Modelling dynamical systems: Learning ODEs with no internal ODE resolution

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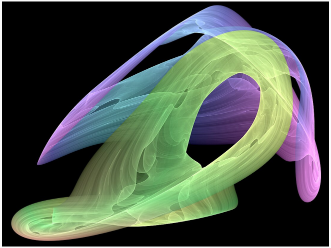
Dynamic system modeling



Goal:

Create a surrogate model for particle accelerators

- Predict beam trajectory from initial state and accelerator settings
- Accelerator trajectories could be anything from beam position, size, emittance along the beamline
- trajectory could be also seen as any times series data
- Model beam trajectory using an **ODE framework**

Problem Description: Supervised Learning for ODE Approximation

Objective: Learn an approximate trajectory of the particle beam based on time measurements and control parameters.

Key Components:

- **Time Measurements:**

  $$(T_i)_{i=1}^N \quad \text{with} \quad T_i \in [t_0, T]$$

  These are the discrete time points where the trajectory is observed.
- **Trajectory Function:**

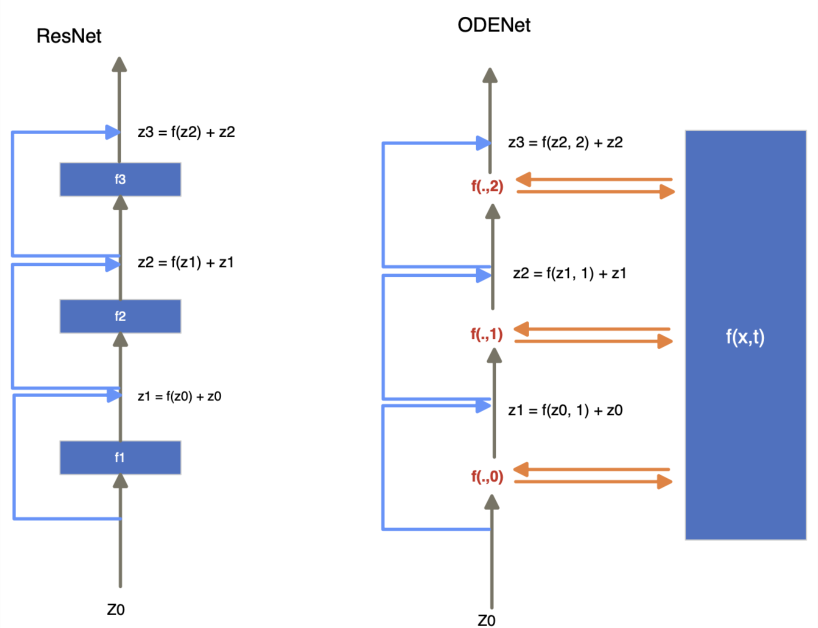
  $$\mathrm{u} : [t_0, T] \times \mathbb{R}^p \to \mathbb{R}^n$$

  The trajectory $\mathrm{u}(t, \mathbf{c})$ maps time t and the initial state/control parameters $\mathbf{c}$ to a position in the n-dimensional space.
- **Control Parameters:**

  $$\mathbf{c} \in \mathbb{R}^m$$

  Control parameters $\mathbf{c}$ influence the trajectory of the beam. These could represent accelerator settings or other system controls.
- **Goal:** Approximate the trajectory $\mathrm{u}(t, \mathbf{c})$ by learning from the initial

Background


ResNet
ODENet
z3 = f(z2) + z2
f3
z2 = f(z1) + z1
f2
z1 = f(z0) + z0
f1
Z0
z3 = f(z2, 2) + z2
f(.,2)
z2 = f(z1, 1) + z1
f(.,1)
z1 = f(z0, 1) + z0
f(.,0)
Z0
f(x,t)

- **Recurrent Neural Networks (RNNs):**

$$\mathrm{u}(t_{i+1}, \mathbf{c}) = \mathrm{u}(t_i, \mathbf{c}) + f_\theta(\mathrm{u}(t_i, \mathbf{c}))$$

  - f_θ is a neural network that captures the system's dynamics.
  - θ refers to the learned weights of the neural network.

- **Neural ODEs (NODEs) Chen-2018:**
  - Unlike RNNs, NODEs model the system's behavior in continuous time:

$$\frac{d\mathrm{u}(t, \mathbf{c})}{dt} = f(\mathrm{u}(t, \mathbf{c}), t, \mathbf{c})$$

  - Here, f_θ is a neural network that approximates the unknown dynamics f.
  - The trajectory $\hat{\mathrm{u}}(t, \mathbf{c})$ is computed by solving the ODE:

$$\frac{d\hat{\mathrm{u}}(t, \mathbf{c})}{dt} = f_\theta(\hat{\mathrm{u}}(t, \mathbf{c}), t, \mathbf{c})$$

  - This approach allows for a more flexible representation of time-evolving processes.

