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Neuromancer:
Differentiable Programming Library for Modeling, Control, and Optimization

The Sixth Autonomous Energy Systems, NREL Workshop, Golden, CO

September 18, 2023

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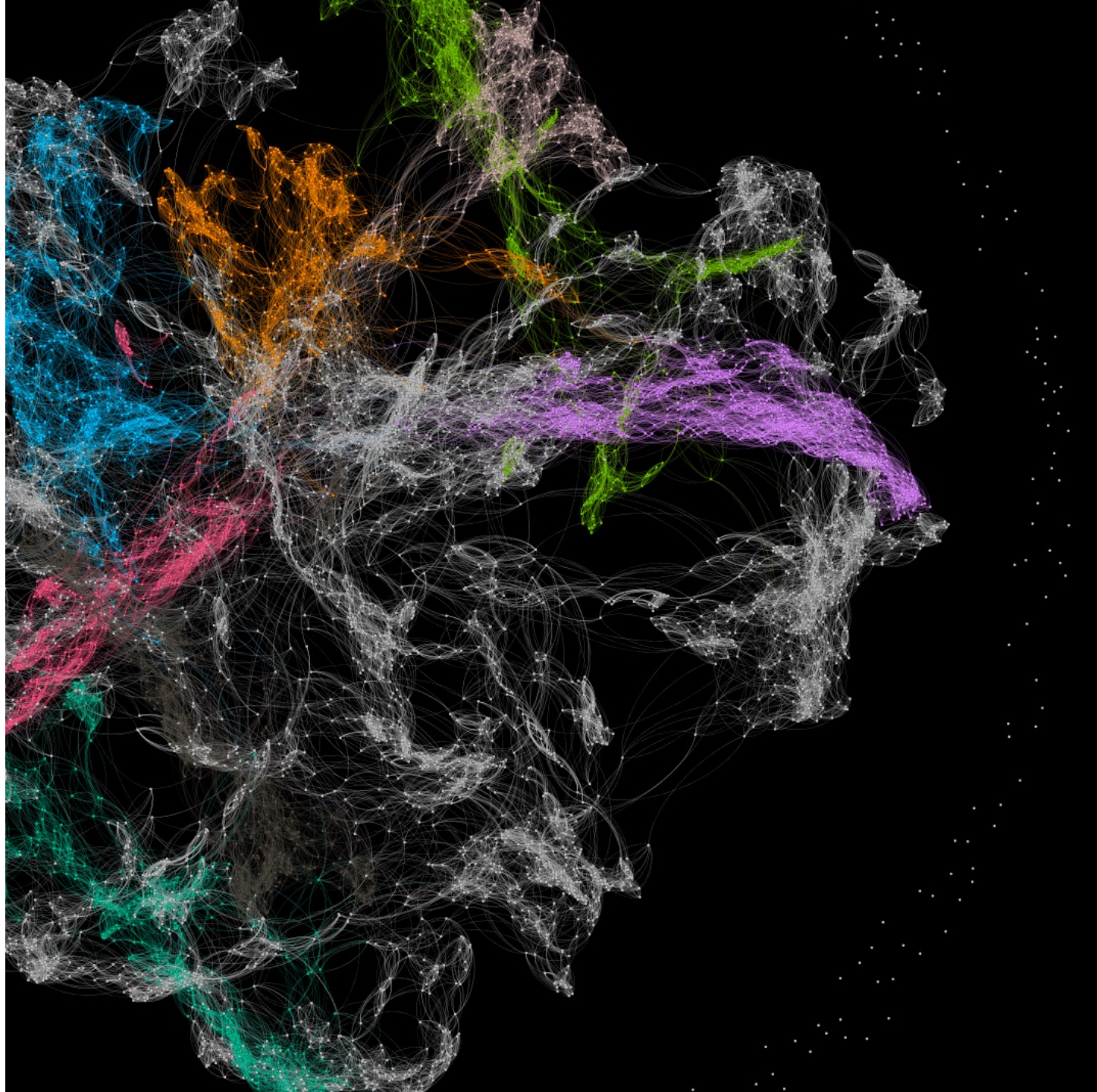

