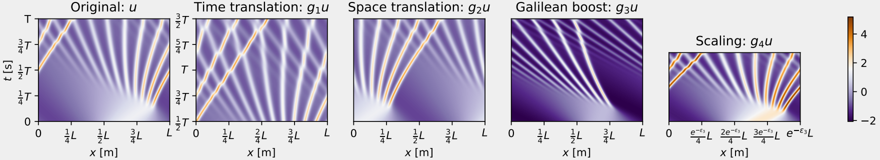
g_4(\epsilon)(x,t,u) &= (e^{\epsilon}x, e^{3\epsilon}t, e^{-2\epsilon}u) && \text{scaling}
\end{aligned}$$



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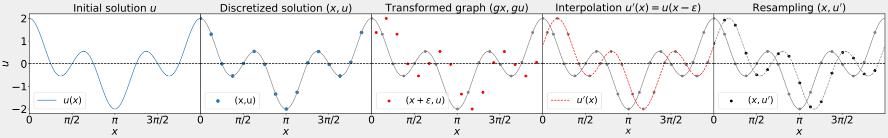

Lie point symmetry data augmentation

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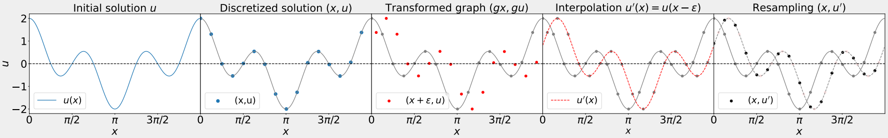

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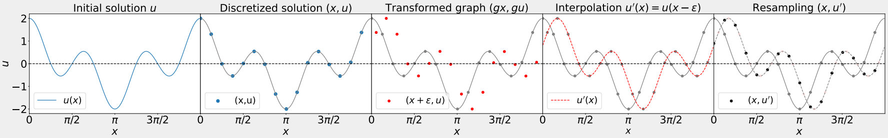

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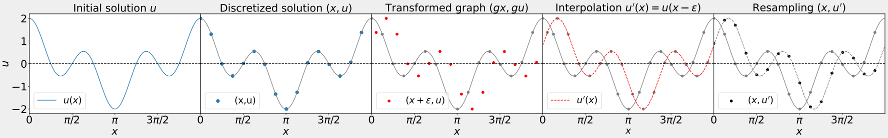

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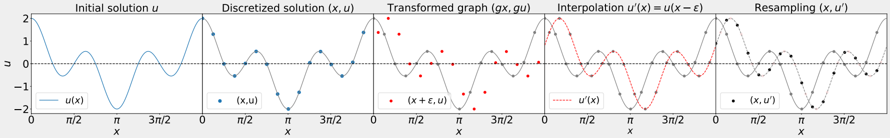
5. Reinterpolate to grid: $\mathbf{u}(\mathbf{x}) \to \mathbf{u}'(\mathbf{x})$



Different PDEs, different symmetries

- Korteweg-de Vries equation:

$$\Delta((x,t),u^{(3)}) = u_t + uu_x + u_{xxx} = 0$$

- Kuramoto-Shivashinsky equation:

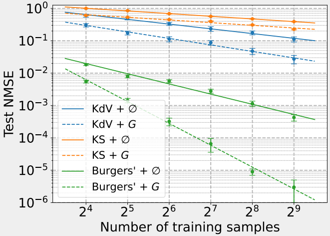
$$\Delta((x,t),u^{(4)}) = u_t + uu_x + u_{xx} + u_{xxxx} = 0$$

- Burgers' equation:

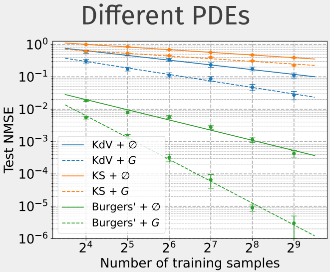
$$\Delta((x,t),u^{(2)}) = u_t + uu_x - \nu u_{xx} = 0$$

Equation	g_1	g_2	g_3	g_4	g_α
KdV	$(x, t+\epsilon, u)$,	$(x+\epsilon, t, u)$,	$(x+\epsilon t, t, u+\epsilon)$,	$(e^{\epsilon}x, e^{3\epsilon}t, e^{-2\epsilon}u)$	
KS	$(x, t+\epsilon, u)$,	$(x+\epsilon, t, u)$,	$(x+\epsilon t, t, u+\epsilon)$		
Burgers'	$(x, t+\epsilon, u)$,	$(x+\epsilon, t, u)$,	$(x, t, u+\epsilon)$,	$(e^{\epsilon}x, e^{2\epsilon}t, u)$,	$\left(u, t, 2\nu \log\left((1-\sigma(\epsilon))e^{\frac{1}{2\nu}u} + \sigma(\epsilon)e^{\frac{1}{2\nu}\alpha}\right)\right)$

