Julia in Research

Albin Heimerson

What I do

PhD student doing ML for datacenter/cloud control

- Controlling large interconnected systems
- A lot of data
- Reinforcement learning for control
- Modelling to improve learning

Why I use Julia

Partly because I just enjoy the language, but also

- Automatic Differentiation for the whole language
- Composability between packages
- High level and high performance
- Transparency in library code, Julia all the way

Trade-offs in Automatic Differentiation

Julia

- ForwardDiff/ReverseDiff - Operator overloading
- Zygote - Source to source reverse mode
- Enzyme - LLVM source to source reverse mode, experimental

Flexible choices good for different things, usable with most packages.

Python

Does not handle dynamic structure of the language.

- Tensorflow - Essentially source to source, but make user write IR
- PyTorch - Operator overloading
- Jax - Non-standard interpretation to create IR, then TF

Fast with standard deep learning, not as fast or flexible outside.

http://www.stochasticlifestyle.com/engineering-trade-offs-in-automatic-differentiation-from-tensorflow-and-pytorch-to-jax-and-julia/

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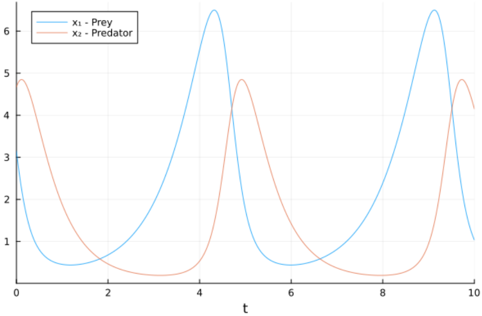
Embedding ML into differential equations

Example: Lotka-Volterra[1]

$$\frac{dx_1}{dt} = \alpha x_1 - \beta x_1 x_2$$
$$\frac{dx_2}{dt} = -\delta x_2 + \gamma x_1 x_2$$

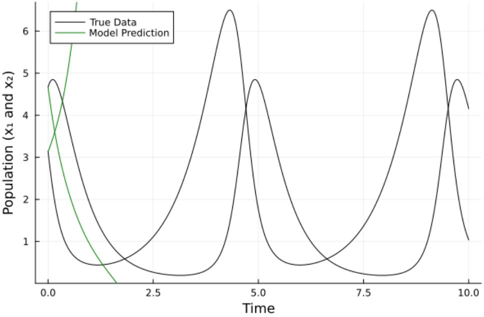


[1] https://docs.sciml.ai/Overview/stable/showcase/missing_physics/

Embedding ML into differential equations

Learn *unknown* dynamics with neural networks

$$\frac{dx_1}{dt} = \alpha x_1 + NN_1^{\boldsymbol{\theta}}(x_1, x_2)$$
$$\frac{dx_2}{dt} = -\delta x_2 + NN_2^{\boldsymbol{\theta}}(x_1, x_2)$$



Embedding ML into differential equations

Loss: difference between simulated $\boldsymbol{x}$ and real $\boldsymbol{x}_{data}$

$$L(\boldsymbol{\theta}) = \frac{1}{N}\sum_{i=1}^{N}\left[\boldsymbol{x}(t_i) - \boldsymbol{x}_{data}(t_i)\right]^2$$

```
function lotka_nn!(dx, x, p, t)
    x_nn = model(x, p)
    dx[1] = alpha * x[1] + x_nn[1]
    dx[2] = -delta * x[2] + x_nn[2]
end
```

```
function loss(p)
    prob = ODEProblem(lotka_nn!, x_train[:, 1], (0, 10), p)
    xhat = Array(solve(prob, saveat=t_train))
    mean(abs2, x_train .- xhat)
end
```

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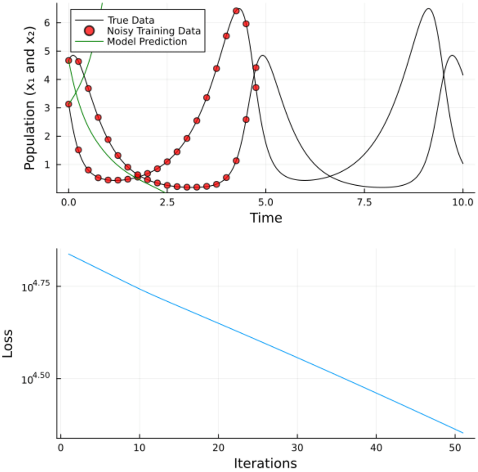