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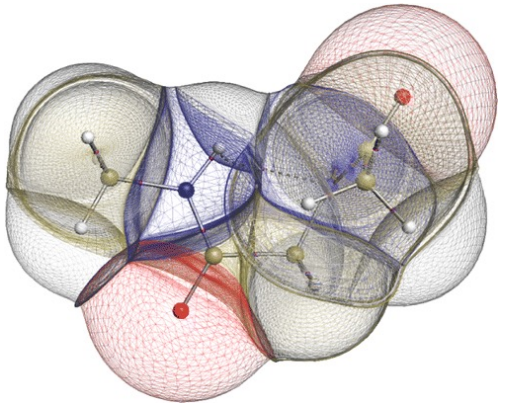
Challenges of Dynamical Systems Modeling and Control

- **Simulations** are crucial for many areas of decision-making and scientific discovery
- **Need**: Improve computational efficiency and scalability for heterogenous scientific simulations
- **Challenges**:
  - Physically-consistent data-driven modeling
  - Fast simulation of complex systems
  - Optimal control and design of complex systems
- **Emerging solution**:
  - Scientific Machine Learning connecting physics and AI domains

Latest Neural Nets Solve World's Hardest Equations Faster Than Ever Before

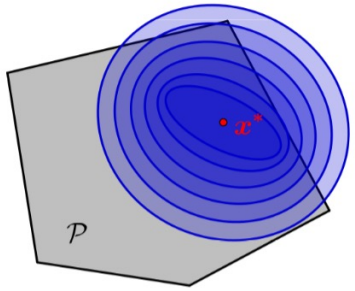
Quantamagazine



Landscape of Solution Methods

Constrained optimization

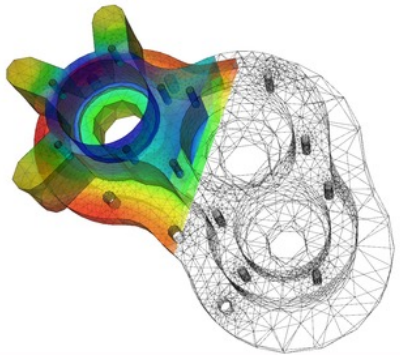
$$\begin{aligned} \min_{x} \quad & f(x) \\ \text{subject to} \quad & b(x) \geq 0 \\ & c(x) = 0. \end{aligned}$$



- Requires prior knowledge of objective function and constraints

Differential equations

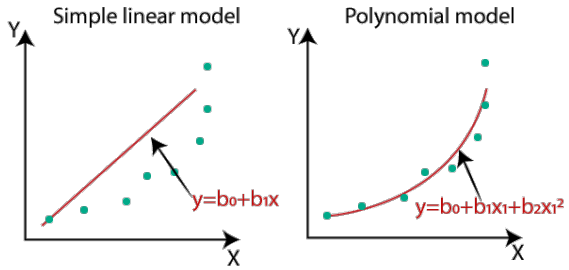
$$\frac{dy}{dx} = f(x)$$



- Requires prior knowledge of the physics to be modeled

Supervised Learning

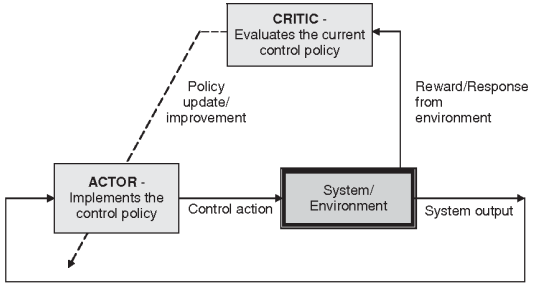
$$\min_{\theta} \frac{1}{N} \sum_{i=1}^{N} L(y^i, f(x^i, \theta))$$



- Requires large labeled datasets

Reinforcement Learning

$$\begin{aligned} \min_{\Theta} \quad & \sum_{i=1}^{m} \mathbf{r}(\mathbf{x}, \Theta) \\ \text{s.t.} \quad & \mathbf{Bellman}(\mathbf{x}, \Theta) = \mathbf{0}, \\ & \mathbf{environment}(\mathbf{x}, \Theta) = \mathbf{0} \\ & \mathbf{x} \in \Xi \end{aligned}$$



