Neural Ordinary Differential Equations With Trainable Solvers

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Outline

- Introduction to Neural ODEs
- Training Neural ODEs, example on learning dynamical systems
- Trainable solvers for (N)ODEs
- Applications
- Conclusion and perspectives

Introduction to Neural ODEs

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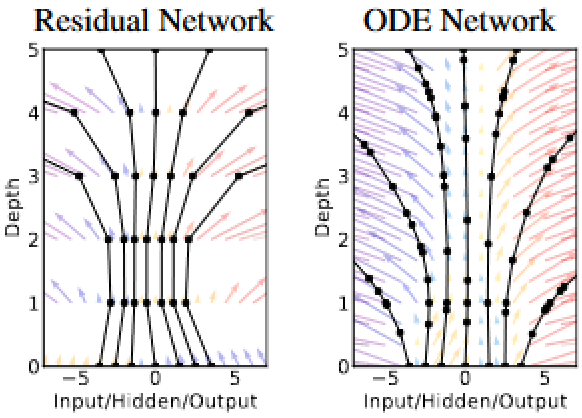

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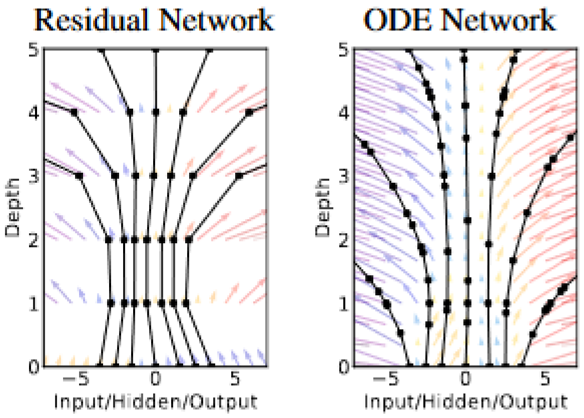

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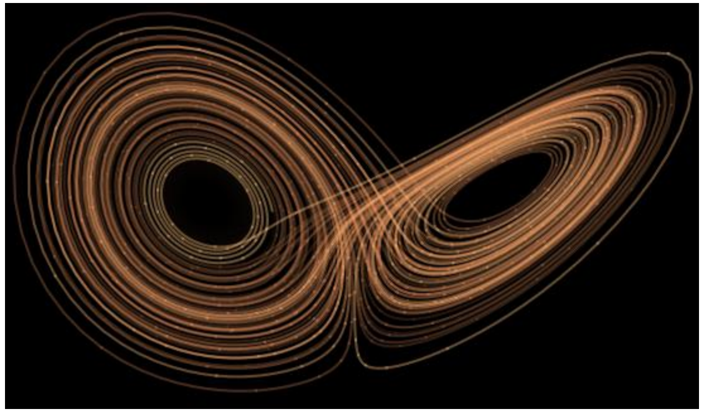

Modeling of time series and dynamical systems

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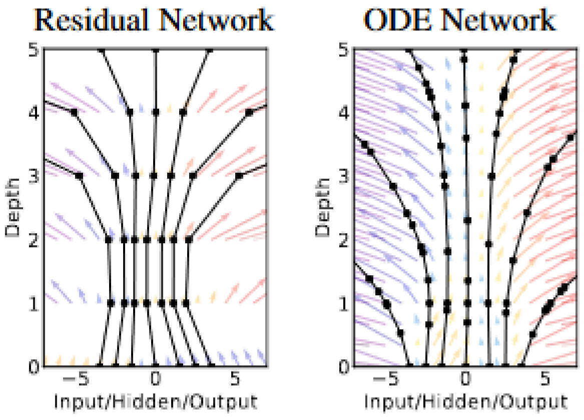

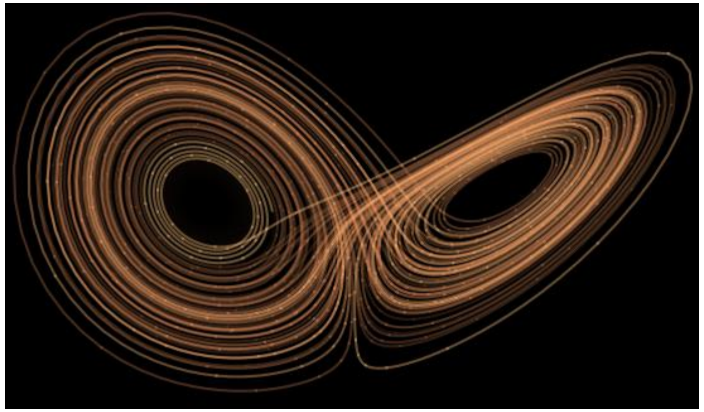

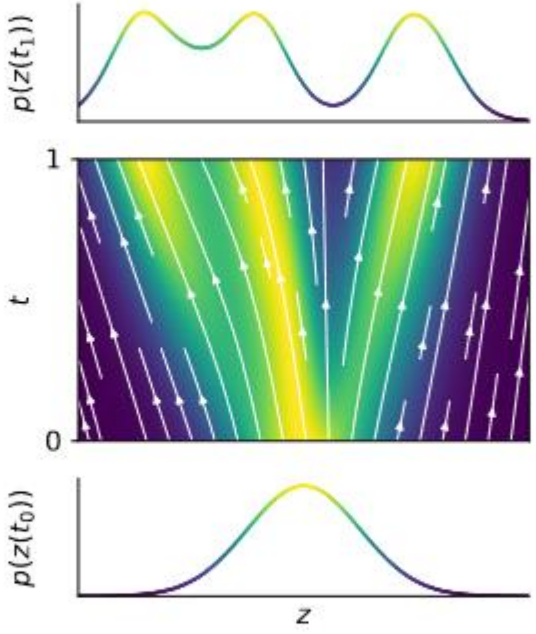

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Density estimation and generative modeling