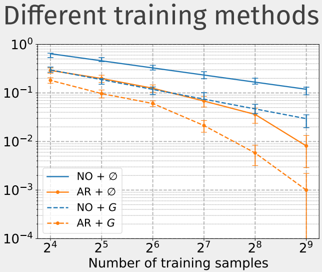
Different PDEs



Results



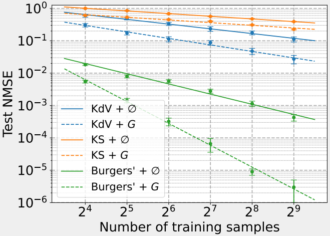
Different PDEs
Test NMSE
Number of training samples
KdV + ∅
KdV + G
KS + ∅
KS + G
Burgers' + ∅
Burgers' + G



Different training methods
Number of training samples
NO + ∅
AR + ∅
NO + G
AR + G

Results

Different PDEs



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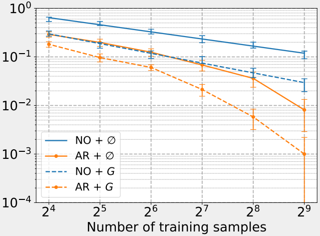
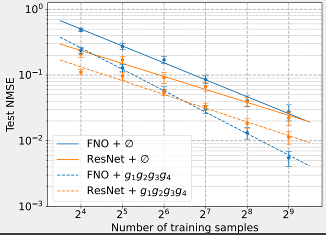


Different models



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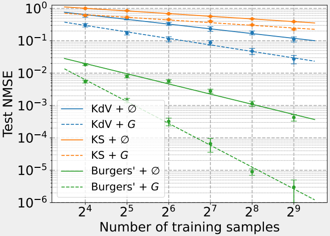

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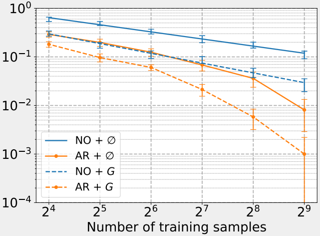

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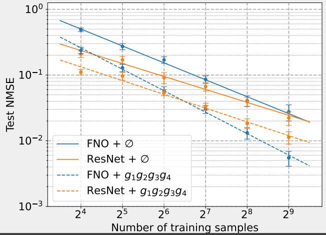
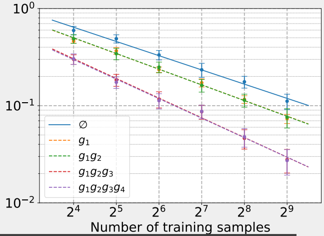
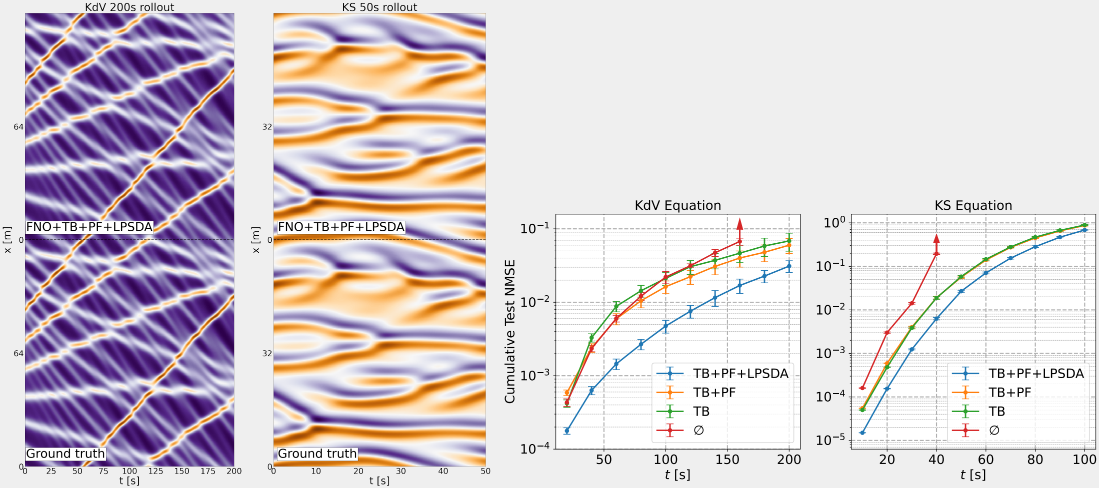


Combining symmetries




KdV 200s rollout
FNO+TB+PF+LPSDA
Ground truth
x [m]
t [s]
KS 50s rollout
FNO+TB+PF+LPSDA
Ground truth
x [m]
t [s]
KdV Equation
Cumulative Test NMSE
t [s]
TB+PF+LPSDA
TB+PF
TB
∅
KS Equation
t [s]
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TB
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- LPSDA comprises the full set of solution-preserving, pointwise, continuous data transformations for any (analytic) PDEs
- LPSDA improves neural PDE solver sample complexity to over an order of magnitude
- Solver-agnostic & PDE-agnostic

Paper: Lie Point Symmetry Data Augmentation for Neural PDE Solvers

arXiv:2202.07643

Code: *https://github.com/brandstetter-johannes/LPSDA*