

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

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# Deep Implicit Layers

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# Deep Implicit Layers

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

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

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

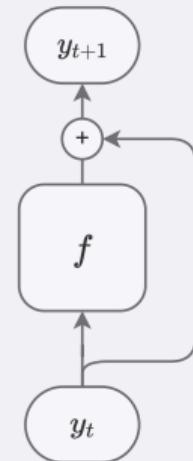
and resembles the Explicit Euler's Method discretization with  $h = 1$

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

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

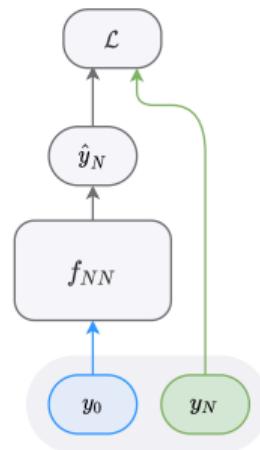
$$y_{t_0}, \dots, y_{t_N} = \text{ODEint}(f, y_0, [t_0, \dots, t_N])$$

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

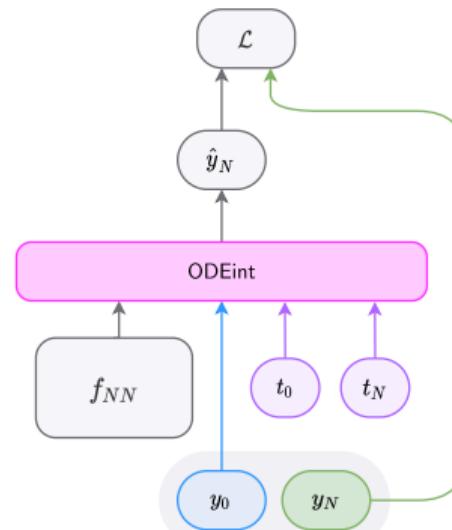
# Architectures differences

## Backpropagation in ODE-Nets

FFNN



ODE-Net

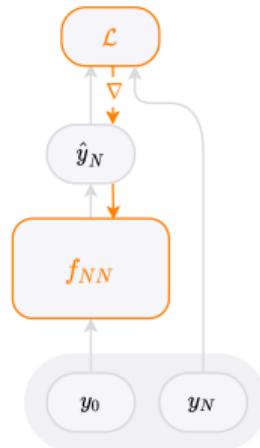


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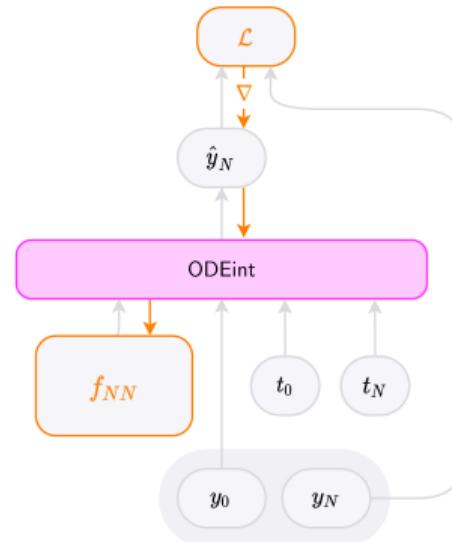
FFNN

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



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  $\theta$ , 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( $[y(t), a(t), \cdot]$ ,  $t, \theta$ ):