Training Neural ODEs, example on learning dynamical systems

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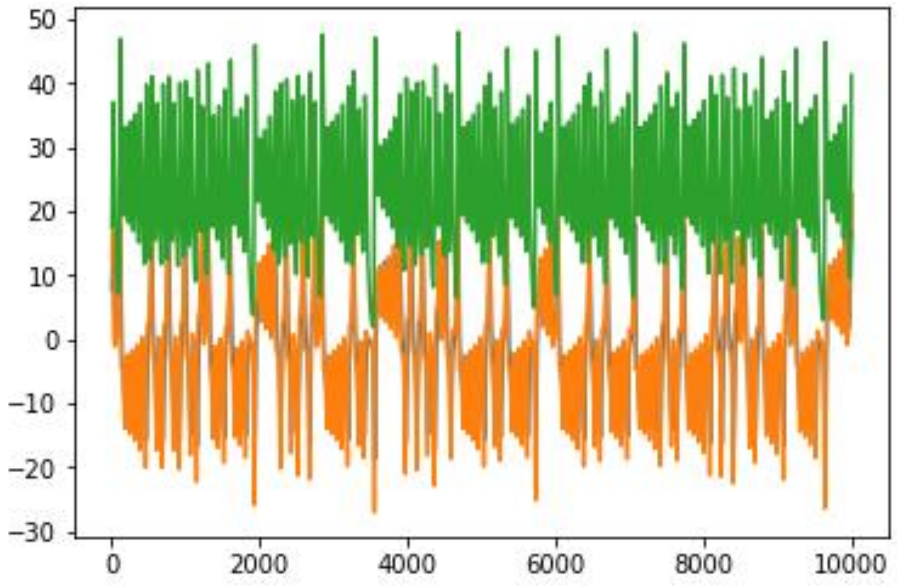

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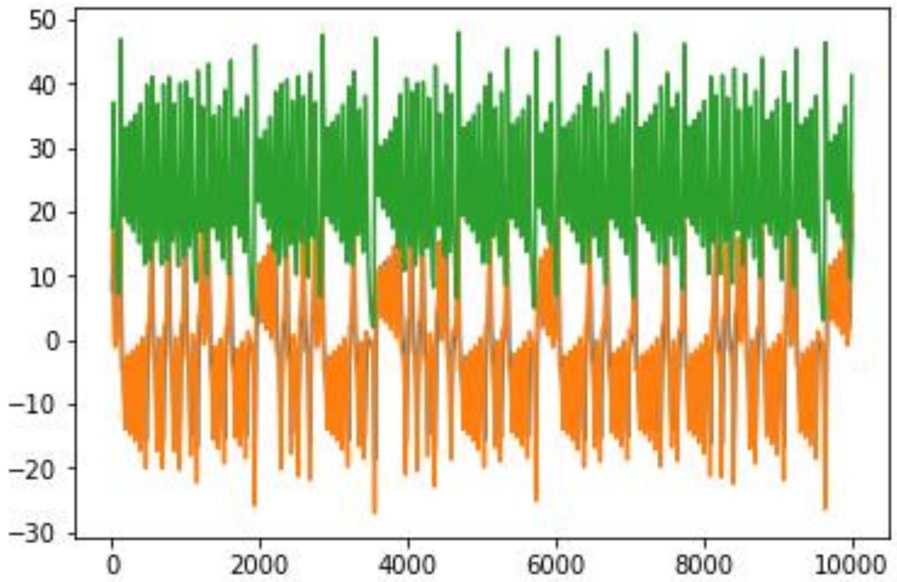

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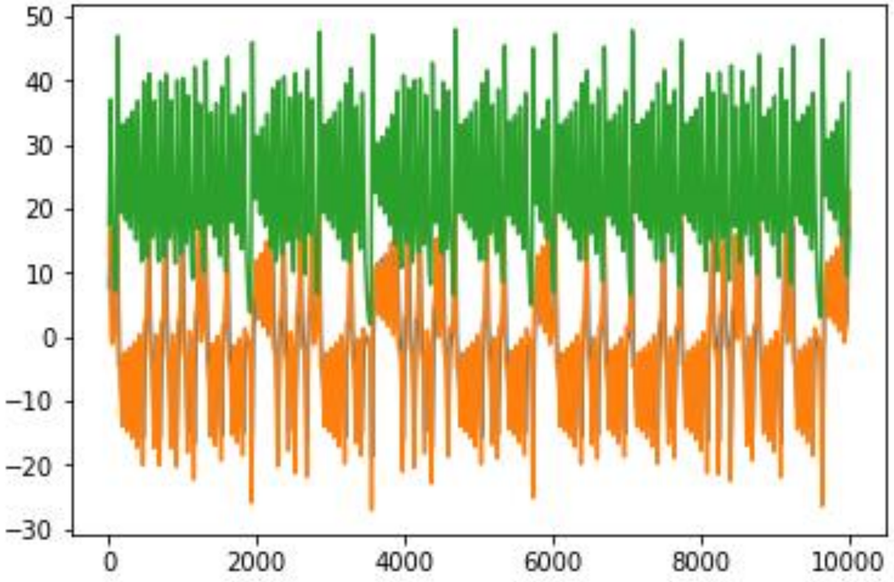

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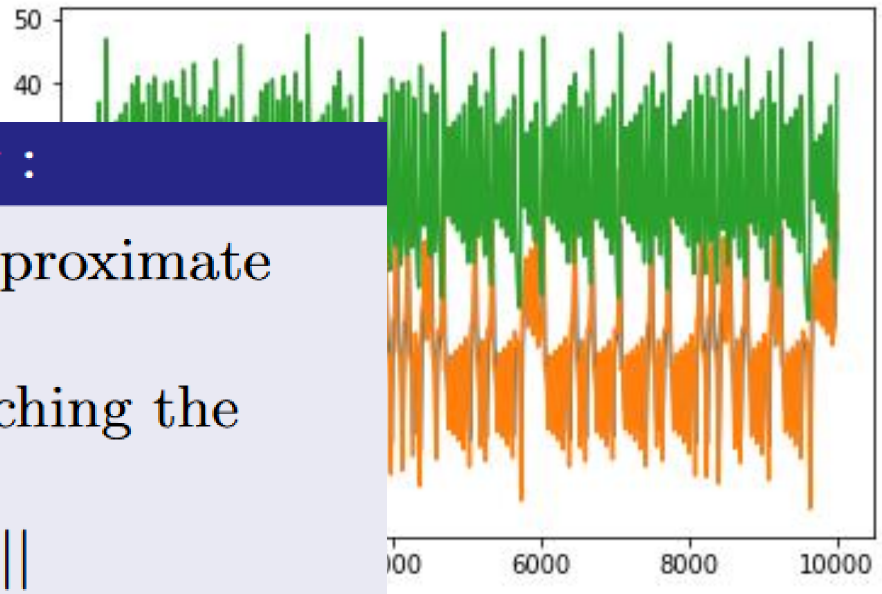

