Equivariant Neural Networks and Differential Invariants Theory for Solving Partial Differential Equations

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Introduction

What is the goal of this paper?

- Using Equivariant Neural Networks (ENN) for solving Partial Differential Equations.
- Exploiting the underlying symmetry groups to strengthen the approximation.
- Generalizing ENN to tackle vector valued function with any given symmetry group.
- Building symmetry preserving Finite Difference methods.
- Illustrating our method on the 2D heat equation.

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Neural Networks applied to PDEs
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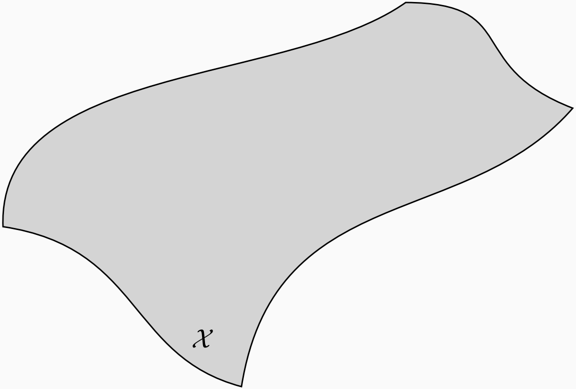
Only one applied to PDEs:
Rui Wang, Robin Walters, and Rose Yu. *Incorporating Symmetry Into Deep Dynamics Models for Improved Generalization* [WWY]. However, only special cases.

PDEs and Symmetries

In what space are we working?

- A smooth manifold $\mathcal{X}$ (coordinate space).



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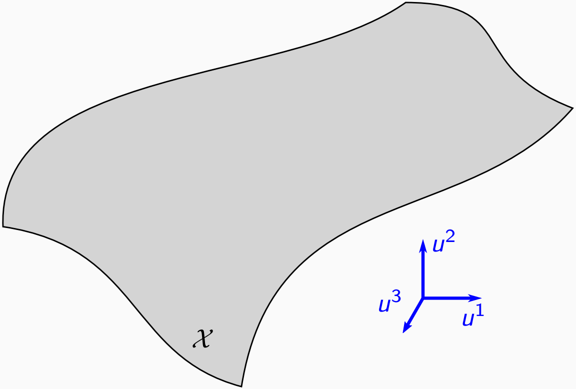

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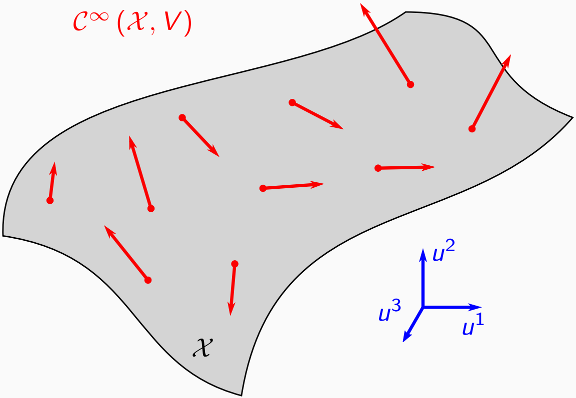

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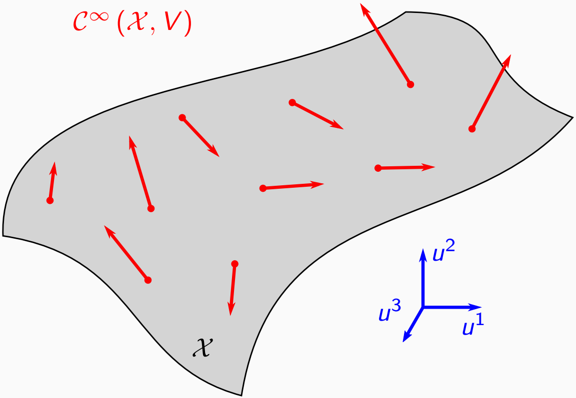
- The Jet space $J^{(n)} = \mathcal{X} \times \mathcal{U} \times \ldots \times \mathcal{U}$



What are we trying to solve?

Definition (PDE System)

$$(E): \quad \begin{cases} \Delta\left(t, x, u^{(n)}\right) = 0 & \forall t, x \in \mathbb{R}^+ \times \mathcal{X} \\ u(t,x) = u_b(t,x) & \forall (t,x) \in B \end{cases}$$

What are symmetries?

Definition (Symmetry Group)
A Lie group G is the *symmetry group* of a PDEs system when if f is a solution, then its transform f_g by the group action is also a solution.