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

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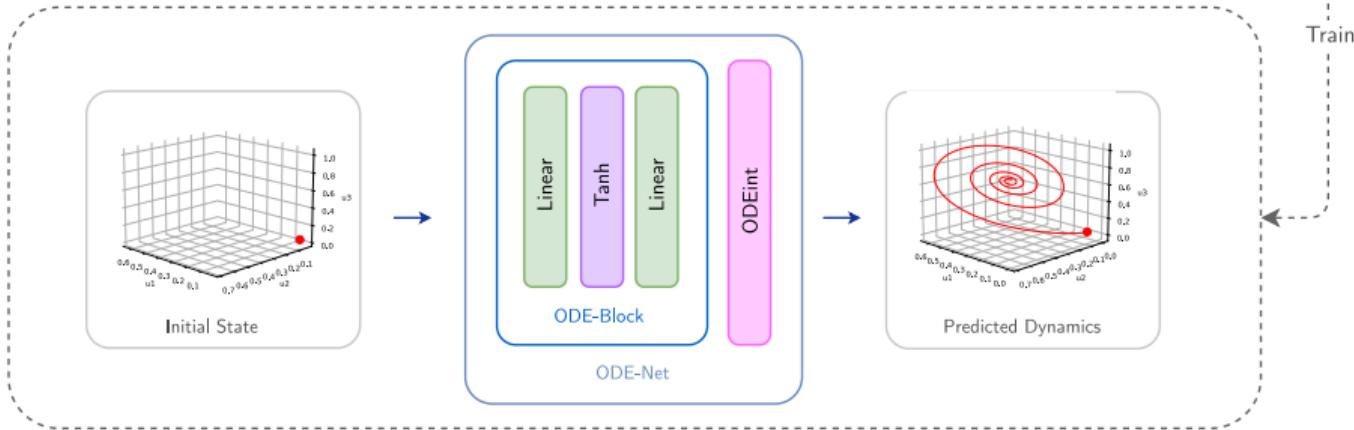
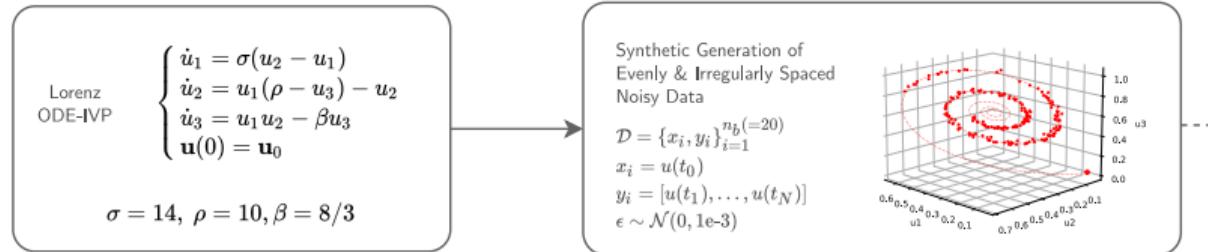
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Observation: the learned function has direct interpretation, we will refer to it as the *learned vector field*.

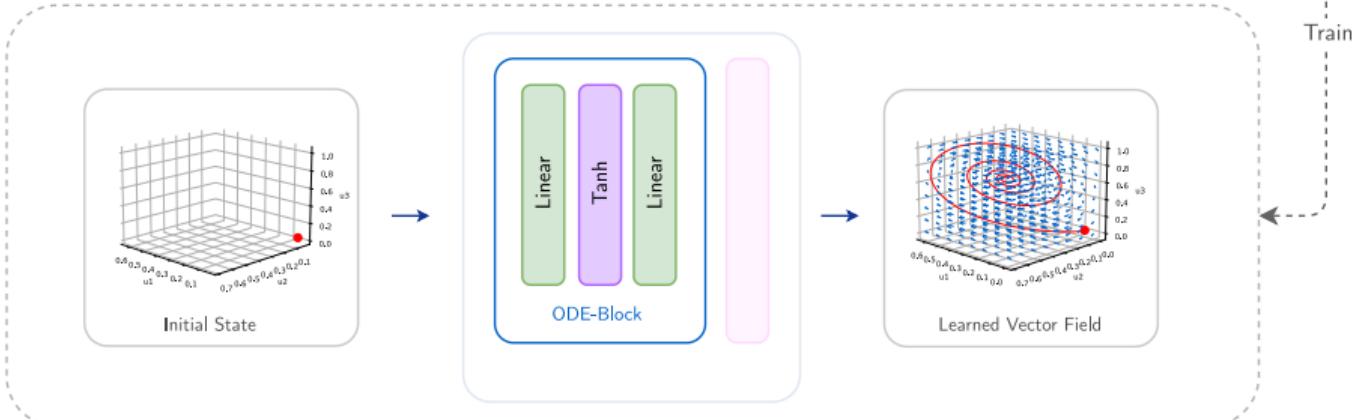
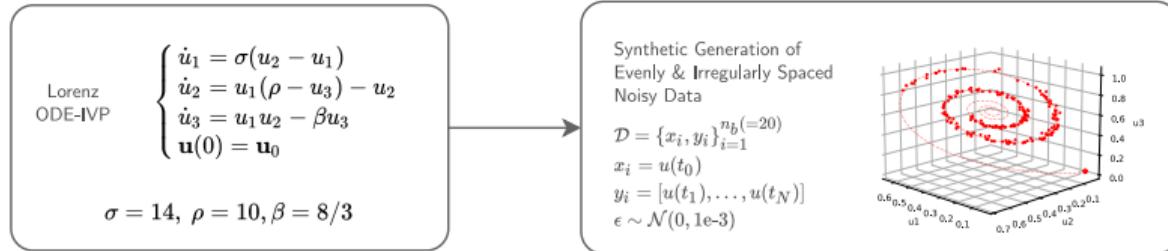
# Spiral ODE