Continuous time setting :

- Direct work on the approximate ODE : $\dot{\mathbf{z}}_t = f_\theta(\mathbf{z}_t)$
- θ is estimated by matching the derivatives *i.e.* $\hat{\theta} = \arg\min_\theta ||f_\theta(\mathbf{z}_t) - \hat{\dot{\mathbf{z}}}_t||$
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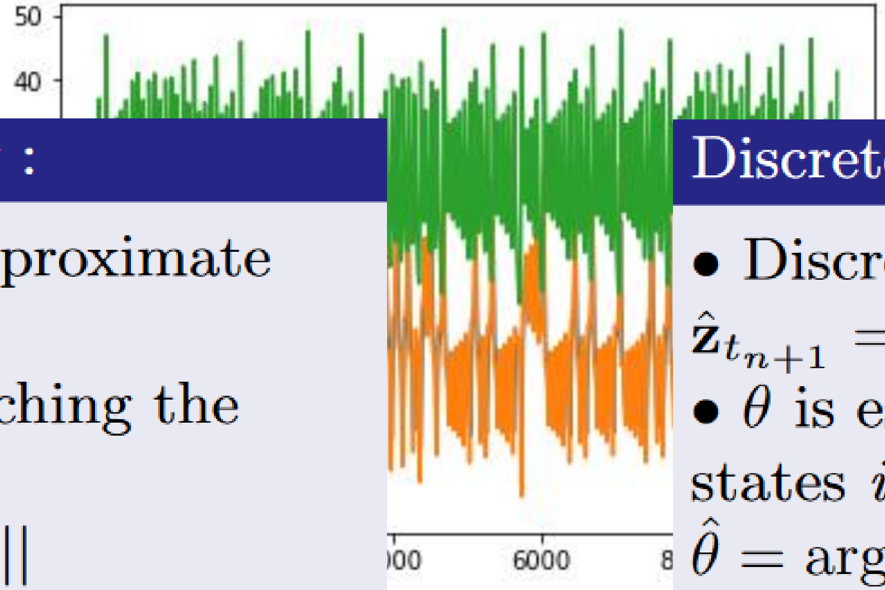

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Discrete time setting :

- Discretized version : $\hat{\mathbf{z}}_{t_{n+1}} = \Phi_{\mathcal{D},t_{n+1}}(\mathbf{z}_{t_n})$
- θ is estimated by matching the states *i.e.* $\hat{\theta} = \arg\min_\theta ||\mathbf{z}_t - \Phi_{\mathcal{D},t_{n+1}}(\mathbf{z}_{t_n})||$
- Issue : which $\Phi_{\mathcal{D},t_{n+1}}$?

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- Need to make sure that the integration is stable with respect to the ODE and the time step.
- Solution : black box adaptive step-size solvers ?
- Adaptive step-size solvers in identification applications (chen et al. 2018) can be subject to memory/instability issues.

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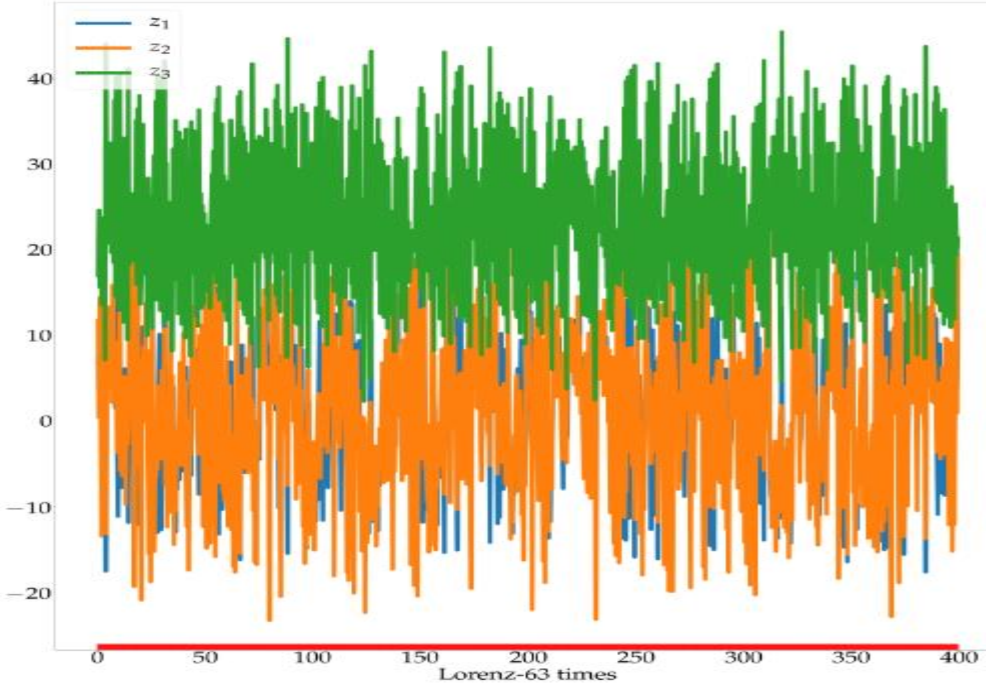

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Adaptive solver

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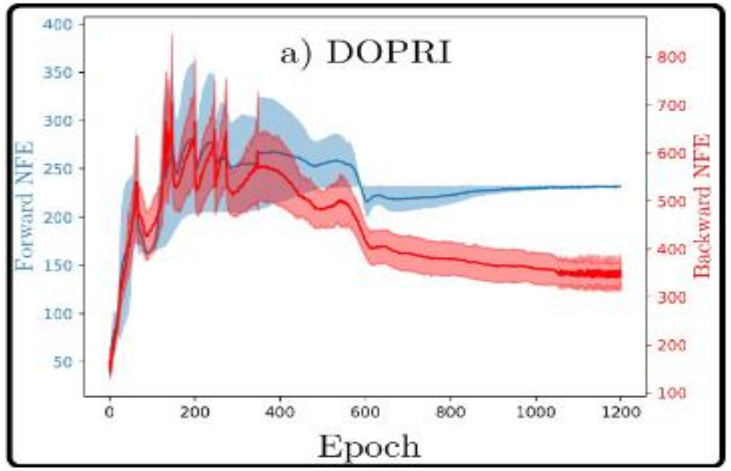