NODE integrates neural networks into the ODE framework by parameterizing the derivative of the state with respect to time using a neural network:

$$\frac{\mathrm{d}\mathrm{u}}{\mathrm{d}t}(t,\mathbf{c}) = f\left(\mathrm{u}(t,\mathbf{c}), t, \mathbf{c}\right) \quad \rightarrow \quad \frac{\mathrm{d}\widehat{\mathrm{u}}}{\mathrm{d}t}(t,\mathbf{c}) = f_\theta\left(\widehat{\mathrm{u}}(t,\mathbf{c}), t, \mathbf{c}\right)$$

NODE Algorithm:

1. Initialize the neural network f_θ with random weights.
2. For a control parameter $\mathbf{c}$ and trajectory $\mathrm{u}(t,\mathbf{c})$:
   - 2.1 Solve the ODE to get $\widehat{\mathrm{u}}(t,\mathbf{c})$.
   - 2.2 Compute the loss: $L(\widehat{\mathrm{u}}(T,\mathbf{c})) = ||\widehat{\mathrm{u}}(T,\mathbf{c}) - \mathrm{u}(T,\mathbf{c})||^2$.
   - 2.3 Calculate the gradient of the loss using the adjoint method.
   - 2.4 Update the network weights based on the gradient.

Resolution: The state estimate $\widehat{u}(t,\mathbf{c})$ at any time t is obtained by numerically solving the ODE.

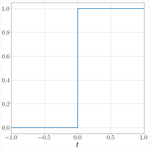
$$\widehat{u}(t,\mathbf{c}) = \mathrm{ODESolve}\left(\widehat{f_\theta}(\cdot,\mathbf{c}), \widehat{u}(t_0,\mathbf{c}), t_0, t, \mathbf{c}\right)$$

Limitations of NODE

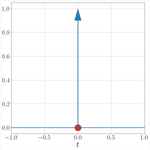
1. Computational Time: NODE relies on numerical ODE solvers to integrate the system's dynamics. This can become computationally intensive, especially for complex models and long-time series.

2. Modeling Discontinuities:

- NODE inherently assumes smooth dynamics governed by the ODEs ($\frac{\mathrm{d}u}{\mathrm{d}t}$ should be well defined everywhere).
- The smooth dynamics assumption makes it challenging to model time series with abrupt changes or discontinuities.



$$\mathrm{u}\left(t, \mathbf{c}\right) = H\left(t\right)$$



$$\frac{\mathrm{d}u}{\mathrm{d}t}\left(t, \mathbf{c}\right) = \delta\left(t\right)$$

Neural Integral Ordinary Differential Equations (NIODE)

Objective: Learn the trajectories u using a model inspired by NODEs.

Additional Information: Incorporate an **extra function** $\mathrm{v} = \mathcal{F}(u)$ that satisfies:

$$\frac{d\mathrm{v}}{dt}(t, \mathbf{c}) = g(\mathrm{u}(t, \mathbf{c}), \mathrm{v}(t, \mathbf{c}), t)$$

where g is called a driving function and must satisfy :

1. **Lipschitz Continuity in State Space:**

$$\|g(\mathrm{u}_2, \mathbf{x}_\mathbf{v}, t) - g(\mathrm{u}_1, \mathbf{x}_\mathbf{v}, t)\| \leq k_\mathrm{u} \|\mathrm{u}_2 - \mathrm{u}_1\|$$

2. **Lipschitz Continuity in Integral State Space:**

$$\|g(\mathrm{u}, \mathbf{x}_{\mathbf{v}2}, t) - g(\mathrm{u}, \mathbf{x}_{\mathbf{v}1}, t)\| \leq k_\mathrm{v} \|\mathbf{x}_{\mathbf{v}2} - \mathbf{x}_{\mathbf{v}1}\|$$

3. **Continuity Over Time:** g is continuous with respect to time.

Different Choices for v and Their Impact on g

1. **Case 1:** If $\mathrm{v}(t, \mathbf{c})$ is the integral of $u(t, \mathbf{c})$:

$$\mathrm{v}(t, \mathbf{c}) = \int_{t_0}^{t} u(s, \mathbf{c})\, ds$$

   Then, $g = u$ (identity with respect to u).

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2. **Case 2:** If $\mathrm{v}(t, \mathbf{c})$ is the exponentially smoothed version of $u(t, \mathbf{c})$:

$$\mathrm{v}(t, \mathbf{c}) = u(t_0, \mathbf{c}) e^{-\lambda(t - t_0)} + \lambda \int_{t_0}^{t} e^{-\lambda(t-s)} u(s, \mathbf{c})\, ds$$

Then, $g = \lambda(u - \mathrm{v})$.

