Diff-SINDy: A Differentiable Framework for Discovering Partial Differential Equations from Data

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Motivation

Discovering the governing equations of complex partial differential equations (PDEs) from data remains a challenging problem.

Traditional approaches such as SINDy [1] and PINN-SR [2] rely on fixed libraries of candidate functions, limiting flexibility.

Evo-SINDy [3] relaxes this constraint by introducing the derivative as a unary operator but remains non-differentiable in training and depends on discrete derivative estimates that are sensitive to noise.

Feature	SINDy	PINN-SR	Evo-SINDy	**Diff-SINDy**
No Functional Library	✗	✗	✓	✓
Differentiability	✗	✓	✗	✓
AD Derivatives	✗	✓	✗	✓
Sparsity	✓	✓	✓	✓
No Pre-training	✓	✗	✗	✓

Diff-SINDy is a differentiable framework for data-driven PDE discovery:

- Separating fully-differentiable training and Symbolic Regression (SR) inference stages
- Using a flexible derivative library rather than a functional library
- Observed solutions are approximated using a deep neural network (DNN) and derivatives calculated using AD

Problem Statement

Consider PDEs linear in their derivatives with spatiotemporal samples (x,t) and partially observed solution data, $u(x,t)$,

$$u_t = f_0 + f_1\,u_x + f_2\,u_{xx} + f_3\,u_{tt} + \cdots + f_j\,u_{xxx} + \ldots \qquad u_{tt} = g_0 + g_1\,u_x + g_2\,u_t + g_3\,u_{xx} + \cdots + g_j\,u_{xxx} + \ldots$$

Many physical systems of interest:

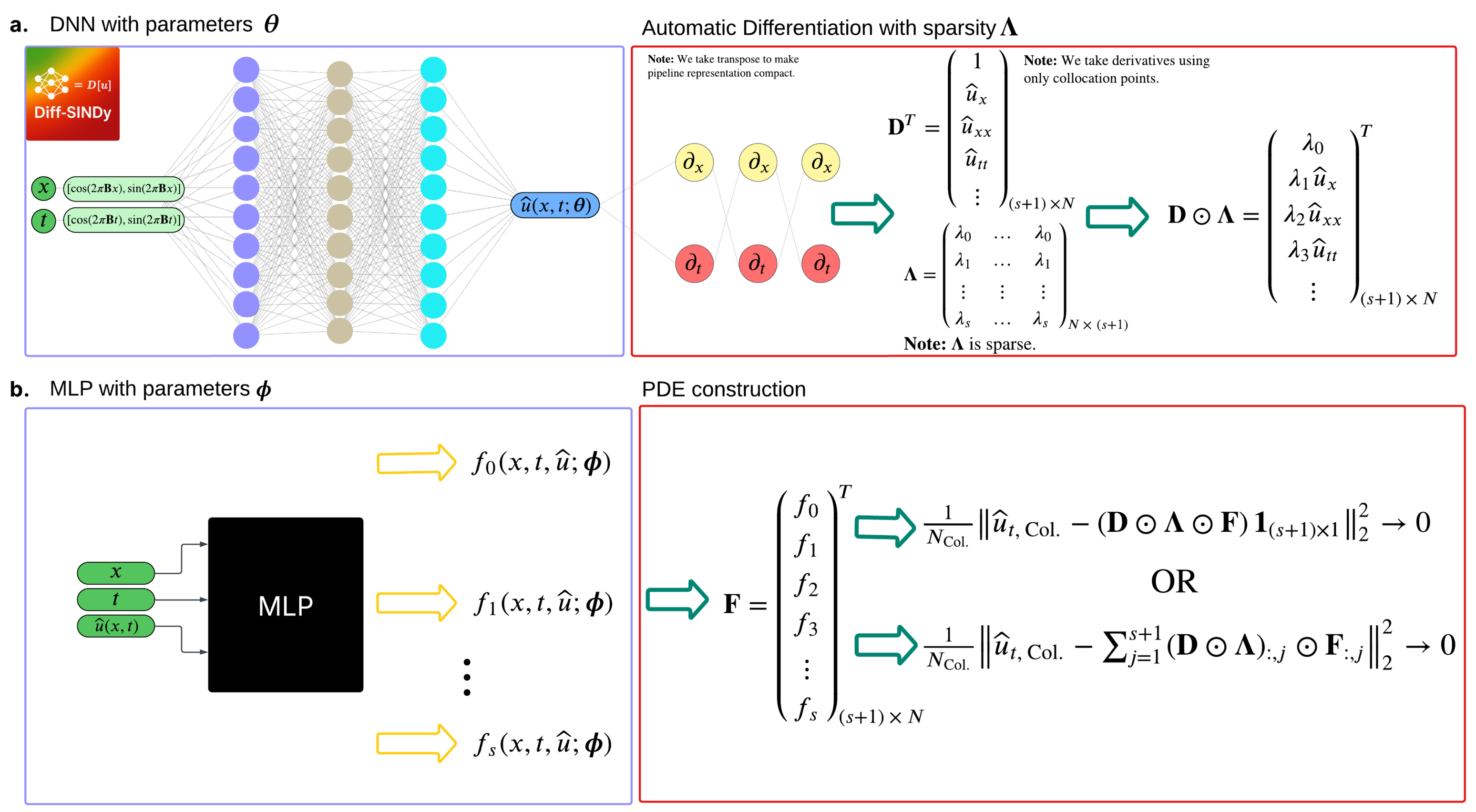
Heat: $u_t = \nu u_{xx}$ — Wave: $u_{tt} = c^2 u_{xx}$

