

Neural Ordinary Differential Equations

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Deep Implicit Layers

Modern deep learning architectures are made by a stack of multiple layers, whose computational structure is explicitly defined, so that, given the input x , the output y of a layer $f : \mathcal{X} \times \mathbb{R}^{|\theta|} \rightarrow \mathcal{Y}$ can be directly computed as

$$y = f(x; \theta)$$

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$$\text{Find } y : f(x; \theta) - y = 0$$

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with $g : \mathcal{X} \times \mathcal{Y} \times \mathbb{R}^{|\theta|} \rightarrow \mathbb{R}^n$.

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⇒ *Root finding problem* → Bisection method, Newton's method...

⇒ Decouple the *definition* of the layer and from its *computational structure*.

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$$\text{Find } y(t^*) : \frac{dy}{dt}(t) = f(t, y(t); \theta), \quad y(0) = y_0$$

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requiring the IVP is satisfied, where $f : \mathbb{R} \times \mathbb{R}^d \times \mathbb{R}^{|\theta|} \rightarrow \mathbb{R}^d$ is a neural network, $\theta = \{(W_l, b_l)\}_{l=1}^L$ is the set of learnable parameters of its L-layers, and $y_0 \in \mathbb{R}^d$.

⇒ **Neural Ordinary Differential Equation.**

Derivating Neural ODEs from ResNets

Continuous-depth architectures

The t -th block in a ResNet architecture consists of

$$y_{t+1} = y_t + f(y_t; \theta_t)$$

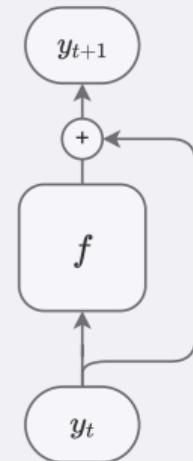
and resembles the Explicit Euler's Method discretization with $h = 1$

$$y_{t+1} - y_t = hf(y_t; \theta_t)$$

corresponding to the continuous formulation

$$\frac{dy}{dt}(t) = f(t, y(t); \theta)$$

ResNet Block



Computing the output of an ODE-Layer

Ordinary Differential Equations Layers

In order to compute the output of the implicitly defined ODE-layers we rely on numerical integration methods

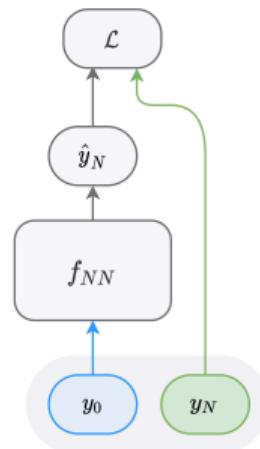
$$y_{t_0}, \dots, y_{t_N} = \text{ODEint}(f, y_0, [t_0, \dots, t_N])$$

implemented in the `torchdiffeq` library, together with the *Adjoint Backpropagation Method* (Chen et al. 2018).

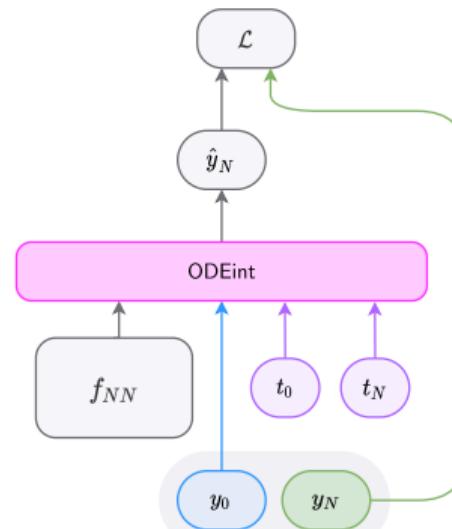
Architectures differences

Backpropagation in ODE-Nets

FFNN



ODE-Net

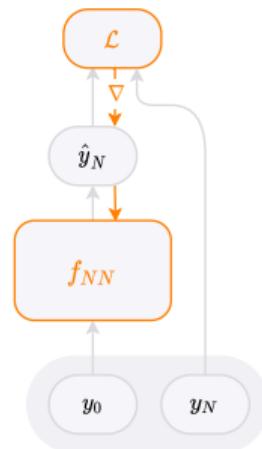


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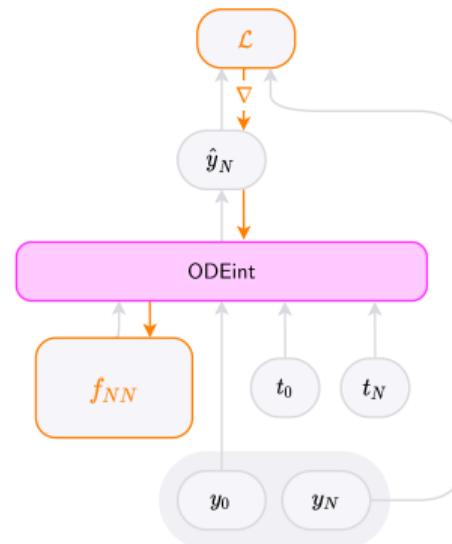
FFNN

$$\mathcal{L}(\hat{y}_N) = \mathcal{L}(f_{NN}(y_0; \theta))$$



ODE-Net

$$\mathcal{L}(\hat{y}_N) = \mathcal{L}(\text{odeint}(f_{NN,\theta}, y_0, t_0, t_N))$$