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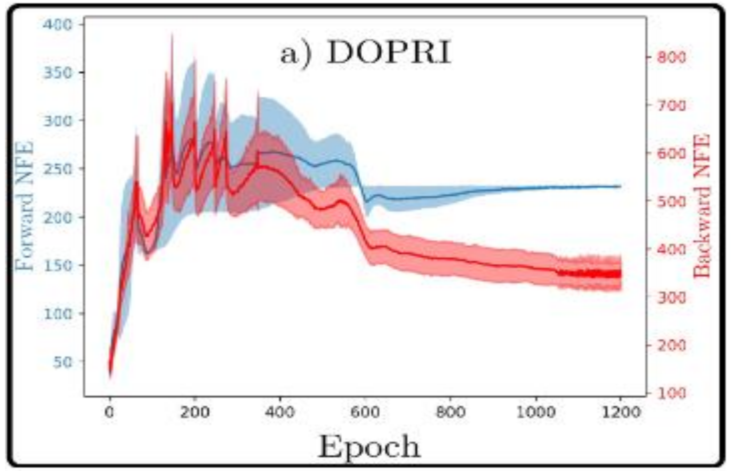

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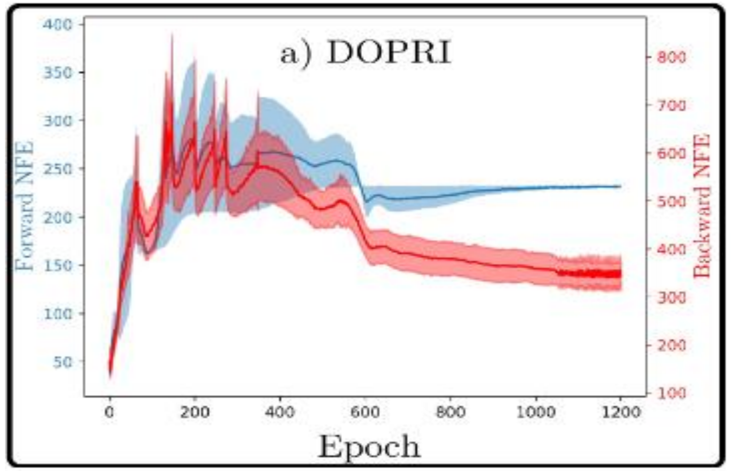
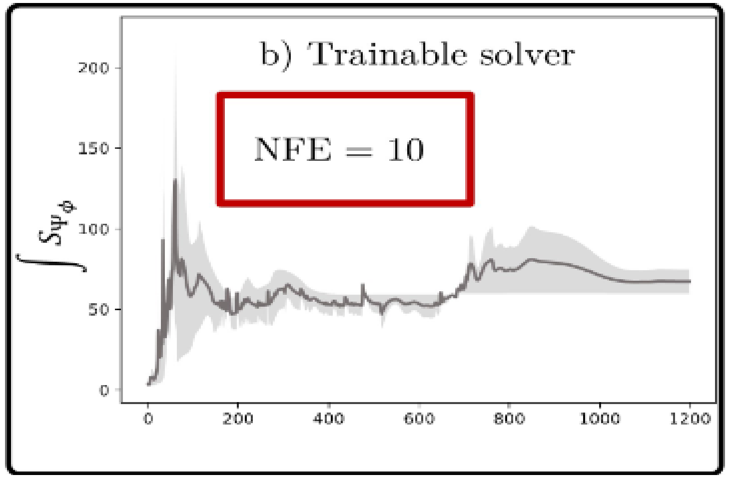


The stability region increases at a fixed NFE!



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- The solution of this equation is computed using a Runge Kutta scheme with q stages

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- where the parameters of the scheme are:

$$\boldsymbol{\phi}_q = \{\mathbf{A} = [a_{i,j}] \in \mathbb{R}^{q\times q}, \mathbf{b} = [b_i] \in \mathbb{R}^q, \mathbf{c} = [c_i] \in \mathbb{R}^q\}$$

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- where $\mathcal{J}$ is a scalar valued loss function that is subject to order/stability constraitns
- The order constraint garentee that the solution of the trainable scheme converges to the analytical solution
- Stability constraints are optional, they can be enforced to garentee the asyptotic stability of the solution

Trainable Solvers for (N)ODEs, order constraints

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- It can be shown assuming mild conditions on the NODE model $\dot{\mathbf{z}}_t = f_\theta(t, \mathbf{z}_t)$ that the order of the Runge-Kutta scheme (in terms of its local truncation error) corresponds to the order of convergence of the Runge-Kutta solution

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- For Runge-Kutta methods, it can be shown that first order constriants (or consistency) can be enforced in terms of the coeficients $\mathbf{b} = [b_i] \in \mathbb{R}^q$ as folows:

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$$\mathcal{C}_{\phi q} : \sum_{i=1}^{q} b_i = 1$$

- This constraint is satisfied exactly in our framework using projected gradient, which makes the trainable schemes at least first order accurate

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- The notion of absolute stability is based on the following linear test equation:

$$\dot{\mathbf{z}}_t = \mathbf{M}\mathbf{z}_t, \qquad \mathbf{z}_{t_0} = \mathbf{z}_0 \quad \text{where} \quad \mathbf{M} \in \mathbb{R}^{s \times s}$$

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- For this equation, the trainable Runge-Kutta scheme can be written as:

$$\begin{cases} \hat{\mathbf{z}}_{t_0} = \mathbf{z}_{t_0} = \mathbf{z}_0 \\ \hat{\mathbf{z}}_{t+h} = \mathcal{R}_{\Psi_\phi}(h\mathbf{M})\hat{\mathbf{z}}_t \end{cases}$$