## 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 & degraded 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

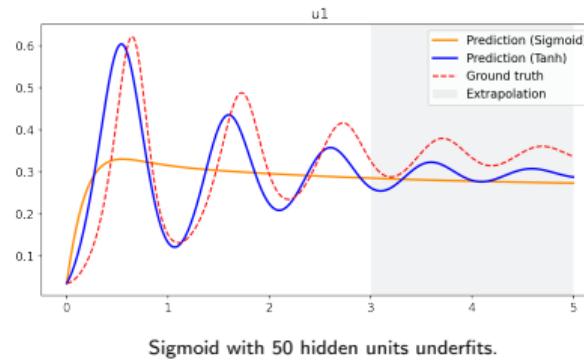
ODE-Block structure:

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

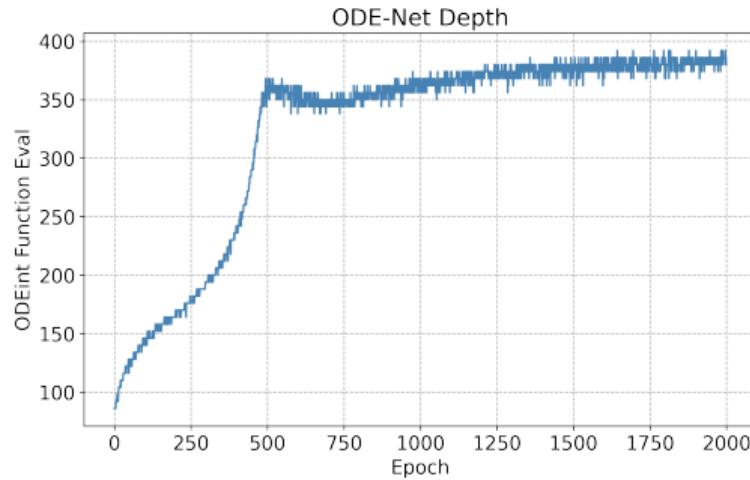


Sigmoid with 50 hidden units underfits.