Architectures differences

Backpropagation in ODE-Nets

Adjoint Backpropagation Method (Chen et al. 2018) can be employed for backpropagating through the ODE solver:

Input: Params θ , start time t_0 , stop time t_N , final state $y(t_N)$, loss gradient $\frac{\partial \mathcal{L}}{\partial y(t_N)}$

$$s_0 = [y(t_N), \frac{\partial \mathcal{L}}{\partial y(t_N)}, 0_{|\theta|}]$$

def AugmentedDynamics($[y(t), a(t), \cdot]$, t, θ):

| **return** $[f(y(t), t, \theta), -a(t)^T \frac{\partial f}{\partial y}, -a(t)^T \frac{\partial f}{\partial \theta}]$;

$$[y(t_0), \frac{\partial \mathcal{L}}{\partial y(t_0)}, \frac{\partial \mathcal{L}}{\partial \theta}] = \text{ODEint}(\text{Augmented Dynamics}, s_0, t_N, t_0, \theta)$$

return $\frac{\partial \mathcal{L}}{\partial y(t_0)}, \frac{\partial \mathcal{L}}{\partial \theta}$;

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```
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    | return [f(y(t), t, θ), -a(t)T ∂f / ∂y, -a(t)T ∂f / ∂θ];
```

$$[y(t_0), \frac{\partial \mathcal{L}}{\partial y(t_0)}, \frac{\partial \mathcal{L}}{\partial \theta}] = \text{ODEint}(\text{Augmented Dynamics}, s_0, t_N, t_0, \theta)$$