- Requires environment model to sample

More domain knowledge

Less domain knowledge

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Landscape of Solution Tools

Constrained optimization

Differential Equations

Supervised Learning

Reinforcement Learning

PYOMO

JUMP

GEKKO DYNAMIC OPTIMIZATION

CVXPY

CasADi

GUROBI OPTIMIZATION

DifferentialEquations.jl

MATLAB®

SciPy

PETSc TAO

NWCHEM

PyTorch

TensorFlow

flux

Gym

More domain knowledge

Less domain knowledge

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Landscape of Solution Tools

Online optimization

PYOMO

JUMP

GEKKO DYNAMIC OPTIMIZATION

CVXPY

CasADi

GUROBI OPTIMIZATION

Differential Equations

DifferentialEquations.jl

MATLAB®

SciPy

PETSc TAO

NWCHEM

Supervised Learning

PyTorch

TensorFlow

flux

Reinforcement Learning

Gym

What comes next? … Differentiable programming (DP): a unifying approach for data-driven modeling and optimization of complex systems based on automatic differentiation (AD)

Differentiable Programming Enables Scientific Machine Learning

- **Differentiable Programming**
  - M. Innes, et al., *A Differentiable Programming System to Bridge Machine Learning and Scientific Computing*, 2019
- **Physics-informed Neural Networks**
  - M. Raissi, et al., *Physics-informed neural networks: A deep learning framework for solving forward and inverse problems involving nonlinear partial differential equations*, 2019
- **Neural Differential Equations**
  - R. T. Q. Chen, et al., *Neural Ordinary Differential Equations*, 2019
  - C. Rackauckas , et al., *Universal Differential Equations for Scientific Machine Learning*, 2021
- **Differentiable Optimization**
  - A. Agrawal, et al., Differentiable Convex Optimization Layers, 2019
  - P. Donti, et al., *DC3: A learning method for optimization with hard constraints*, 2021
  - S. Gould, et al., *Deep Declarative Networks: A New Hope*, 2020
  - J. Kotary, et al., *End-to-End Constrained Optimization Learning: A Survey*, 2021
- **Differentiable Control**
  - B. Amos, et al., *Differentiable MPC for End-to-end Planning and Control*, 2019
  - S. East, et al., *Infinite-Horizon Differentiable Model Predictive Control*, 2020

NeuroMANCER: a Scientific Machine Learning Library

1. Mathematical formulation

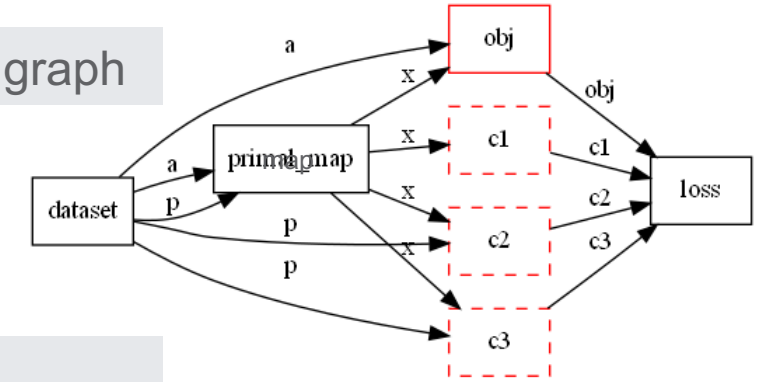
$$\min_{\Theta} (1-\mathbf{x})^2 + \boldsymbol{p}(\mathbf{y}-\mathbf{x}^2)^2$$
$$\text{s.t. } (\boldsymbol{p}/2)^2 \leq \mathbf{x}^2 + \mathbf{y}^2 \leq \boldsymbol{p}^2, \quad \mathbf{x} \geq \mathbf{y}$$
$$\mathbf{x} = \boldsymbol{\pi}_{\Theta}(\boldsymbol{p})$$