# What about ODE-Nets' depth?

## Application I

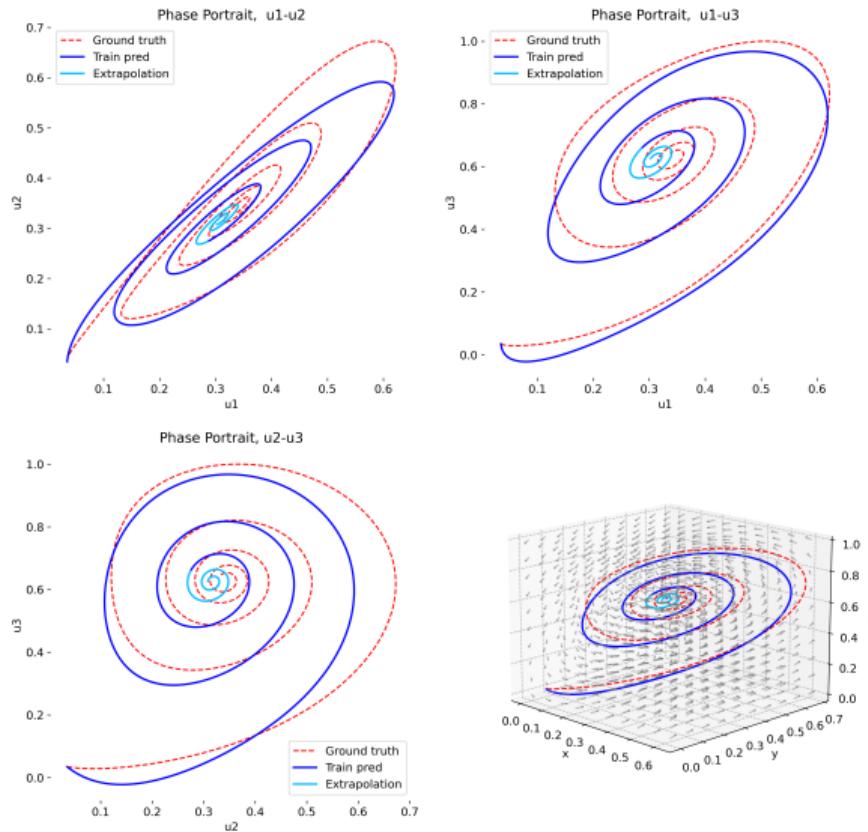
ODE-Nets' depth depends on the number of function evaluations taken by the adaptive-step solver, and it grows as the training proceeds, resulting in 4x deeper networks, wrt classical ResNets.



# 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.

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

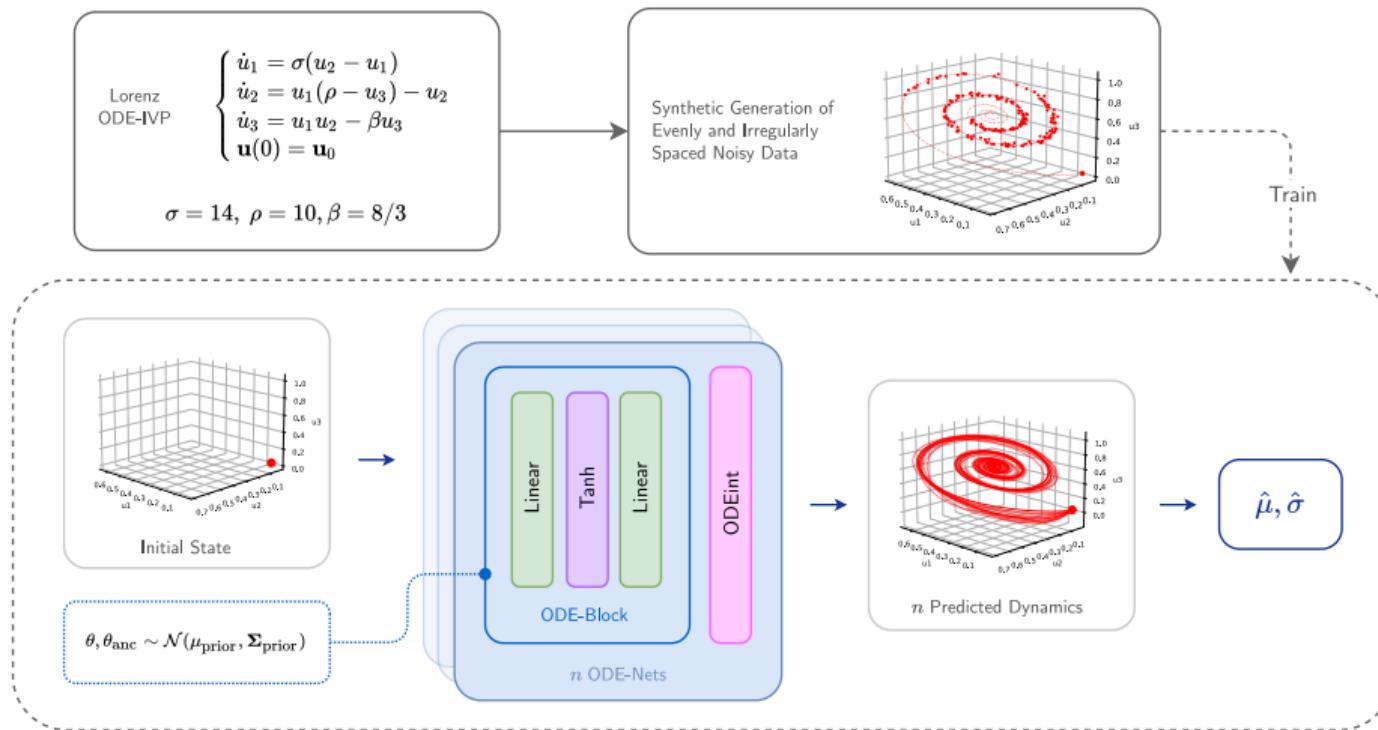
**Problem:** Regularization reduces diversity between differently initialized models, reducing the ensemble's capabilities to capture uncertainty.