```
return ∂L / ∂y(t_0), ∂L / ∂θ;
```

Practically we already know how to backpropagate through some solvers since they can be viewed as a ResNet (i.e. Euler).

Learning Latent ODE

Framework

The aim of the project is to employ Neural ODEs to learn the latent dynamics of time-dependent processes, by exploiting NODEs' continuous-depth (time-continuous) architecture:

$$\dot{u} = f(t, u(t); \mu)$$

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Learning Latent ODE

Framework

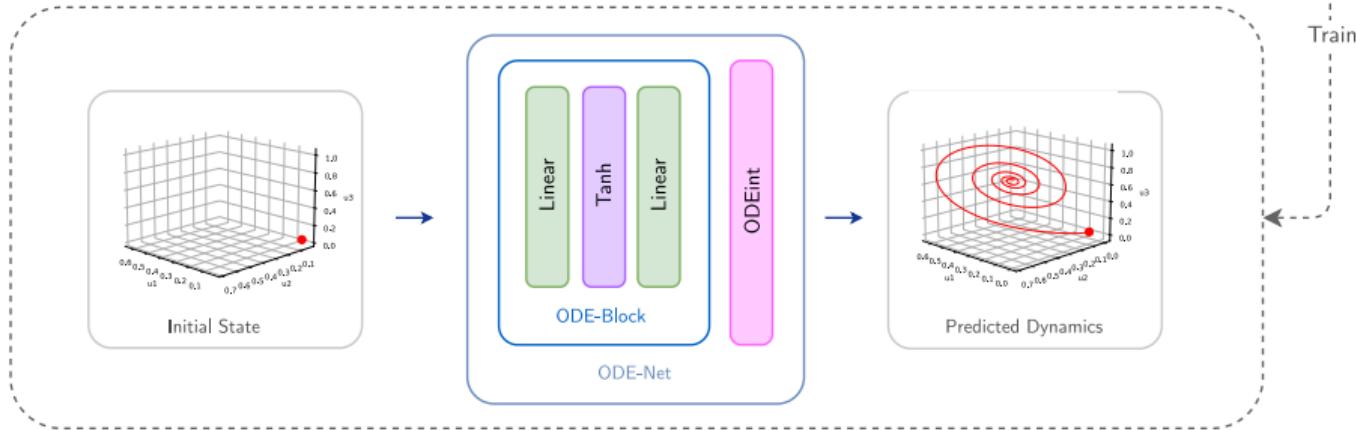
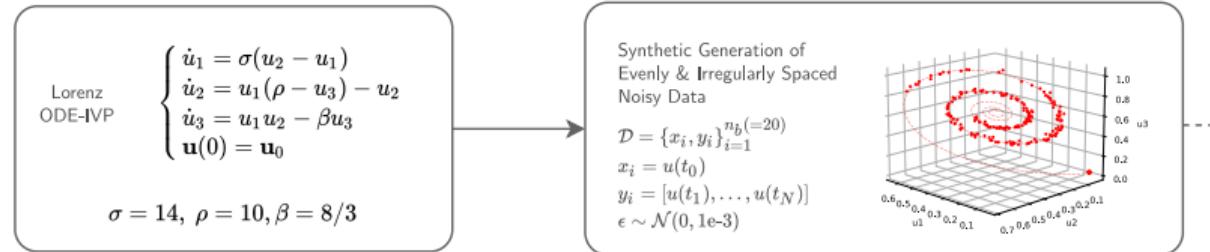
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Observation: the learned function has direct interpretation, we will refer to it as the *learned vector field*.

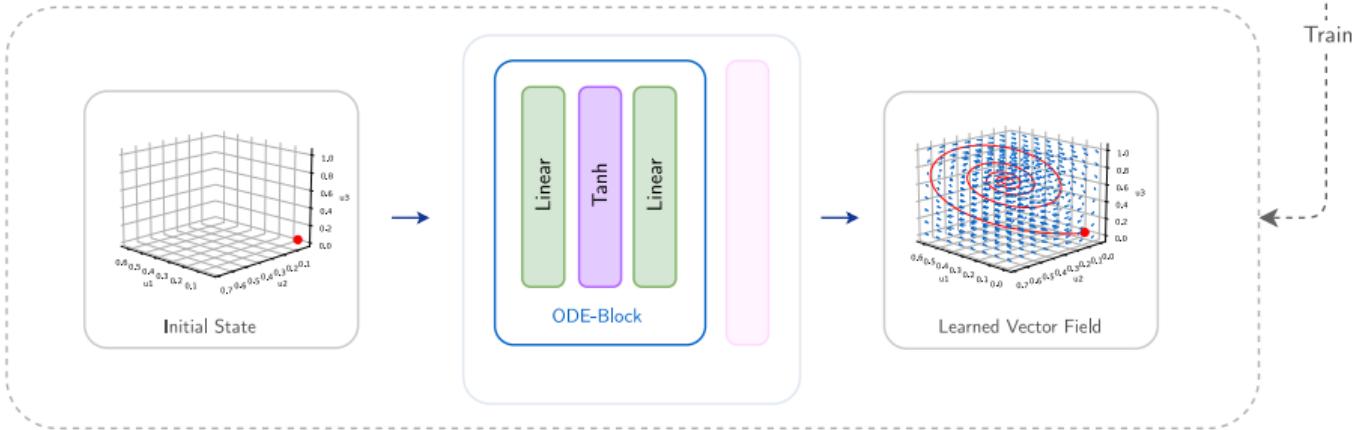
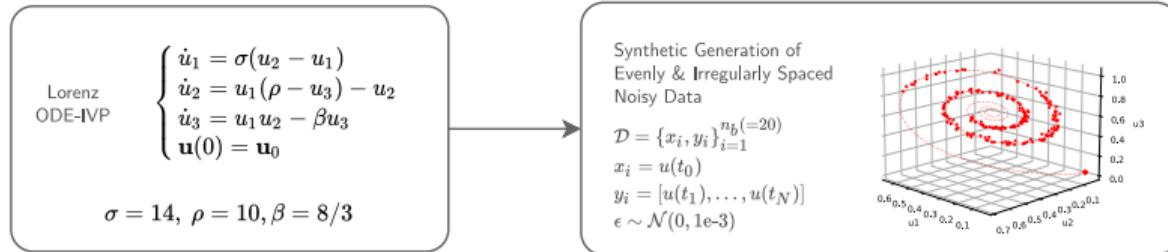
Spiral ODE

Application I - Framework



Spiral ODE

Application I - Framework



Integration Methods Comparison

Application I - Training

Evenly spaced										Irregularly spaced			
	Method	Training time [min]	Time/Epoch [s]	MSE	Max NFE	Training time [min]	Time/Epoch [s]	MSE	Max NFE				
Fixed	Euler	7.721	0.231	7.62e-03	199	7.987	0.239	9.17e-03	199				
	Euler+Adjoint	17.283	0.518	1.37e-02	398	17.339	0.520	1.45e-02	398				
