A tutorial on SciML

What is scientific machine learning and how do you use it?

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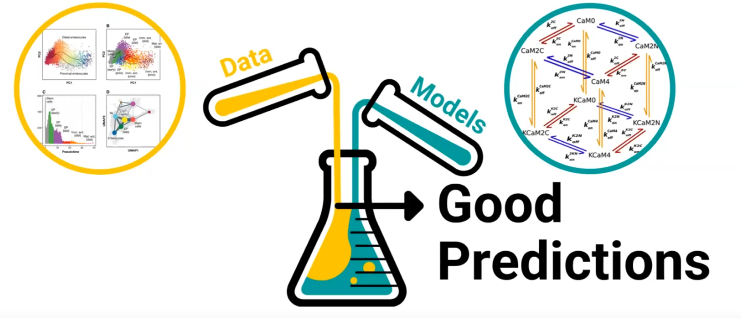
What is SciML?



Scientific Computing + Machine Learning[1]

[1] C. Rackauckas (2023). *Generalizing Scientific Machine Learning and Differentiable Simulation Beyond Continuous Models*. presentation at The Alan Turing Institute

Why?

Why not!

- Improved accuracy
- Data efficiency
- Physical consistency
- Better generalization
- Interpretability
- Uncertainty quantification
- From extrapolation to interpolation
- Cheaper surrogate models

Agenda

a. Approaches (10 min)
b. Practical example in Julia
   1. Quick intro to Julia (10 min)
   2. Lotka-Voltera SciML example (35 min)
   3. Controlled bouncing ball (15 min)
c. Challenges and opportunities (15 min)
d. Questions (? min)

01

Approaches

Physics-Informed Neural Network

Partial differential equation

$$\frac{\partial u}{\partial t} + \mathcal{N}[u] = 0, \quad t \in [0, T], x \in \Omega$$

subject to

$$u(0, x) = g(x), \quad x \in \Omega \qquad \text{(Initial conditions)}$$
$$\mathcal{B}[u] = 0, \quad t \in [0, T], x \in \Omega \qquad \text{(Boundary conditions)}$$

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Idea: Let a neural network represent an unknown solution to the PDE.

Physics-Informed Neural Network

If $u_\theta(t, x)$ is a neural network, then PINN optimizes the following objective[2]:

$$\mathcal{L}(\theta) = MSE\left(\frac{\partial u_\theta}{\partial_t}(t^i, x^i) + \mathcal{N}[u_\theta](t^i, x^i)\right) +$$

$$MSE(u_\theta(0, x^i) - g(x^i)) +$$

$$MSE(\mathcal{B}[u_\theta](t^i, x^i))$$

[2] S. Wang, S. Sankaran, H. Wang, and P. Perdikaris (2023). *An Expert's Guide to Training Physics-informed Neural Networks*. arXiv: 2308.08468

Universal Differential Equations[3]

$$\mathcal{N}[u(t), u(\alpha(t)), W(t), U_\theta(u, \beta(t))] = 0$$

[3] C. Rackauckas, Y. Ma, J. Martensen, C. Warner, K. Zubov, R. Supekar, D. Skinner, A. Ramadhan, and A. Edelman (2021). *Universal Differential Equations for Scientific Machine Learning*. arXiv: 2001.04385

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Specializations

- ODEs
- SDEs
- DDEs
- DAEs
- PDEs

Generalizations

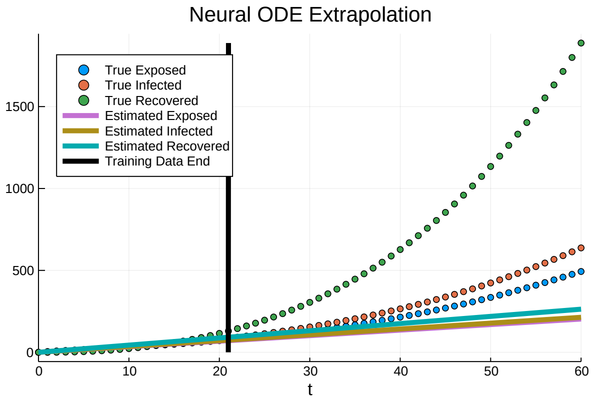
- Hybrid and jump equations
- Uncertainty quantification
- Discrete random processes
- Chaotic systems
- Non-linear mixed effect models