**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

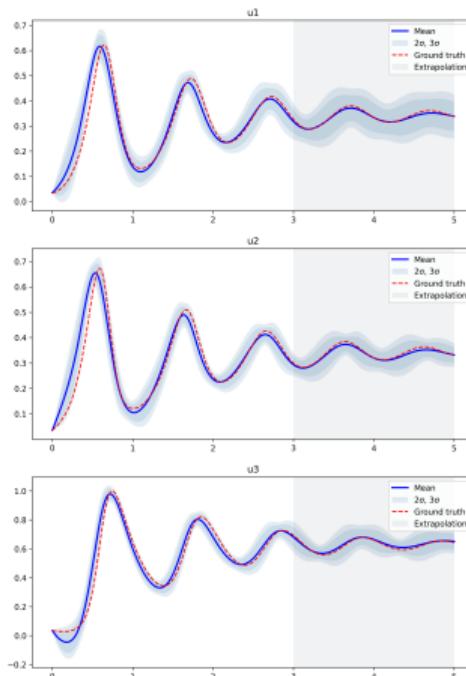
## Application II - Framework



# Results

## Application II

20 ODE-Net Ensemble

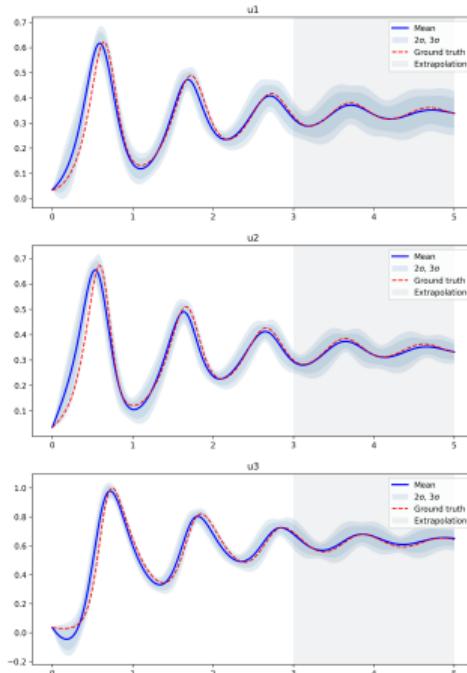


$\sigma_{\text{prior}}^2$	Ensemble Size	Training Time	Mean Prediction		% within $\pm 2\sigma$		
			Train MSE	Test MSE	$u_1$	$u_2$	$u_3$
1	3	~45 min	8.39e-03	7.33e-04	40.2%	62.2%	23.8%
	5	~1h 15 min	1.06e-02	8.31e-04	39.7%	58.4%	32.0%
	10	~2h 30 min	1.01e-02	8.90e-04	34.5%	51.4%	27.3%
	20	~5h	1.05e-02	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%
	20	~5h	2.30e-03	5.36e-05	94.5%	88.3%	87.7%