	Step	RK4	22.984	0.689	6.31e-03	796	23.838	0.715	1.12e-02	796			
Adaptive	RK4+Adjoint	25.541	0.765	1.02e-02	1592	25.612	0.768	1.12e-02	1592				
	Bosh3	39.452	1.183	4.89e-03	1007	58.671	1.760	4.91e-03	1883				
	Bosh3+Adjoint	112.364	3.370	2.88e-03	3328	140.651	4.219	4.16e-03	5230				
Step	DorPri5	12.263	0.367	2.83e-03	212	17.311	0.519	3.70e-03	380				
	DorPri5+Adjoint	73.300	2.198	1.10e-02	1786	87.391	2.621	6.43e-03	2578				

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- Adjoint Backprop Method: up to 4x slower training & worsen predictive performances.

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- Adjoint Backprop Method: up to 4x slower training & worsen predictive performances.
- Dormand-Prince 5 has been selected due to training performances and low MSE.

ODE-Block: Linear/Tanh/Linear, 50 hidden units per layer.

Data noise $\varepsilon \sim \mathcal{N}(0, 1e-3)$ added to globally max-scaled data. Irregular spacing obtained by uniformly sampling from a fixed batch time interval of 200 time-steps.

ODE-Block Configurations

Application I - Hyperparameters Tuning

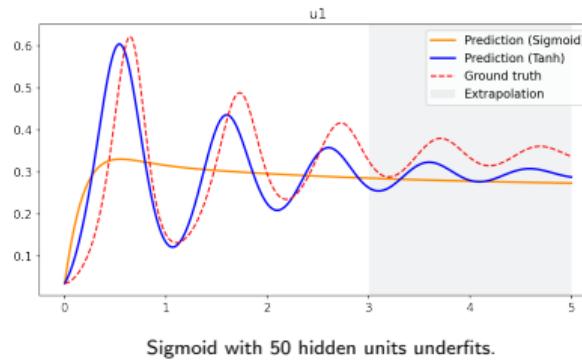
ODE-Block structure:

Layer	Input Size	Output Size
1	3	n hidden units
		activation