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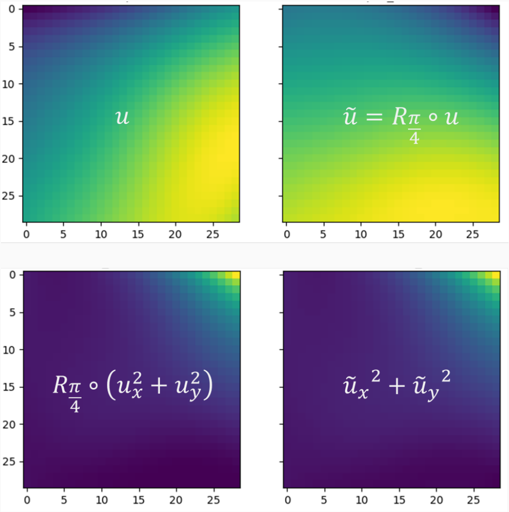
Definition (Differential Invariant)
The algebraic invariants I_G of the prolonged group action $\mathrm{pr}^{(n)}\, G$ are called the *differential invariants* of order n of the group G. A complete set of independent differential invariants of order n will be denoted by $\partial\phi^G_{u,n} = \left\{\partial\phi^{G,1}_{u,n}, \ldots, \partial\phi^{G,k}_{u,n}\right\}$.

What are symmetries?



Equivariant Neural Networks

What is the operation behind G-CNN?

Definition (Group Convolution)

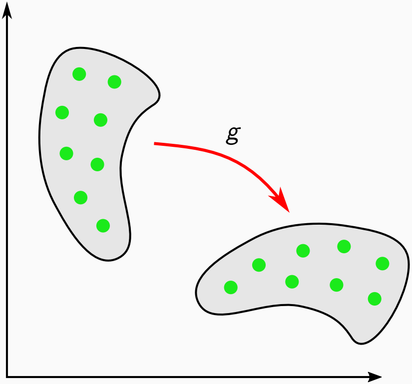
Let G be a compact Group and $V_1,\ V_2$ two vector spaces. Let $K : G \to \mathcal{L}(V_1, V_2)$ be a kernel, $f : G \to V_1$ be a feature function, and μ the Haar measure on G. We define the *group convolution* for any $s \in G$ by

$$(K * f)(s) = \int_G K\left(r^{-1}s\right) f(r) d\mu(r).$$

Why is it interesting?

Proposition
If the actions of G on V_1^G and V_2^G has regular representations, then the group convolution defined before is G-equivariant.

Why is it not enough?



Regular representation $\rho(g) = 1$ on scalars.

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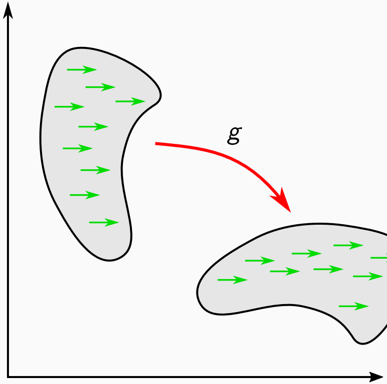

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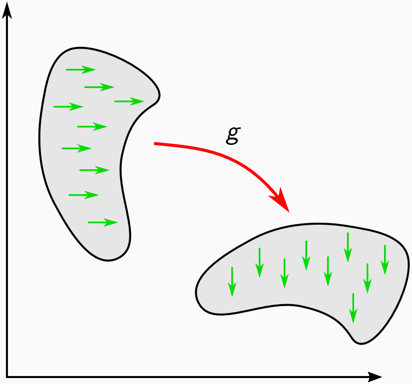

Non-regular representation on vectors.

A New Convolution

Definition (Representative Group Convolution)

Let G be a compact Group and $V_1,\ V_2$ two vector spaces. Let $K : G \to \mathcal{L}(V_1, V_2)$ be a kernel, $f : G \to V_1$ be a feature function, and μ the Haar measure on G. If $\rho_1 : G \to \mathcal{L}(V_1)$ and $\rho_2 : G \to \mathcal{L}(V_2)$ are the linear representations of the action of G on V_1 and V_2 respectively, we define the *representative group convolution* for any $s \in G$ by

$$(K \circledast f)(s) = \int_G \rho_2(r) K\left(r^{-1}s\right) \rho_1\left(r^{-1}\right) f(r) d\mu(r) \tag{1}$$

Finally enough

Theorem

If G acts on V^G by

$$\rho(g)f\left(g^{-1}r\right) \qquad \forall g, r \in G \text{ and } f : G \to V,$$

then the representative group convolution is G-equivariant.

Equivariant Neural Network

G-CNN

$$
\begin{aligned}
\text{input layer:} \quad & \mathcal{N}^0 = f \in V_0^G, \\
\text{convolution layers:} \quad & \mathcal{N}^\ell = K^\ell \circledast \mathcal{N}^{\ell-1} \in V_\ell^G, \\
& \text{with } \rho_{\ell-1},\ \rho_\ell, \text{ for } 1 \leq \ell \leq L.
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Remark
One can use non-equivariant pointwise function between layers as long as $\rho_\ell = I_d$.