Matrix polynomial

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- Stability region of a trainable Runge-Kutta scheme can be defined as:

$$S_{\Psi_\phi} = \{x \in \mathbb{C} : \|\mathcal{R}_{\Psi_\phi}(x)\| \leq 1\}$$

Trainable Solvers for (N)ODEs, stability constraints 2

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- Stability constraints of a trainable Runge-Kutta scheme can be defined as:

$$\mathcal{S} : \|\mathcal{R}_{\Psi_\phi}(\lambda h)\| - 1 \leq 0$$

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- Where the matrix polynomial of the Runge-Kutta scheme can be written as a function of the Runge-Kutta parameters as follows:

$$\mathcal{R}_{\Psi_\phi}(\lambda h) = \mathbf{b}^T(\mathbf{I} - (\lambda h)\mathbf{A})^{-1}\mathbf{1}$$

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- Stability constraints are inequality constraints, they can be satisfied efficiently using the penalty method

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- Until which values of λh, a trainable Runge-Kutta scheme is able to integrate a linear test equation $\dot{\mathbf{z}}_t = \lambda \mathbf{z}_t$?

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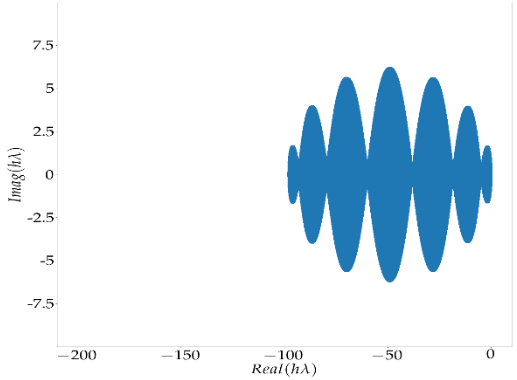
Real λ

\# stages = 7



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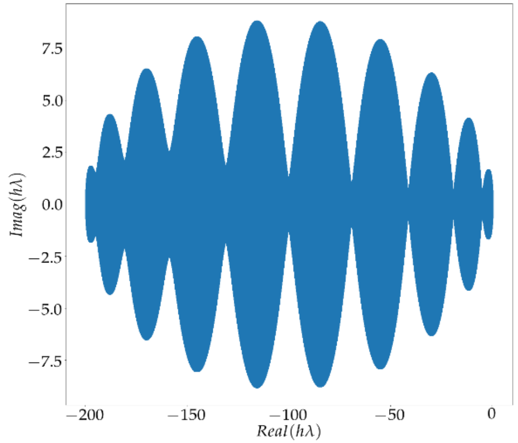

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Real λ

Imaginary λ

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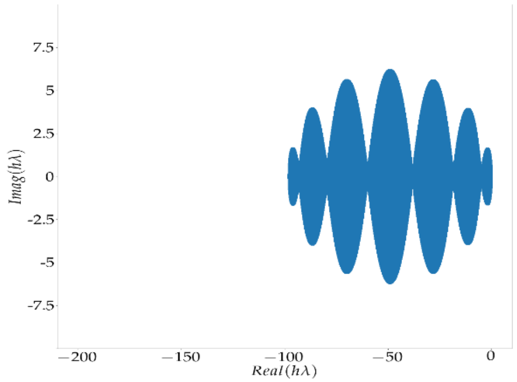

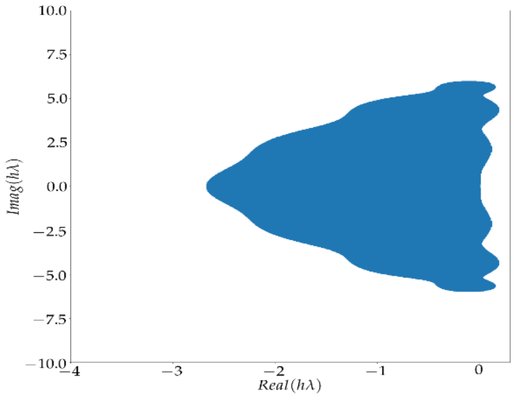

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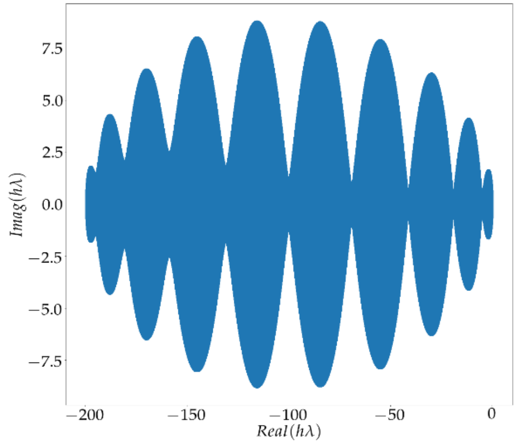