2. Python code interface

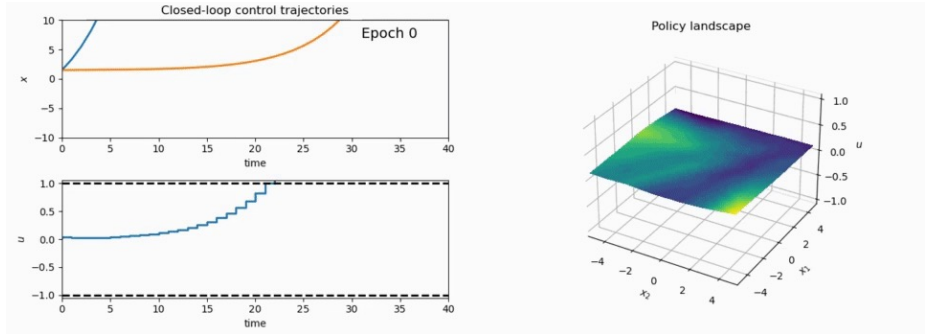
PyTorch

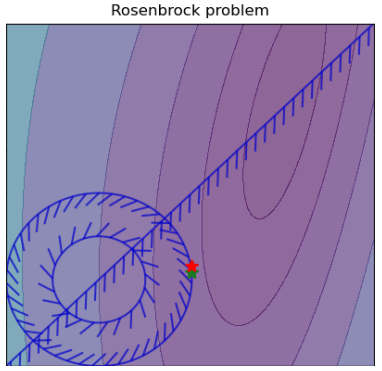
```
import neuromancer as nm

p = nm.variable('p')
x = nm.variable('x')
y = nm.variable('y')

obj = ((1-x)**2 + p*(y-x**2)**2).minimize(weight=1.0, name='obj')
c1 = (p/2)**2 <= x**2 + y**2
c2 = x**2 + y**2 <= p**2
c3 = x >= y

net = nm.MLP(insize=2, outsize=2, hsizes=[80]*4)
map = nm.Node(net, input_keys=['p'], output_keys=['x','y'])

loss = nm.PenaltyLoss([obj], [c1, c2, c3])
problem = nm.Problem([map], loss)
optimizer = torch.optim.AdamW(problem.parameters())
trainer = nm.Trainer(problem,data,optimizer)
best_model = trainer.train()
```