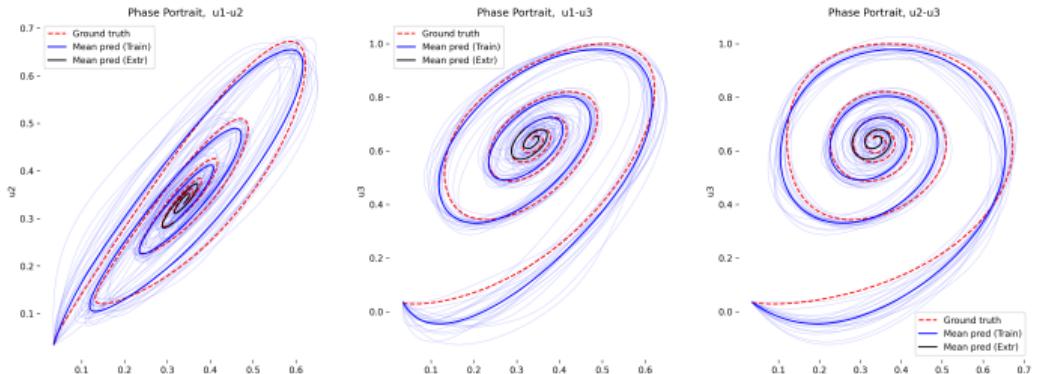
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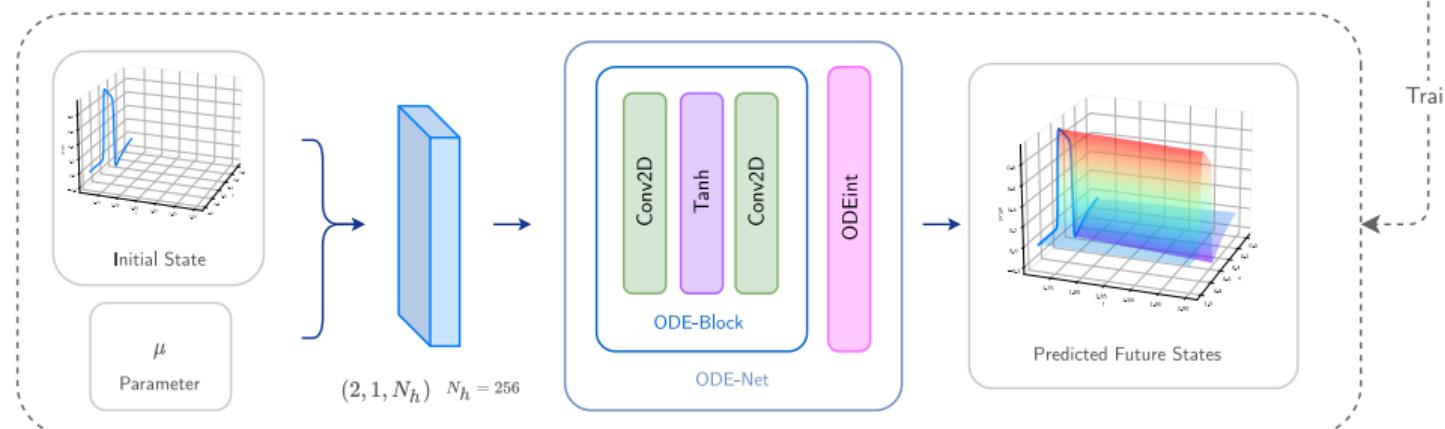
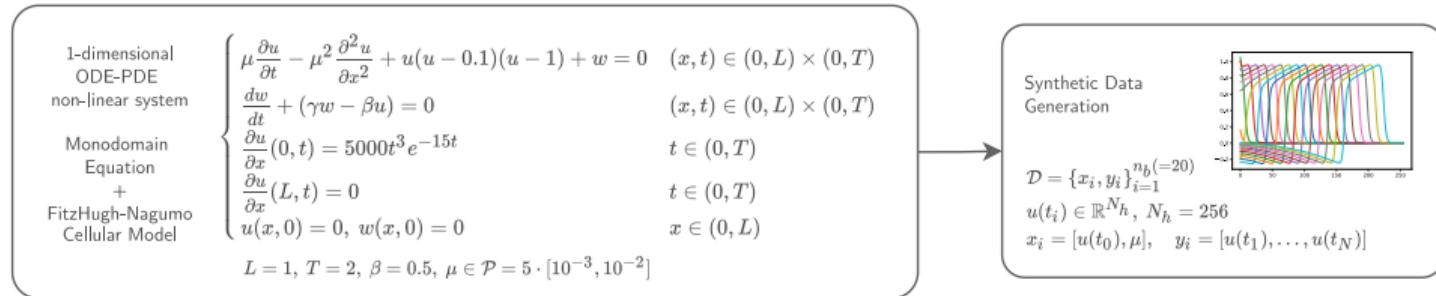