2	n hidden units	3

Tested configurations:

- Hidden Units: 20, 50, 100
- Activations: Sigmoid, Tanh

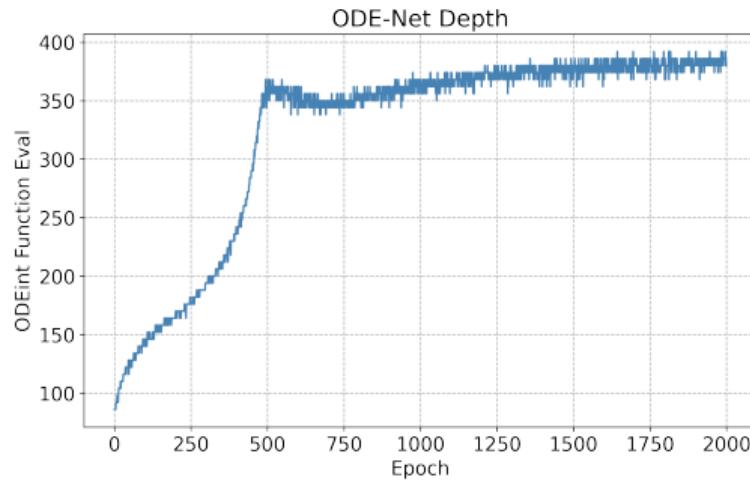
Activation	Hidden units	Time/Epoch [s]	Train MSE	Test MSE
Sigmoid	20	0.151	1.58e-02	1.51e-03
	50	0.336	2.45e-02	2.01e-03
	100	0.350	2.68e-02	3.97e-03
Tanh	20	0.401	1.99e-02	1.88e-03
	50	0.453	2.38e-03	8.97e-04
	100	0.484	6.96e-03	8.24e-04



What about ODE-Nets' depth?

Application I

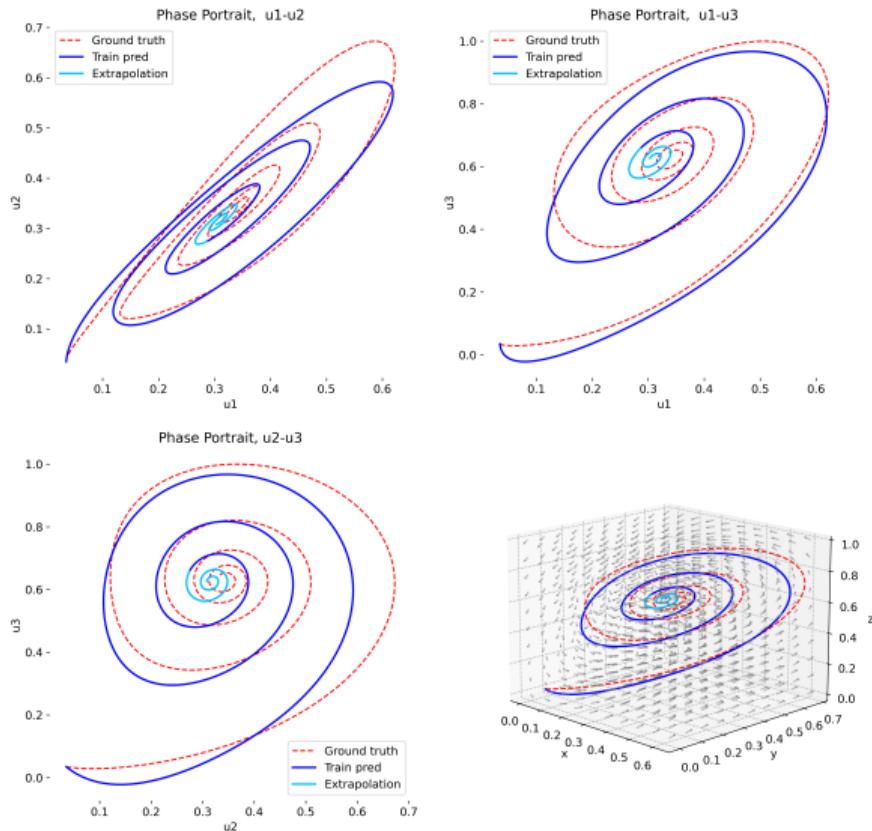
ODE-Nets' depth depends on the number of function evaluations taken by the adaptive-step solver, and it grows as the training proceeds, resulting in 4x deeper networks, wrt classical ResNets.



Observations

Application I

- ODE-Nets are able to capture the general behavior of the true underlying dynamics.
- A major role is played by the employed integration method, both in terms of training performances and predictive capabilities.



Augmenting Neural ODE Framework

- ① Improve predictive accuracy and robustness wrt irregularly sampled data
- ② Quantify predictions' uncertainty

A natural way to model uncertainty in a NN-framework is to employ Bayesian Neural Networks (BNNs), enabling to model weights and biases as distributions.