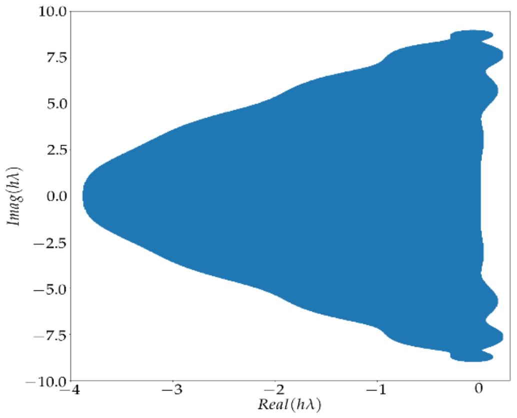

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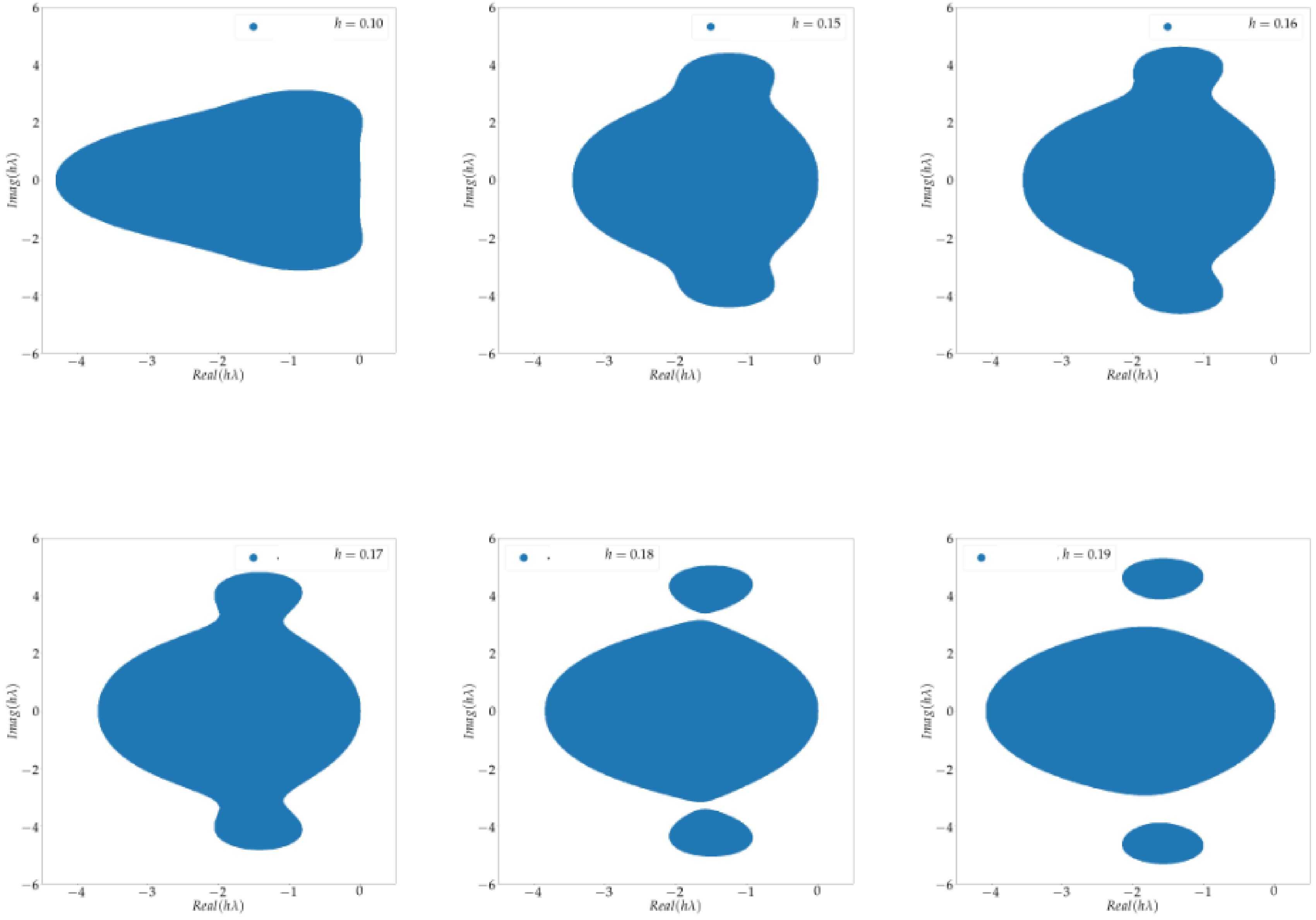
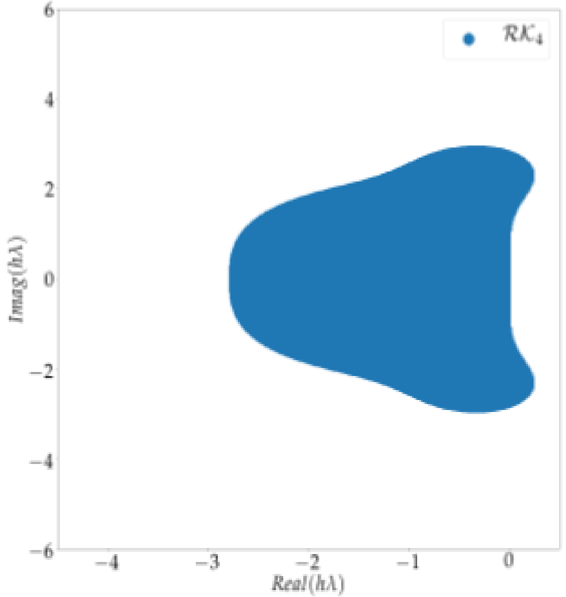
h	0.1	0.15	0.16	0.17	0.18	0.19
TRK4	✓	✓	✓	✓	X	X
RK4	✓	X	X	X	X	X

Integration ability of both the classical RK4 and a trainable Runge Kutta with 4 stages (TRK4) on the Lorenz 63 system with different integration time steps



Stability regions of the TRK4 schemes trained on integration time steps ranging from h = 0.1 to h = 0.19



Stability region of the classical RK4

Numerical experiments, Identification of dynamical systems

Numerical experiments, Identification of dynamical systems

- Can we learn a numerical scheme that adapts to the dynamics of a unknown ODE ?

Numerical experiments, Identification of dynamical systems

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- Learn a numerical scheme that is able to identify the dynamics of the Lorenz 63 model given training data with decreasing sampling rate

$$\left\{\begin{array}{lcl} \frac{dz_{t,1}}{dt} & = & \sigma\left(z_{t,2}-z_{t,2}\right) \\ \frac{dz_{t,2}}{dt} & = & \rho z_{t,1}-z_{t,2}-z_{t,1}z_{t,3} \\ \frac{dz_{t,3}}{dt} & = & z_{t,1}z_{t,2}-\beta z_{t,3} \end{array}\right.$$

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Coarser sampling →

Model		$h_1 = 0.2$	$h_2 = 0.3$	$h_3 = 0.4$
SR	$t_0 + h$	9.06	> 10	9.34
	$t_0 + 4h$	6.02	5.81	6.97
Euler	$t_0 + h$	4.27	2.57	1.99
	$t_0 + 4h$	> 10	> 10	7.89
$\mathcal{RK}_4$	$t_0 + h$	2.05	3.10	2.48
	$t_0 + 4h$	3.82	7.33	> 10
Dopri8	$t_0 + h$	**0.005**	**0.0001**	3.1305
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$\mathcal{TRK}_{10}$	$t_0 + h$	0.017	0.077	**0.189**
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Forecasting performance of data-driven models for Lorenz-63 dynamical model. Mean Root Mean Squared Error (RMSE) for different forecasting time-steps of the tested models.