Burgers': $u_t = -\alpha u u_x + \nu u_{xx}$ — Klein–Gordon: $u_{tt} = c^2 u_{xx} - m^2 u$

KdV: $u_t = -\alpha u u_x - \nu u_{xxx}$ — Sine–Gordon: $u_{tt} = c^2 u_{xx} - m^2 \sin u$

Diff-SINDy learns symbolic expressions for coefficients $f_j(x,t,u)$, $g_j(x,t,u)$, providing a closed-form parsimonious PDE that describes the data.

Model Architecture and Training



First, a DNN is trained to approximate the solution using an initial condition (IC), boundary condition (BC), and interior data (Data) losses.

$$\mathcal{L}_{\mathrm{IC}}(\theta;\ \overbrace{u_{\mathrm{IC}}}^{\text{measured}}\ ) = \frac{1}{N_{\mathrm{IC}}}\Big\|\overbrace{\widehat{u}_{\mathrm{IC}}}^{\text{predicted}} - u_{\mathrm{IC}}\Big\|_2^2;\ \mathcal{L}_{\mathrm{Data}}(\theta; u_{\mathrm{Data}}) = \frac{1}{N_{\mathrm{Data}}}\|\widehat{u}_{\mathrm{Data}} - u_{\mathrm{Data}}\|_2^2;\ \mathcal{L}_{\mathrm{BC}}(\theta; u_{\mathrm{BC}}) = \frac{1}{N_{\mathrm{BC}}}\|\widehat{u}_{\mathrm{BC}} - u_{\mathrm{BC}}\|_2^2$$

The solution network is warmed by minimizing the loss:

$$\mathcal{L}_{\mathrm{warm}} = \lambda_{\mathrm{IC}}\mathcal{L}_{\mathrm{IC}} + \lambda_{\mathrm{BC}}\mathcal{L}_{\mathrm{BC}} + \lambda_{\mathrm{Data}}\mathcal{L}_{\mathrm{Data}}$$

Then, the approximate solutions for the derivatives are calculated via AD. A sparse matrix Λ is used to select active and non-active derivatives.

The final component is the coefficient network, implemented with an MLP architecture in one of three forms: a single MLP for all coefficients, a multi-task MLP with a shared backbone and separate heads, or individual MLPs for each coefficient. It receives spatiotemporal coordinates and predicted solutions at the collocation points as input.