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# Parametrized Neural ODE

## Application III - Framework

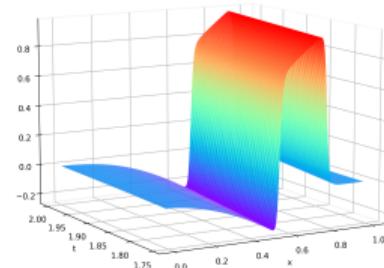


# Parametrized ODE-Block Architecture

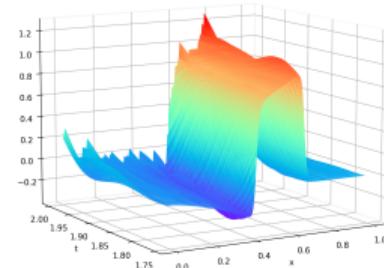
## Application III

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

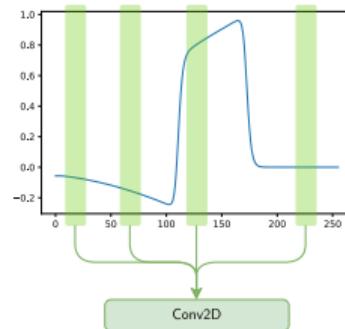
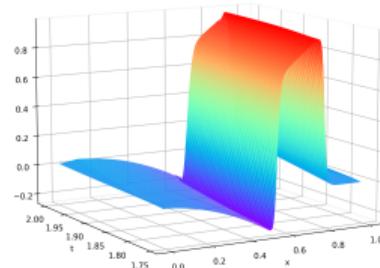
Ground Truth



Predicted (Dense)