Solving of PDEs with ENN

What Neural Network to use for PDEs?

Loss

$$\mathcal{L}(\theta, \mathcal{T}) = w_f \mathcal{L}_f(\theta, \mathcal{T}_f) + w_b \mathcal{L}_b(\theta, \mathcal{T}_b) \tag{2}$$

with

$$\mathcal{L}_f(\theta, \mathcal{T}_f) = \frac{1}{|\mathcal{T}_f|} \sum_{x \in \mathcal{T}_{\boldsymbol{f}}} \left\| \Delta\left(t, x, \hat{u}^{(n)}\right) \right\|_2^2 \tag{3}$$

$$\mathcal{L}_b(\theta, \mathcal{T}_b) = \frac{1}{|\mathcal{T}_b|} \sum_{x \in \mathcal{T}_{\boldsymbol{b}}} \left\| \mathcal{B}(\hat{u}_\theta, x) \right\|_2^2 \tag{4}$$

How can we simplify the problem with differential invariants?

Problem

$$\sum_{i=1}^{k_{\boldsymbol{t}}} a_i \partial_{\boldsymbol{t}}^i u = \Delta\left(t, x, u_x^{(n)}\right) \tag{5}$$

Theorem

$$\Delta\left(t, x, u_x^{(n)}\right) = F\left(\partial\phi_{u,n}^{G,1}, \ldots, \partial\phi_{u,n}^{G,k}\right) \tag{6}$$

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known unknown

How do we use the ENNs now?

Approximation

$$\mathcal{N}_G\left(\left(f^{(i)(\ell)}\right)_{\ell=1}^{n_x}\right)^j \approx \partial\phi_f^{G,(i,j)} = \partial\phi_f^G(t^{(i)}, x^{(j)}) \tag{7}$$

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New problem

$$\sum_{i=1}^{k_t} a_i \partial_t^i u \approx F\left(\mathcal{N}_G^1\left(\left(u^{(i,\ell)}\right)_{\ell=1}^{n_x}\right)^j, ..., \mathcal{N}_G^k\left(\left(u^{(i,\ell)}\right)_{\ell=1}^{n_x}\right)^j\right) \tag{8}$$

Numerical Experiments

How close can we get with SE(2) differential invariants?

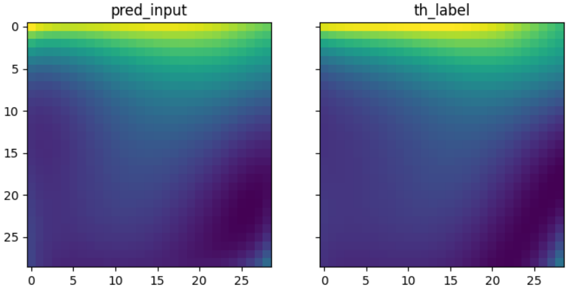

Figure 1: The SE(2) differential invariant $u_x^2 + u_y^2$ computed for the function u depicted in Frame 5 with an SE(2)-CNN (left) and its theoretical value (right)

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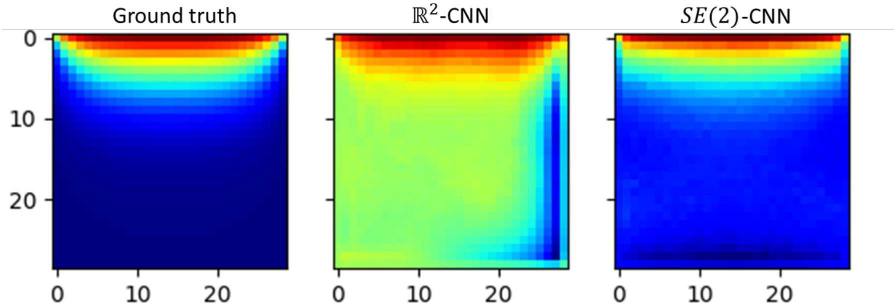

Figure 1: Comparison of the theoretical heat profile of the 2D heat equation with a top 100°C boundary condition with those obtained through simulation with two symmetry preserving FD schemes by leveraging on $\mathbb{R}^2$ (middle) and SE(2) (right) equivariant neural networks.

Conclusion and Further Work

Contributions

- Use of G-CNN to generalize the PINN architecture to encode generic symmetries ;
- Use of ENN to approximate differential invariants of a given symmetry group ;
- Build of symmetry preserving Finite Difference methods.

To go further

- Perfom proper benchmarking between the two approaches and other conventional numerical schemes for PDEs integration ;
- Test on more complex PDEs with richer symmetry groups (e.g. Maxwell).

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Questions?

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