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Forecasting performance of data-driven models for Lorenz-63 dynamical model. Mean Root Mean Squared Error (RMSE) for different forecasting time-steps of the tested models.

- Continuous time formulation
- Data are sparse, impossible to estimate the derivatives

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Forecasting performance of data-driven models for Lorenz-63 dynamical model. Mean Root Mean Squared Error (RMSE) for different forecasting time-steps of the tested models.

- Fixed step size algorithms fail
- Stability region is too small to integrate the data at the sampling rate of the observations

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Forecasting performance of data-driven models for Lorenz-63 dynamical model. Mean Root Mean Squared Error (RMSE) for different forecasting time-steps of the tested models.

- Adaptive solver and trainable schemes are able to get the most accurate results

Numerical experiments, Identification of dynamical systems

Numerical experiments, Identification of dynamical systems

- Comparing the Number of Function Evaluation (NFE) for both the TRK scheme and the adaptive solver

Numerical experiments, Identification of dynamical systems

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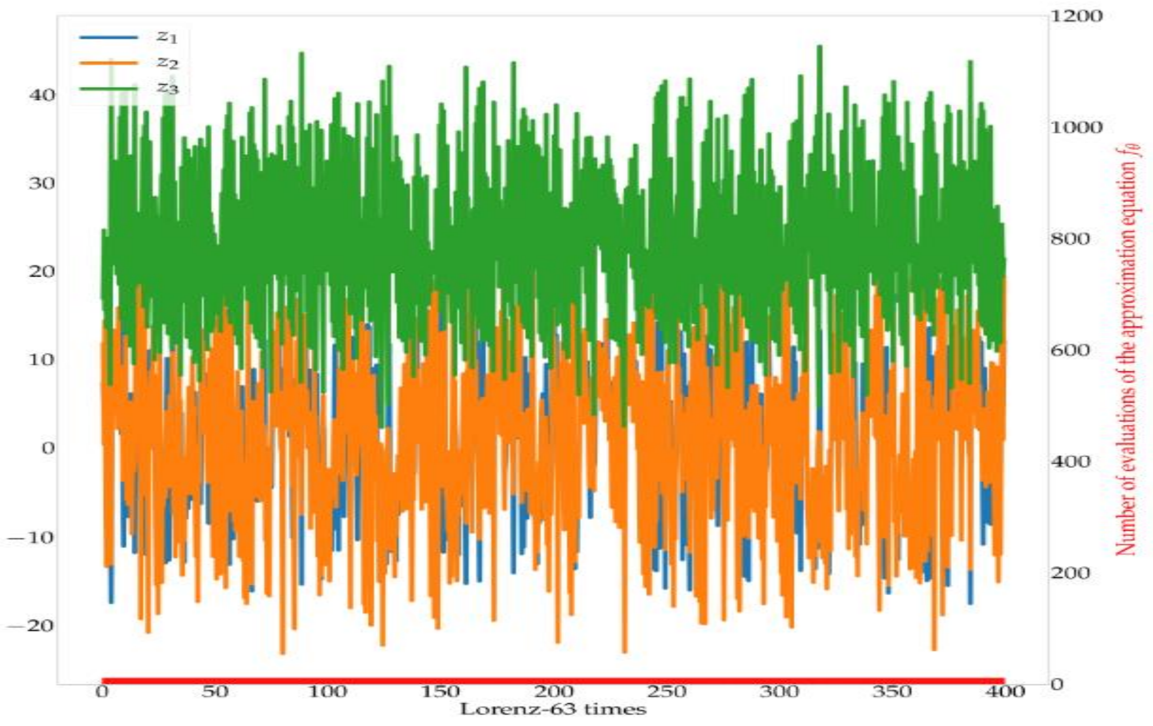

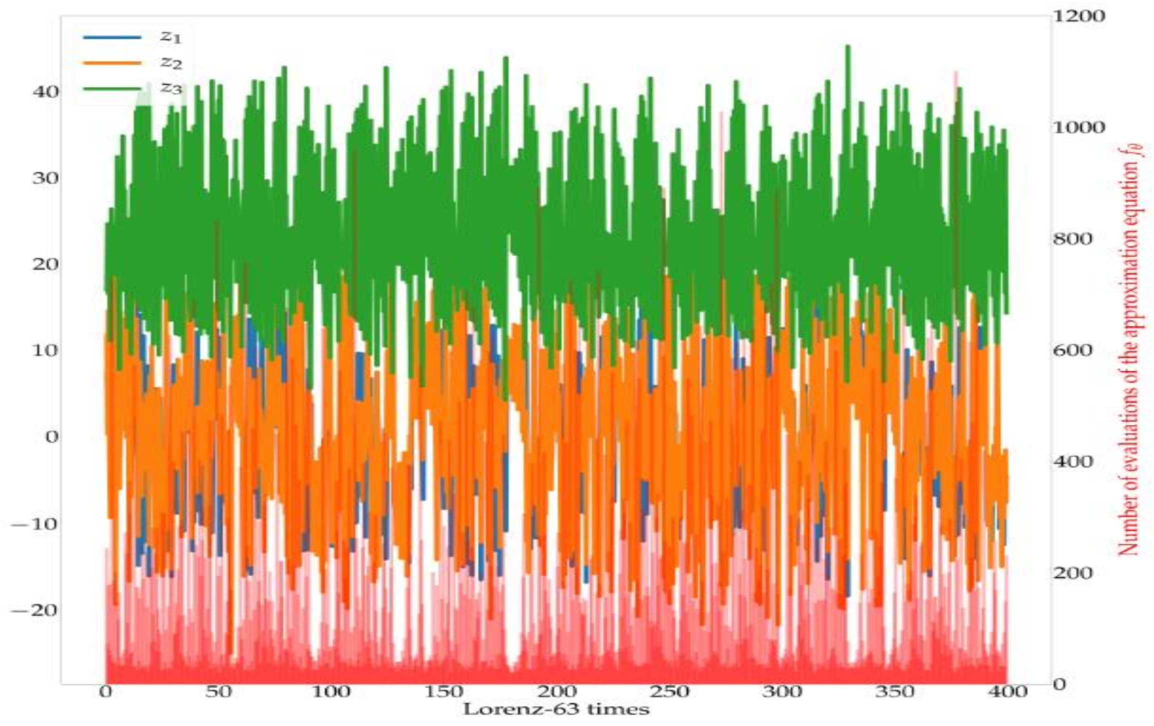

Numerical experiments, Identification of dynamical systems

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- Evaluating the order and stability properties of the trained Runge-Kutta schemes