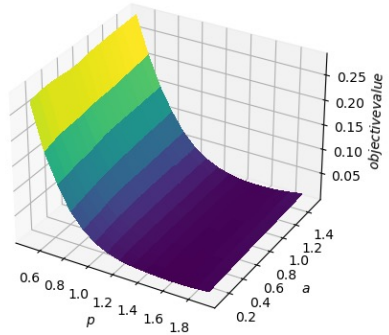
3. Problem graph



4. Results

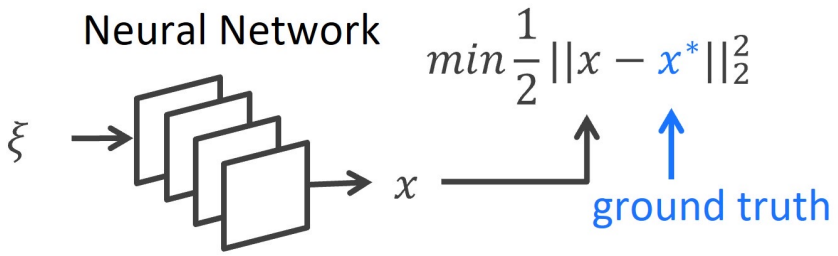




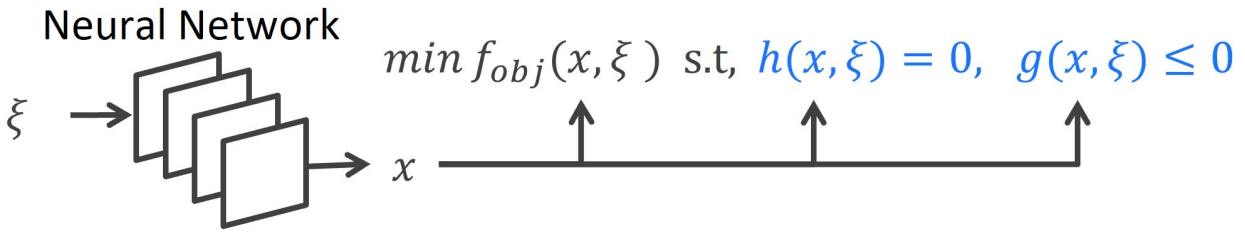


Parametric Constrained Optimization Capabilities in Neuromancer

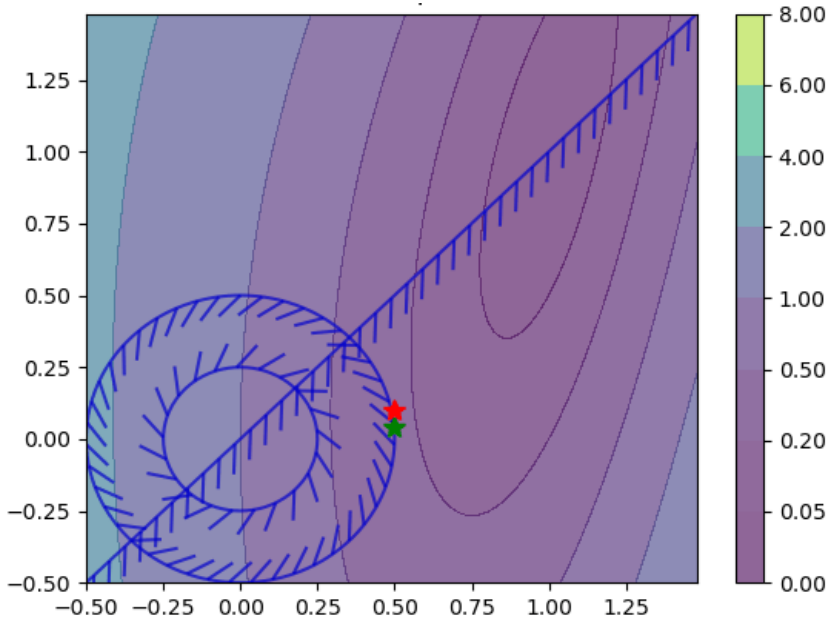
Imitation Learning



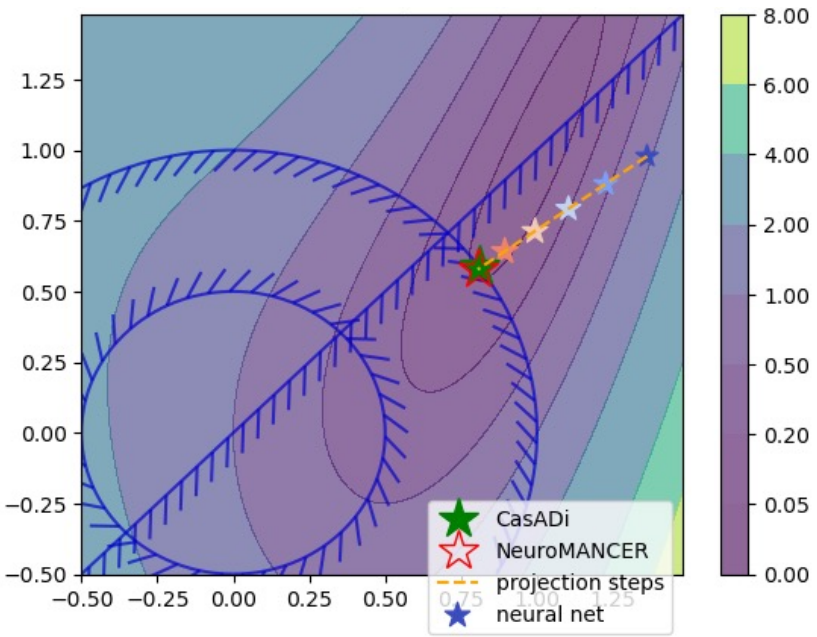
Differentiable Parametric Programming
or, Constrained Deep Learning, End-to-end NN