Problem: BNNs are computationally demanding, thus the training process is critically slowed down when dealing with very deep architectures (like ODE-Nets).

Solution: Employ an *ensembling*-based approximated Bayesian NNs framework.

Approximately Bayesian Ensembling

The framework employed, introduced by Pearce et al. 2018, exploits the fact that by adding a regularization term to the loss, the parameters that minimize the regularized loss can be interpreted as MAP estimates.

$$\mathcal{L}(y_i, \hat{y}_i) = \|y_i - \underbrace{\text{odeint}(f_\theta, x_i, t_0, t_N)}_{\hat{y}_i}\|^2 + \lambda \|\theta\|^2$$

Problem: Regularization reduces diversity between differently initialized models, reducing the ensemble's capabilities to capture uncertainty.

Anchored Bayesian Ensembling

The framework employed, introduced by Pearce et al. 2018, exploits the fact that by adding a regularization term to the loss, the parameters that minimize the regularized loss can be interpreted as MAP estimates.

$$\mathcal{L}_{\text{anc}}(y_i, \hat{y}_i) = \|y_i - \underbrace{\text{odeint}(f_\theta, x_i, t_0, t_N)}_{\hat{y}_i}\|^2 + \lambda \|\theta - \theta_{\text{anc}}\|^2$$

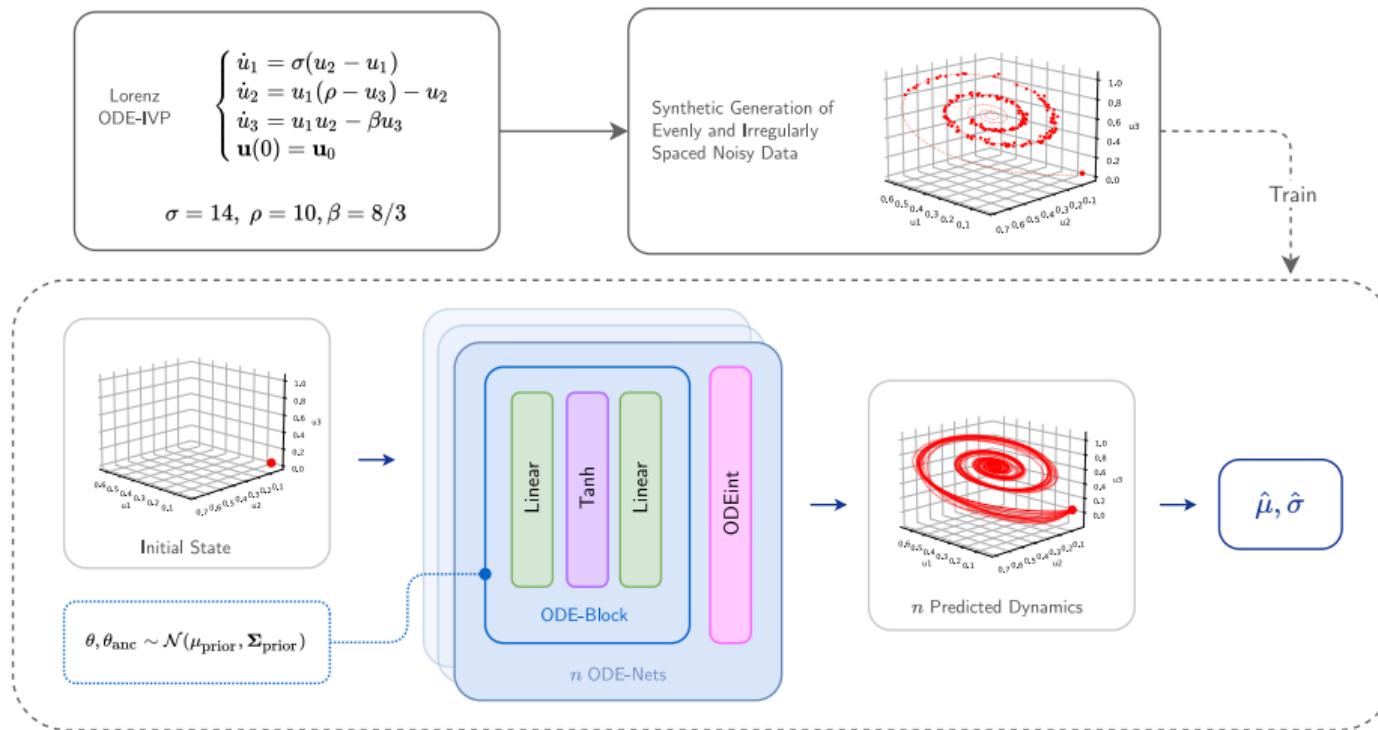