Framework:

We consider an **extra function** $\mathrm{v}(t, \mathbf{c})$ that evolves according to the differential equation, where the **driving function** g verifies certain properties :

$$\frac{\mathrm{d}\mathrm{v}(t,\mathbf{c})}{\mathrm{d}t} = g(\mathrm{u}(t,\mathbf{c}), \mathrm{v}(t,\mathbf{c}), t) \tag{1}$$

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- Compute $\mathsf{v}(t, \mathbf{c})$ from all observable trajectories $\mathsf{u}(t, \mathbf{c})$.
- Train a neural network f_θ to learn $\mathsf{u}(t, \mathbf{c})$ from $\mathsf{v}(t, \mathbf{c})$:

$$\mathsf{u}(t, \mathbf{c}) = f_\theta(\mathsf{v}(t, \mathbf{c}), t, \mathbf{c})$$

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$$\mathrm{u}(t, \mathbf{c}) = f_\theta(\mathrm{v}(t, \mathbf{c}), t, \mathbf{c})$$

- This defines a new ODE:

$$\frac{\mathrm{dv}(t, \mathbf{c})}{\mathrm{d}t} = g(f_\theta(\mathrm{v}(t, \mathbf{c}), t, \mathbf{c}), \mathrm{v}(t, \mathbf{c}), t) = g_\theta(\mathrm{v}(t, \mathbf{c}), t, \mathbf{c})$$

Step 1: Operator preprocessing:

- Compute $\mathrm{v} = \mathcal{F}(\mathrm{u})$ from training data.

Step 2: Learning the ODE:

- Train neural network f_θ to minimize the discrepancy between observed trajectories $\mathrm{u}(t, \mathbf{c})$ and predicted trajectories $f_\theta(\mathrm{v}(t, \mathbf{c}))$:

$$\min_{f_\theta} \|\mathrm{u}(t, \mathbf{c}) - f_\theta(\mathrm{v}(t, \mathbf{c}))\|$$

  This is a classic regression problem

Step 3: Evaluation:

- Solve the ODE defined by g_θ to compute the predicted auxiliary function $\widehat{\mathrm{v}}(t, \mathbf{c})$.
- Estimate the trajectory $\widehat{\mathrm{u}}(t, \mathbf{c})$ as $\widehat{\mathrm{u}}(t, \mathbf{c}) = f_\theta(\widehat{\mathrm{v}}(t, \mathbf{c}))$.

Preliminary Experiment Results

- $u(z, c)$ is the evolution of a beam in a linear particle accelerator
- z is the longitudinal position of the beam (equivalent of$t$ in the equations above)
- $c \in \mathbb{R}^{108}$ is a control parameter of the simulation

Goal:

- Learn $c \to u(\cdot, c)$

Method:

- Learn $\widehat{f}$ s.t. $u(z, c) = \widehat{f}\left(\int_{s=0}^{z} u(s, c)\, \mathrm{d}s, z, c, \theta\right)$

Dataset

- Linac dataset **ThomX-2024** contains 4000 simulations generated by Astra.
- Control settings dimension ($\mathbf{c}$) is 36 **Purwar-2023**.
- Each trajectory consists of 4000 points: $(t_j, \mathrm{u}(t_j, \mathbf{c}_j))$, $t_j \in [0, 9.393]$.

Experiment Set-up

- Compare three variants against baselines (LSTM, NODE).

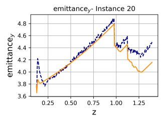
Performance Measurement

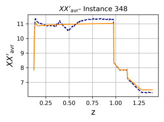
- Use the coefficient of determination R^2 to evaluate model performance:

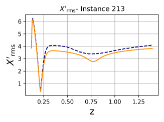
$$R^2 = 1 - \frac{\sum_{i=1}^{n}(y_i - \hat{y}_i)^2}{\sum_{i=1}^{n}(y_i - \bar{y})^2}$$

Preliminary Results

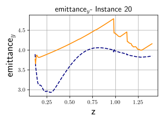
LSTM

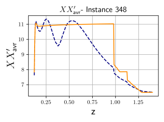


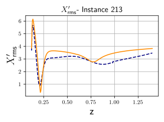




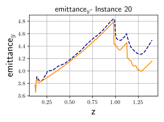
NODE

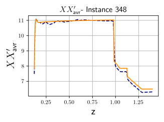


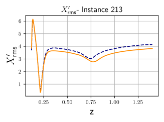




INODE







Emittance over time | XX'_{avr} over time | X'_{ms} over time

(The orange curve represents the ground truth trajectory)

Conclusion

INode Framework:

- Extends Neural ODEs to handle systems with discontinuous behavior.
- Efficient for data-driven ODEs, avoiding the need to directly solve complex ODEs during training.
- Uses integral operators to process input data, addressing challenges of discontinuities. **Other families of operators could be explored !**

Key Results:

- Theoretical guarantees
- Improved computational efficiency
- Provides a foundational approach that can be extended for future work

Questions ?

Thanks you for your attention

Bibliography

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