[3] C. Rackauckas, Y. Ma, J. Martensen, C. Warner, K. Zubov, R. Supekar, D. Skinner, A. Ramadhan, and A. Edelman (2021). *Universal Differential Equations for Scientific Machine Learning*. arXiv: 2001.04385

Universal ODE: COVID-19 modeling

SEIRHD-model

$$\dot{S} = -\eta(t)S$$
$$\dot{E} = \eta(t)S - \alpha E$$
$$\dot{I} = \alpha E - (\gamma_1 + \delta)I$$
$$\dot{R} = \gamma_1 I + \gamma_2 H$$
$$\dot{H} = \delta I - (\mu + \gamma_2)H$$
$$\dot{D} = \mu H$$



https://github.com/ChrisRackauckas/universal_differential_equations/tree/master/SEIR_exposure

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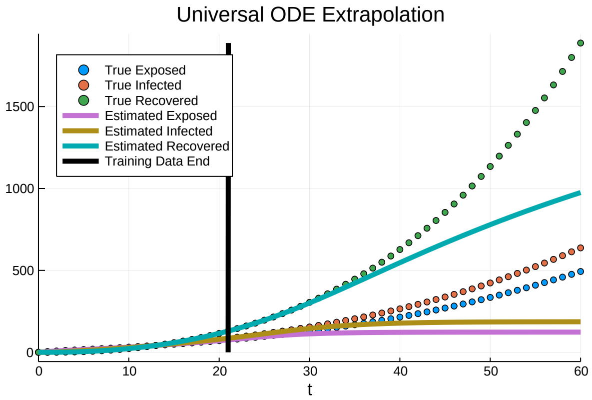

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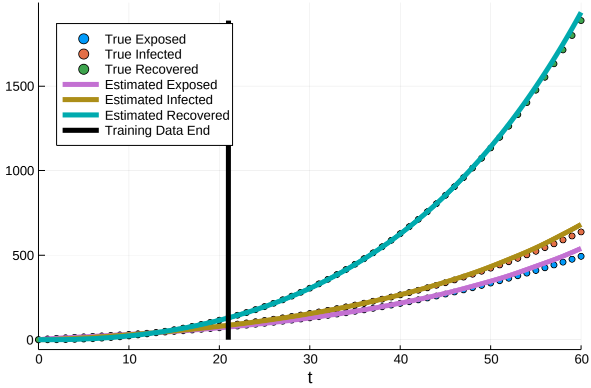

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How do we train UDEs?

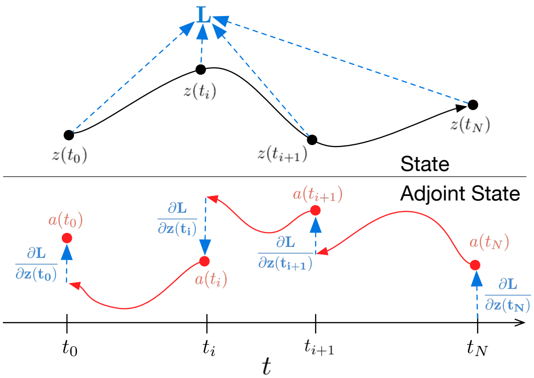
- Using derivative-data directly?
- Differentiable simulators

$$\mathcal{L}(\theta) = \int_0^T \|u_\theta(t) - r(t)\| \, dt \qquad \text{(Distance-based)}$$

Chain-rule: $\frac{d\mathcal{L}}{d\theta} = \frac{\partial \mathcal{L}}{\partial u_\theta(t)} \frac{\partial u_\theta(t)}{\partial \theta}$

Adjoint: $\frac{da(t)}{dt} = -a(t)^\top \frac{\partial f(z(t), t, \theta)}{\partial z}$ where $a(t) = \frac{\partial L}{\partial z(t)}$

Gradients![4] [5]