Training proceeds in two steps:

1. The solution network is trained with sparsity and coefficient network(s) frozen. The PDE is gradually introduced (i.e. λ_{PDE} gradually increases to 1).

$$\mathcal{L}\,(\overbrace{\boldsymbol{\theta}}^{\text{unfrozen}};\ x, t, u, \overbrace{\boldsymbol{\phi}, \boldsymbol{\Lambda}}^{\text{frozen}}) = \lambda_{\mathrm{IC}}\mathcal{L}_{\mathrm{IC}} + \lambda_{\mathrm{BC}}\mathcal{L}_{\mathrm{BC}} + \lambda_{\mathrm{Data}}\mathcal{L}_{\mathrm{Data}} + \lambda_{\mathrm{PDE}}(\mathrm{epoch})\mathcal{L}_{\mathrm{PDE}}$$

2. The coefficient network with sparsity (STRidge) is trained with solution network frozen.

$$\mathcal{L}(\overbrace{\boldsymbol{\phi}, \boldsymbol{\Lambda}}^{\text{unfrozen}}; x_{\mathrm{Col.}}, t_{\mathrm{Col.}}, u_{\mathrm{Col.}}, \overbrace{\boldsymbol{\theta}}^{\text{frozen}}) = \mathcal{L}_{\mathrm{PDE}} + \beta\|\boldsymbol{\Lambda}\|_0$$

Inference

After sparsity is applied, the active coefficients are passed to PySR (Python Symbolic Regression) [4] which infers closed-form expressions by a combination of a genetic evolutionary search algorithm, symbolic manipulation, pruning, and heuristics.

The expressions from PySR are ranked by symbolic complexity. The *score* of the ith expression balances the trade off between its fit quality from the mean squared error (MSE) loss and its simplicity, quantified by its comparison to the next simplest $i-1$ expression.

Complexities ($\mathcal{C}$)	MSE Loss	Score
`[const, +, -, *]`: 1 `[/, sin, cos]`: 2 `[exp]`: 4	$\mathcal{L}_{SR,i}(u) = \big\|f_{SR,i} - f_i\big\|_2^2$	$-\dfrac{\log(\mathcal{L}_{SR,i} - \mathcal{L}_{SR,i-1})}{\mathcal{C}_i - \mathcal{C}_{i-1}}$.

Experiments

We trained the model using a 200-epoch warm start followed by 1,000 epochs in a two-stage procedure. Training required 30 minutes and inference 10 minutes on a single T4 GPU. For the Burgers', heat, and wave equations, the predicted terms differed from the true equations by 0.5%/6% (u_x/u_{xx}), 1%, and 0.3%, respectively.

	Burgers' equation	Heat equation	Wave equation
Exact	$u_t = -1uu_x + \frac{0.01}{\pi}u_{xx}$	$u_t = 0.005\,u_{xx}$	$u_{tt} = 1\,u_{xx}$
Diff-SINDy	$u_t = -0.995uu_x + 0.00298u_{xx}$	$u_t = 0.00494\,u_{xx}$	$u_{tt} = 0.997\,u_{xx}$

Diff-SINDy results for coefficients of u_x and u_{xx} of Burger's equation.

Complexity	Expression	MSE	Score
	$\alpha u = -1u$		
1	x	0.2787	0.000
3	$-0.995\,u$	3.451×10^{-4}	3.346
5	$-0.982\,u + 0.003$	3.392×10^{-4}	0.0099
7	$-0.958(-0.028\,x + u)$	1.835×10^{-4}	0.510
	$\nu = 0.01/\pi \approx 0.0318$		
1	0.00298	2.148×10^{-7}	0.000
5	$0.0009x + 0.003$	1.962×10^{-7}	0.242
7	$0.004\cos(x - 0.303)$	1.334×10^{-7}	0.191
8	$0.0005(x - 0.668)^3 + 0.003$	9.729×10^{-8}	0.316

References

[1] S. L. Brunton, J. L. Proctor, and J. N. Kutz, "Discovering governing equations from data by sparse identification of nonlinear dynamical systems,"

[2] Z. Chen, Y. Liu, and H. Sun, "Physics-informed learning of governing equations from scarce data,"

[3] Y. Jiang and J. Sun, "Evo-sindy: Universal discovery of partial differential equations using cooperative evolutionary computation,"

[4] M. Cranmer, "Interpretable Machine Learning for Science with PySR and SymbolicRegression,"