Training neural networks as explicit solutions

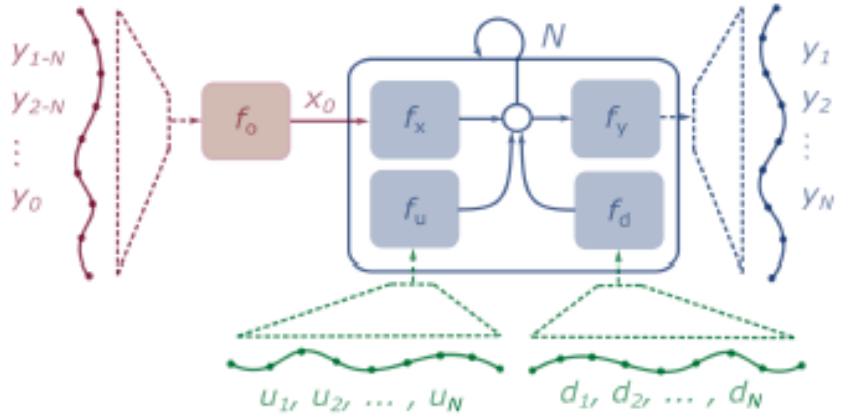


Feasibility restoration with implicit layers

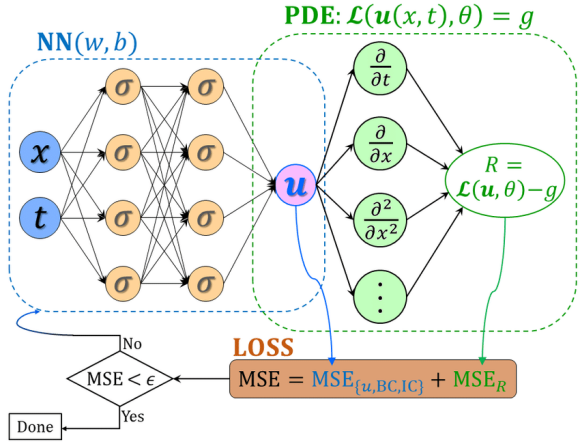


Data-driven Modeling Capabilities in Neuromancer

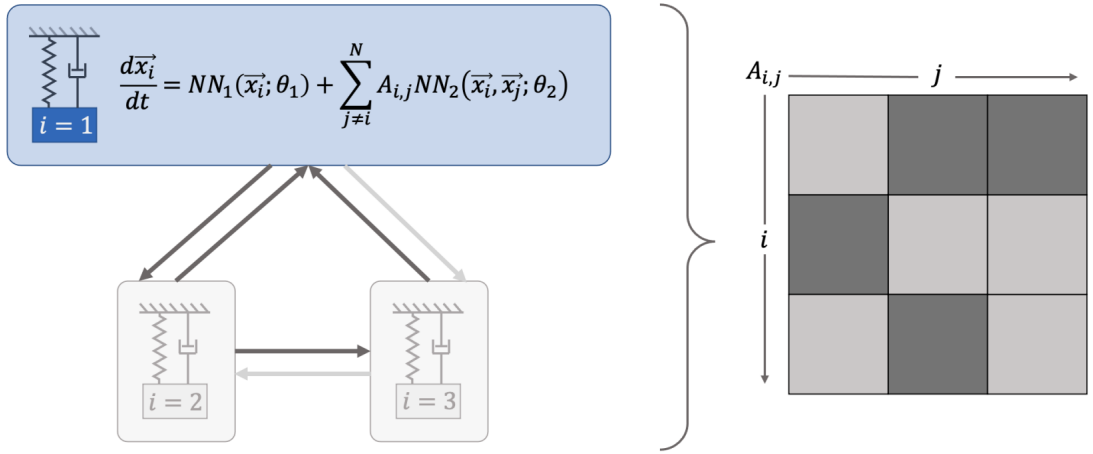
Component-based Physics-informed Machine Learning