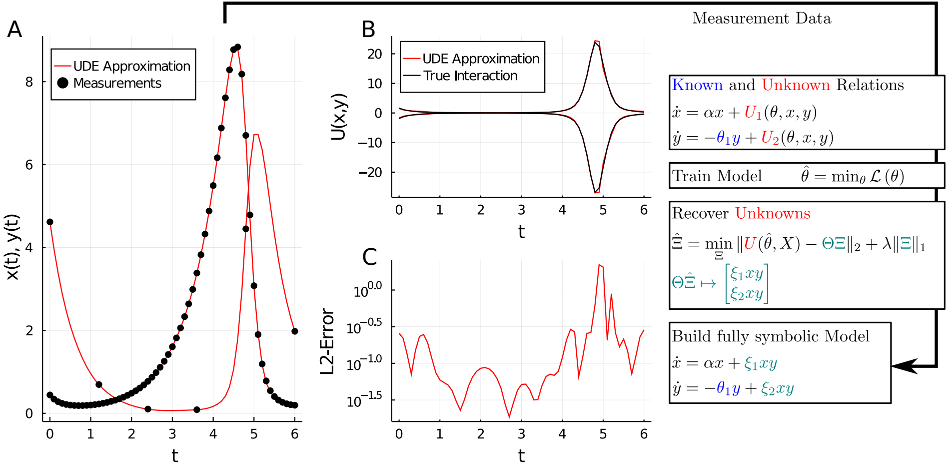
[4] S. Kim, W. Ji, S. Deng, Y. Ma, and C. Rackauckas (2021). "Stiff neural ordinary differential equations". In: *Chaos: An Interdisciplinary Journal of Nonlinear Science*

[5] R. T. Q. Chen, Y. Rubanova, J. Bettencourt, and D. Duvenaud (2019). *Neural Ordinary Differential Equations*. arXiv: 1806.07366

02

Practical example

Process for dynamics discovery



03

Challenges and opportunities

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More on gradients! [6]

Adjoint methods

Method	Stability	Memory usage
BacksolveAdjoint	Poor	Low. $O(1)$.
InterpolatingAdjoint	Good	High. Requires full continuous solution of forward.
QuadratureAdjoint	Good	Higher. Requires full continuous solution of forward and Lagrange multiplier.
BacksolveAdjoint (checkpointed)	Okay	Medium. $O(c)$ where c is the number of checkpoints.
InterpolatingAdjoint (checkpointed)	Good	Medium. $O(c)$ where c is the number of checkpoints.
ReverseDiffAdjoint	Best	Highest. Requires full forward and reverse AD of solve.
TrackerAdjoint	Best	Highest. Requires full forward and reverse AD of solve.

[6] Y. Ma, V. Dixit, M. Innes, X. Guo, and C. Rackauckas (2021). *A Comparison of Automatic Differentiation and Continous Sensitivity Analysis for Derivatives of Differential Equation Solutions*. arXiv: 1812.01892

Tricks of the trade: neural networks

Figure: Trouble Shooting Deep Neural Networks - Josh Tobin

Figure: A Recipe for Training Neural Networks - Andrej Karpathy

`http://josh-tobin.com/assets/pdf/troubleshooting-deep-neural-networks-01-19.pdf`

`https://karpathy.github.io/2019/04/25/recipe/`

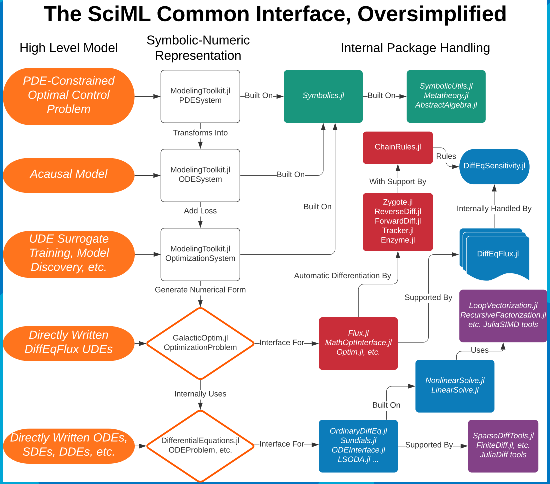
Successful applications

- Learning relativistic physics for binary black hole dynamics
- COVID-19 epidemiological models
- Pharmaceutical modeling
- Battery degradation models
- Combustion models
- Controlling qubits in quantum circuits
- Crash test system modeling
- Williams Formula 1 team!!

Chris Rackauckas: Accurate and Efficient Physics-Informed Learning
Through Differentiable Simulation

More on differentiable programming

LinearSolve.jl	$A(p)x = b$
NonlinearSolve.jl	$f(u, p) = 0$
DifferentialEquations.jl	$\dot{u} = f(u, p, t)$
Integrals.jl	$\int_a^b f(p, t)\, dt$
Optimization.jl	$\min f(u, p)$ s.t. $g(u, p) \leq 0$
(I)MDPs?	$V^{\star}_{M(p)}(s)$



State of Julia's SciML Ecosystem, Chris Rackauckas, JuliaCon 2024

Thank you for your attention

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