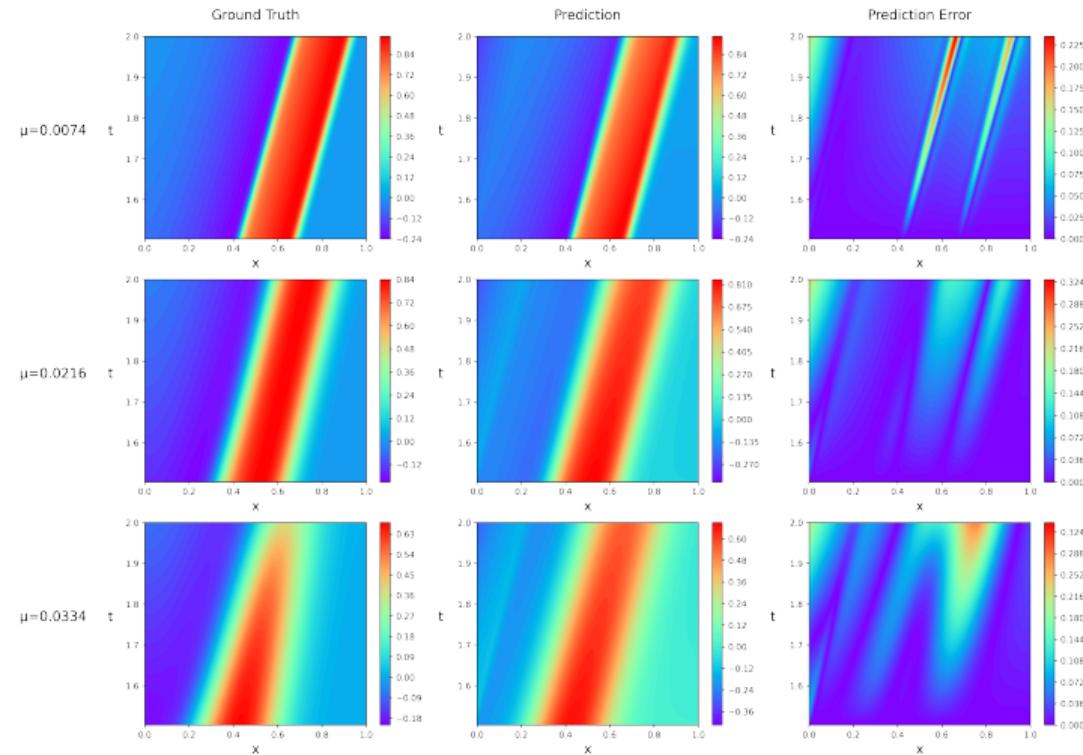


Predicted (Conv)



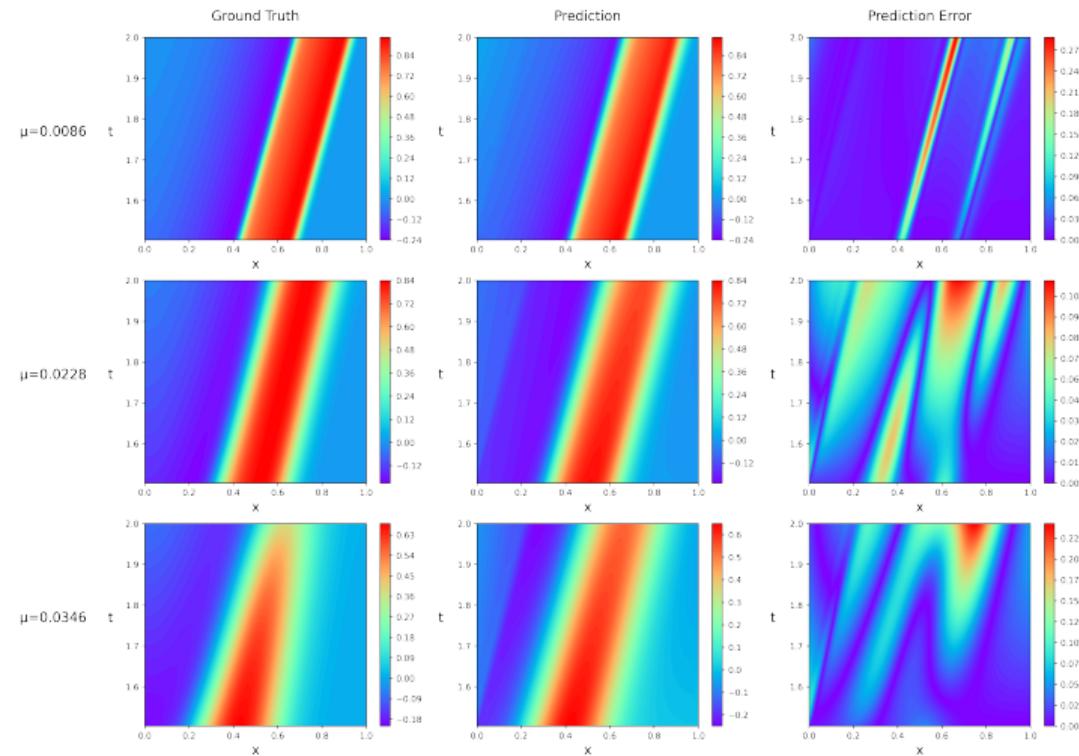
# Results - Time Extrapolation

## 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.
- Parametrized Neural ODEs represent a promising *data-driven* approach to build surrogate models in the field of model-order reduction.

# Thanks!

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