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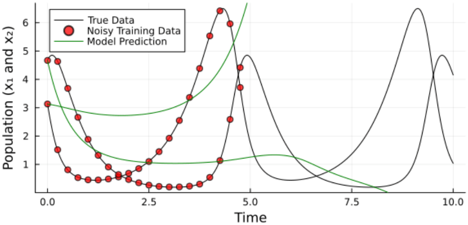

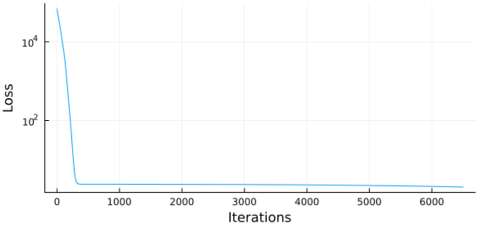

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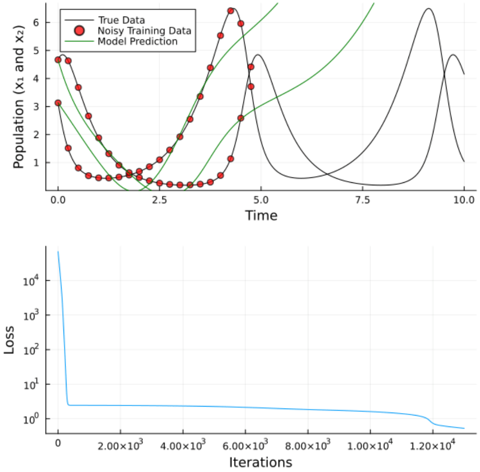

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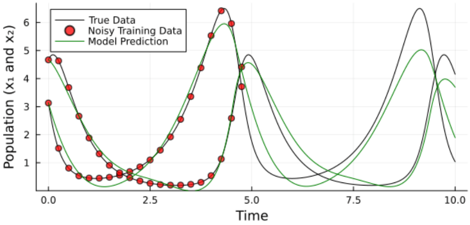

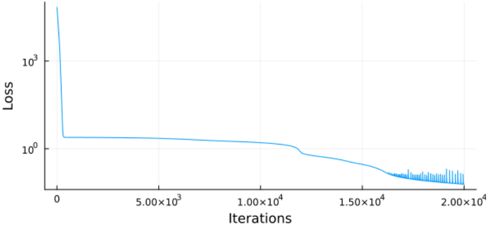

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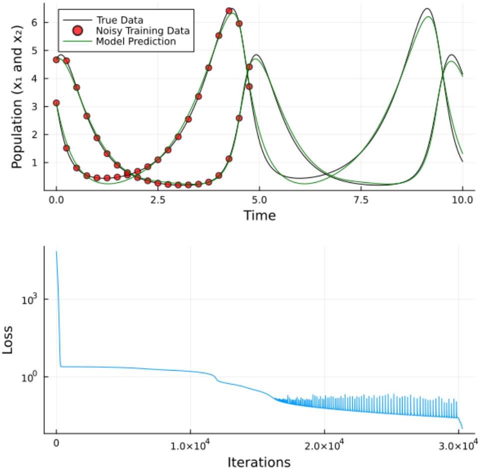

Embedding ML into differential equations

Remarks on the example:

- Found missing dynamics with NN
- Symbolic regression
- More effect in more complex models

Composability and Specialization

Performant composability, specialized code if types are inferred

Some interesting types

- Extended and arbitrary precision numbers
- Dual numbers for AD
- Intervals for interval arithmetic
- Distributions represented by number types
- GPU-arrays and distributed arrays
- Matrices with structure that can be exploited for performance, e.g. diagonal/banded/sparse

Performance

A few of the nice points

- Fast specialized code when type-stable
- Vectorized code vs for loops
- Built in parallelism

Some possible pitfalls

- Type instabilities
- Allocations
- Global scope

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Introspection

- Open source language and package ecosystem
- One language all the way down
- Useful tools (debugging, profiling) and macros
  - `@show func(a, b, c)`
  - `@edit func(a, b, c)`
  - `@code_llvm func(a, b, c)`

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