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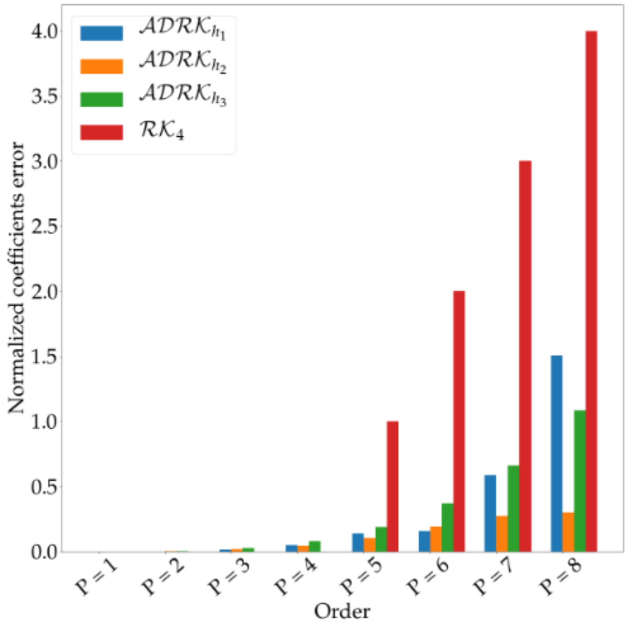
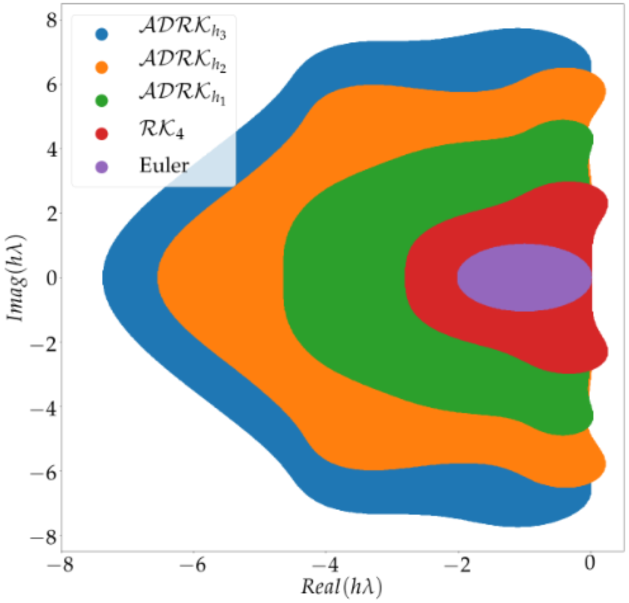


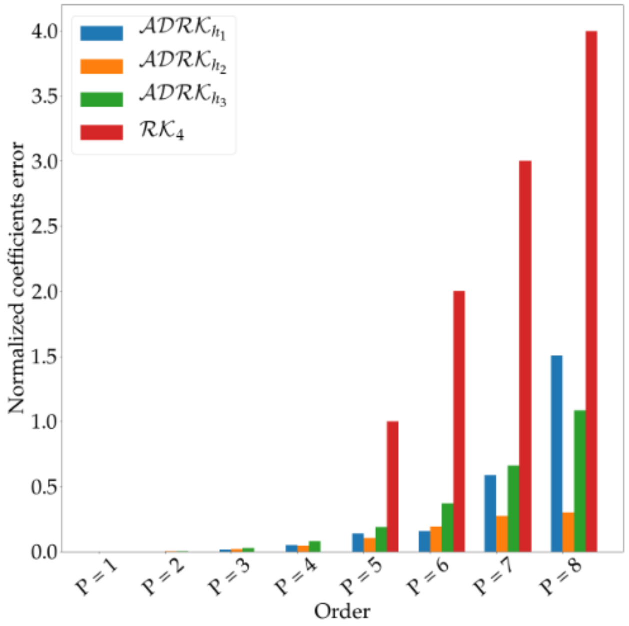
Order coefficients error



Stability region of the learnt schemes

Numerical experiments, Identification of dynamical systems

- Evaluating the order and stability properties of the trained Runge-Kutta schemes



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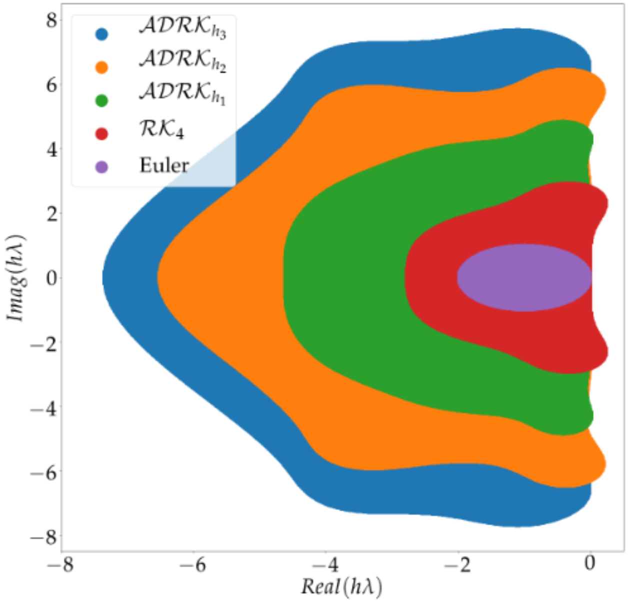

Stability region of the learnt schemes

- The trainable schemes adapt to the dynamics of the learned ODE

Conclusion and perspectives

- Training Numerical schemes jointly with NODE models allows to reduce the computational complexity of NODEs at learning and inference time
- The trained numerical schemes are constrained to guarantee convergence of the solution of the ODE to the analytical one (through the order constraint)
- The order and the stability region of the scheme adapts to the complexity of the ODE, leading to simulations that can operate at a fixed NFE
- Future applications on large scale diffusion models, and high dimensional Partial Differential Equations