Problem: Regularization reduces diversity between differently initialized models, reducing the ensemble's capabilities to capture uncertainty.

Solution: Introduce an anchoring r.v. $\theta_{\text{anc}} \sim \mathcal{N}(\mu_{\text{prior}}, \Sigma_{\text{prior}})$ to:

- inject noise into the regularization term, ensuring diversity
- anchor the learned distribution to the prior

Anchored Bayesian Ensembling

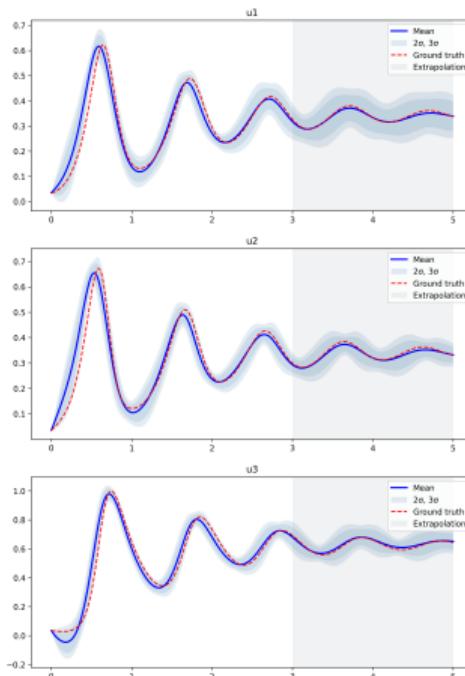
Application II - Framework



Results

Application II

20 ODE-Net Ensemble

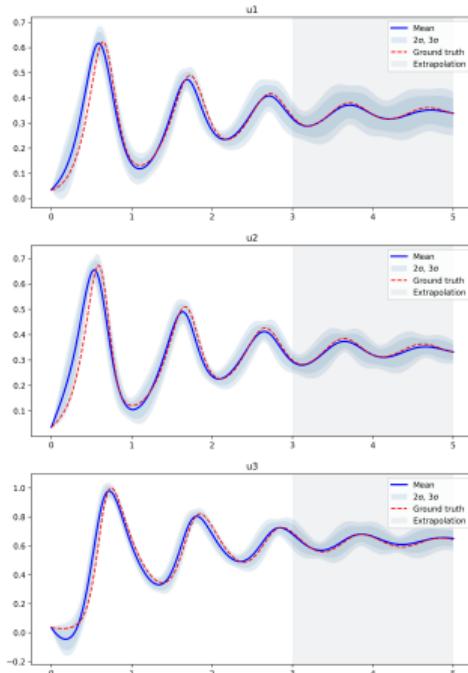


σ_{prior}^2	Ensemble Size	Training Time	Mean Prediction		% within $\pm 2\sigma$		
			Train MSE	Test MSE	u_1	u_2	u_3
1	3	~45 min	8.39e-03	7.33e-04	40.2%	62.2%	23.8%
	5	~1h 15 min	1.06e-02	8.31e-04	39.7%	58.4%	32.0%
	10	~2h 30 min	1.01e-02	8.90e-04	34.5%	51.4%	27.3%
	20	~5h	1.05e-02	8.52e-04	34.2%	52.6%	29.0%
20	3	~45 min	3.17e-03	1.38e-03	80.4%	83.9%	72.7%
	5	~1h 15 min	2.43e-03	1.24e-03	85.6%	81.4%	79.6%
	10	~2h 30 min	2.27e-03	9.02e-05	88.9%	83.0%	78.5%
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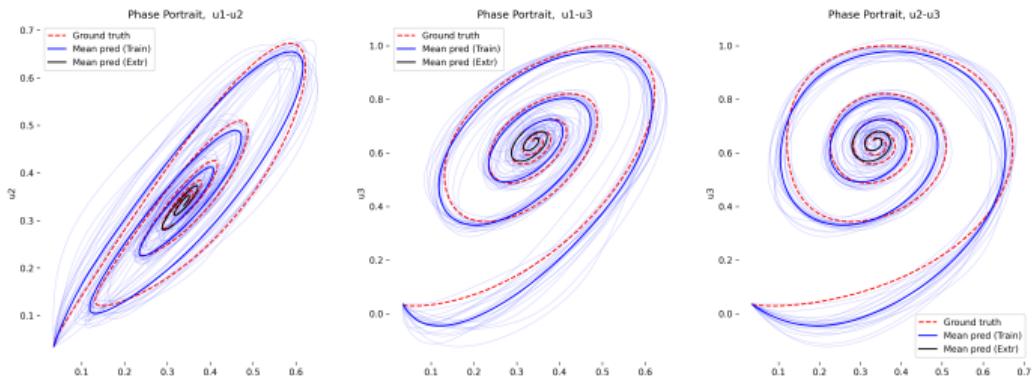
Results

Application II

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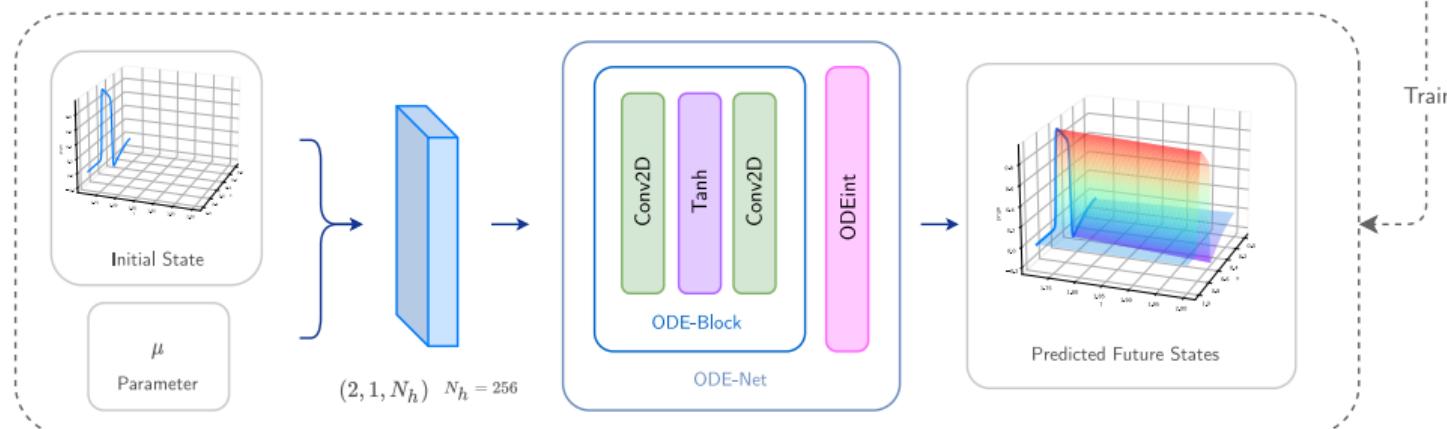
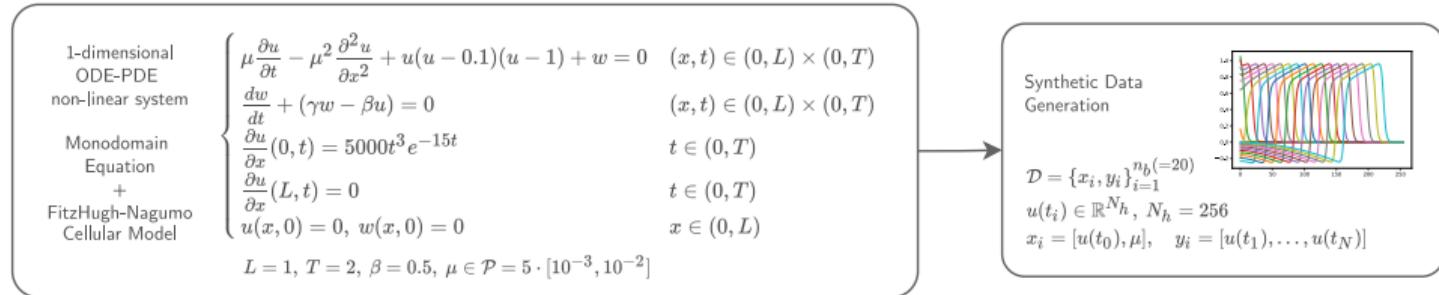