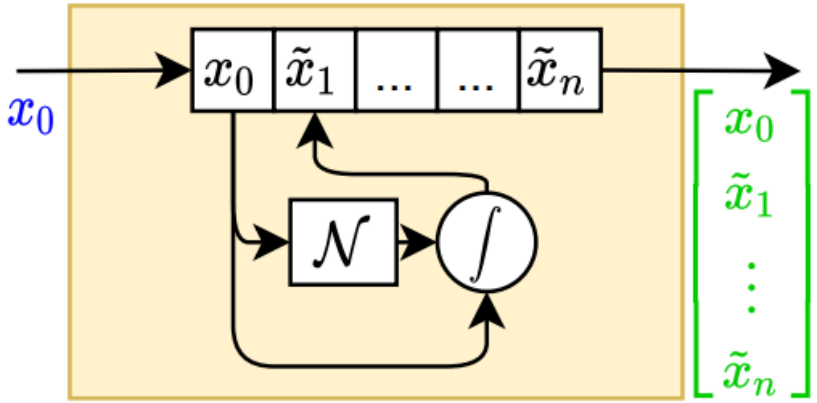
Physics-Informed Neural Networks



Networked Dynamical systems

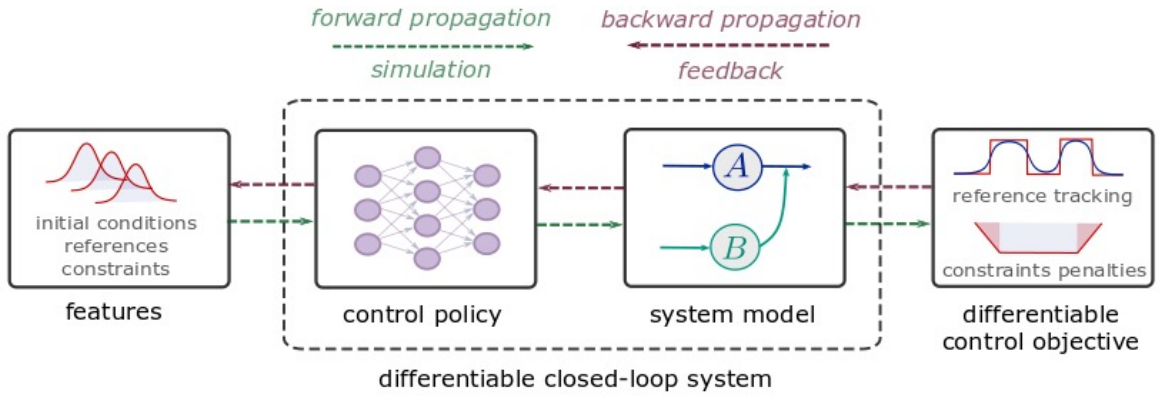


Neural differential equations

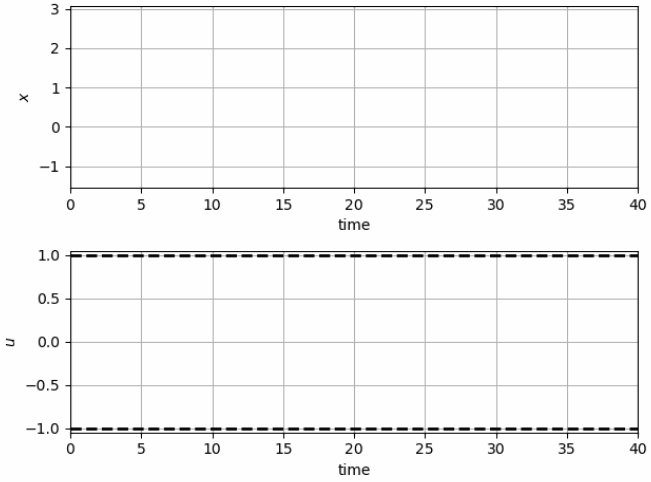


Optimal Control Capabilities in Neuromancer

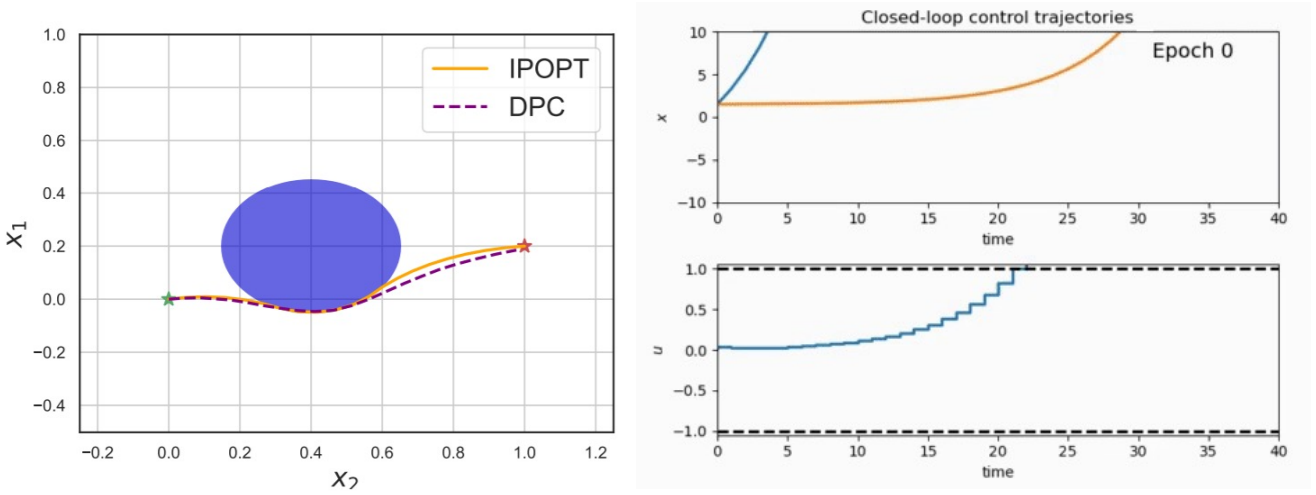
Learning constrained model-based control policies with differentiable control methods



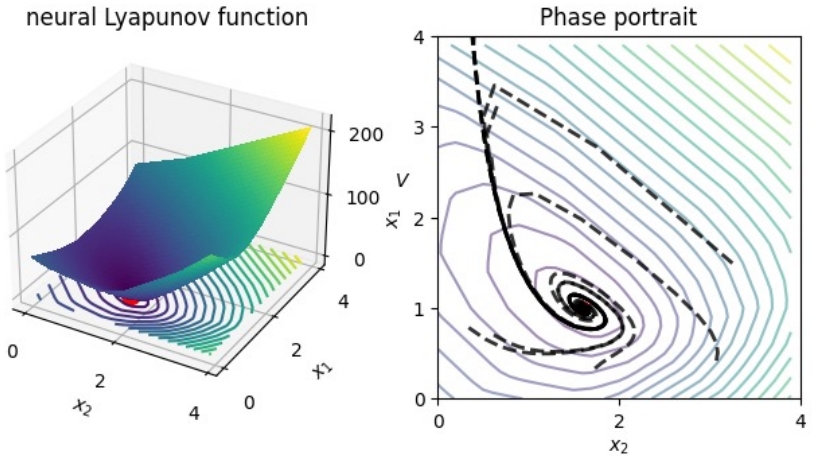
Learning stabilizing controllers



Trajectory optimization and obstacle avoidance



Learning Neural Lyapunov Functions



NeuroMANCER

Open-source scientific machine learning (**SciML**) toolbox in PyTorch for integrating deep learning, constrained optimization, and physics-based modeling

- **Physics-informed machine learning**
- **Data-driven modeling of dynamical systems**
- **Model-based policy optimization**
- **Parametric constrained optimization**

github.com/pnnl/neuromancer

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Acknowledgements


Aaron Tuor


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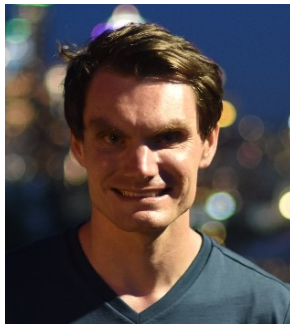
Stefan Dernbach


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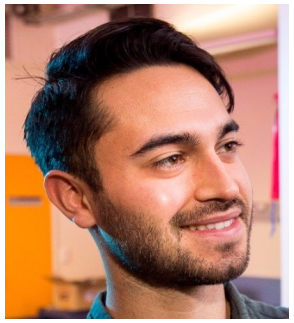
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