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Parameterized Neural ODE

Application III - Framework

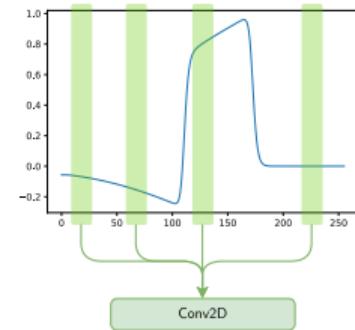


Parameterized ODE-Block Architecture

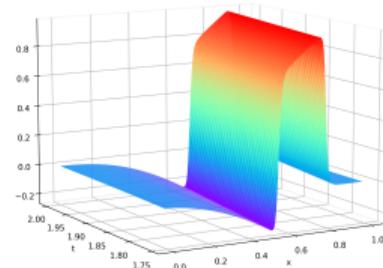
Application III

Layer	Input Shape	Output Shape	Kernel Size	n Filters	Stride	Padding
1	[2,1,256]	[16,1,256]	[1,3]	16	1	Same
Tanh						
2	[16,1,256]	[1,1,256]	[1,3]	1	1	Same

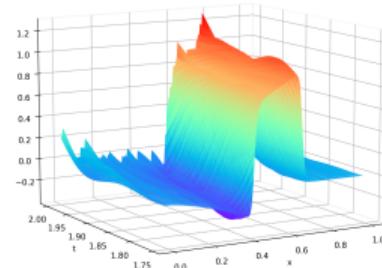
(1500 epochs, training time $\sim 10 \div 15$ min, dopri5)



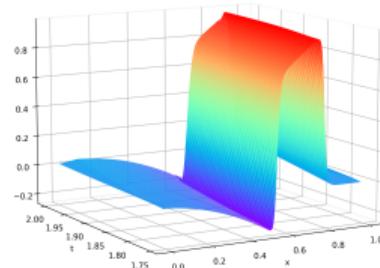
Ground Truth



Predicted (Dense)

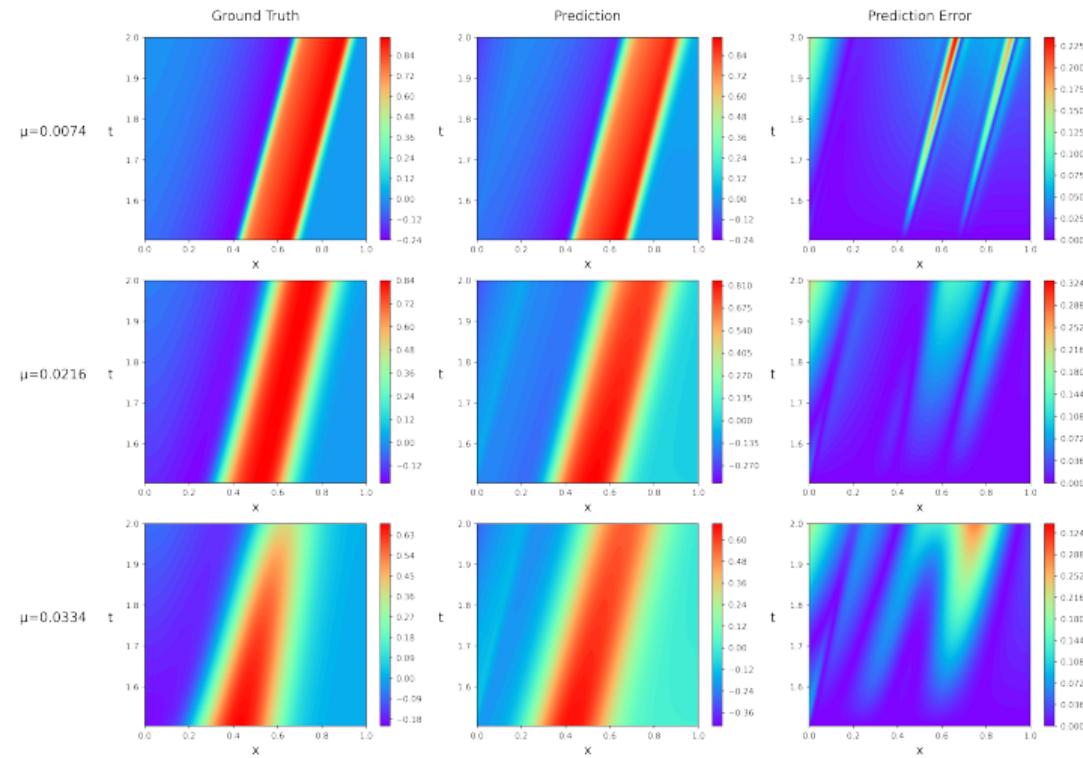


Predicted (Conv)



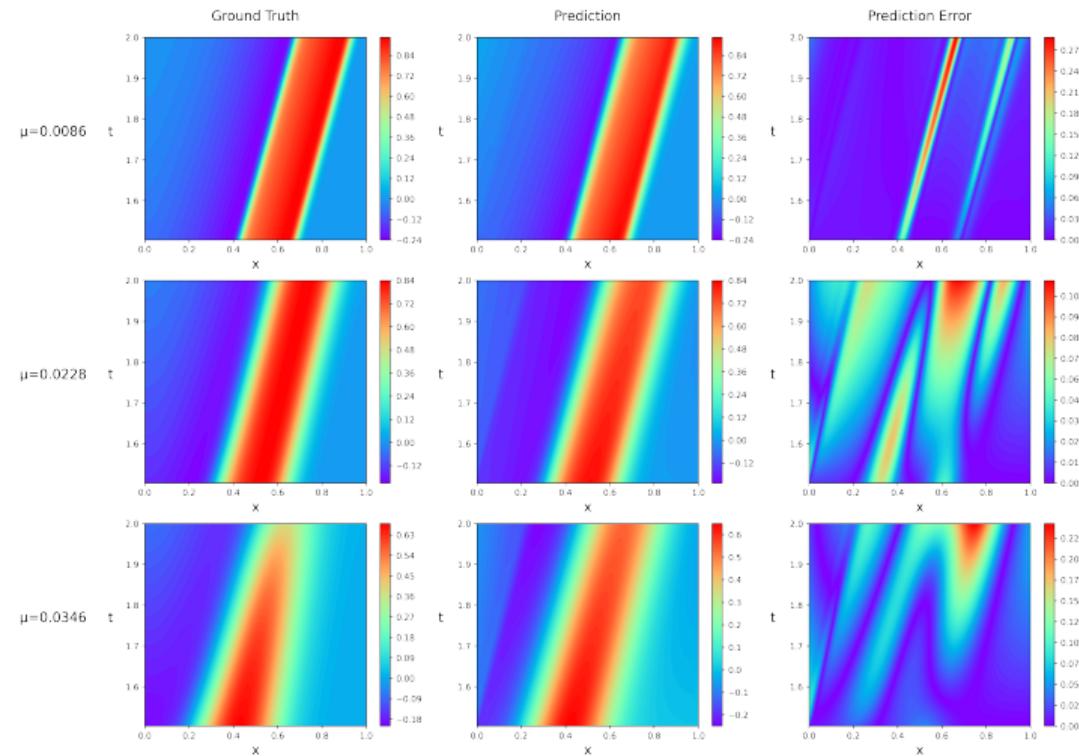
Results - Time Extrapolation

Application III



Results - Out-of- \mathcal{P} Predictions

Application III



Conclusions

- Neural ODEs provide interpretability together with performances comparable to SotA DL approaches.
- *Ensembling*-based techniques (e.g. ABE) allow to both quantify predictions' uncertainty and to achieve better predictive performances.
- Parameterized Neural ODEs represent a promising *data-driven* approach to build surrogate models in the field of model-order reduction.

Thanks!

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