The Error Analysis of Numerical Integrators for Deep Neural Network Modeling of Differential Equations

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Summary

Motivation: Modeling unknown dynamics

Target dynamics :

$$\frac{\mathrm{d}x}{\mathrm{d}t} = f(x)$$

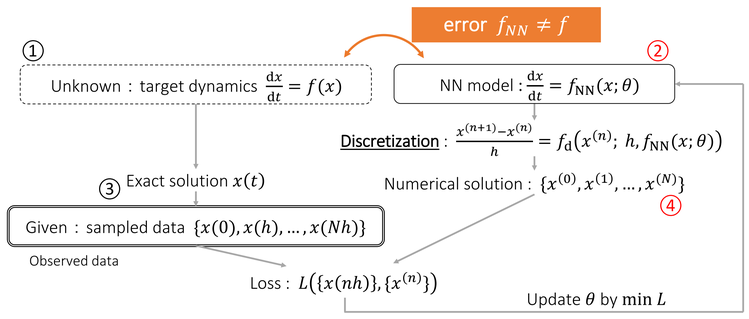
Many systems of physics are written in this form

$\{x(t_1), x(t_2), \dots, x(t_n)\}$: given data
$f(x)$: unknown

Problem :
Construct continuous model $f_{NN}(x;\theta)$ which approximates $f(x)$

Related works: NODE[Tian et al. (2018)], HNN[Greydanus et al. (2019)], etc…

Point :
absence of $\{\dot{x}(t_1), \dot{x}(t_2), \dots, \dot{x}(t_n)\}$
→ need for **discretization** of $f_{NN}(x;\theta)$ in learning process
→ causes **modeling error** $f_{NN} \neq f$



Contribution:

- Defined the modeling error as the “learnability coefficient”
- Formulated the way of learnability analysis
- Proposed the new viewpoint of designing numerical methods other than the consistency, stability, and convergence

How to use the result:

1. Roughly estimate the damping/oscillation behavior of the target dynamics (e.g. by spectrogram)
2. Select a discretization method that has good “learnability” for the behavior
3. Or, design a new method that is good in terms of “learnability”

Learnability analysis enables us to do step 2 and 3

Theory

Setup 1: The model equation

Target dynamics f is too general
-> Introduce the linear “model equation” as a benchmark problem

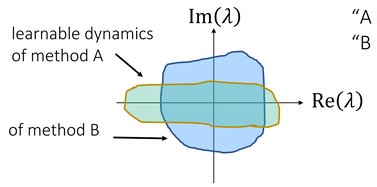
$$\text{model equation*} : \frac{\mathrm{d}x}{\mathrm{d}t} = \lambda x \quad (\lambda \in \mathbb{C})$$

*commonly used in stability analysis of numerical methods

λx represents linearized and diagonalized f
$\mathrm{Re}(\lambda)$: damping, $\mathrm{Im}(\lambda)$: oscillation

The idea of “learnability analysis”

learnable region $\{\lambda$: learnability(λ) < threshold $\}$



“A is better than B for learning damping dynamics”
“B is better than A for learning vibrating dynamics”
↑
to say like these, calc the learnability **for each discretization method** and **for each λ**

what’s “learnability”?

Setup 2: Definition of the learnability coefficient

To know the error that remains even if the learning is successful, suppose that the learned model f_{NN} is linear : $f_{NN}(x) = \alpha x \ \ (\alpha \in \mathbb{C})$

Define the relative error as “learnability coefficient” $\left|\frac{\alpha-\lambda}{\lambda}\right|$

Main result : equation of learned model

Theorem

If we learned the **model eq.** $\frac{\mathrm{d}x}{\mathrm{d}t} = \lambda x$ with the **Runge-Kutta methods**,
There exists a **linear model** $f_{\mathrm{NN}}(x) = \alpha x$ that the numerical solution of f_{NN} **matches the sampled exact solution** $x(nh) = x_0 \mathrm{e}^{n\lambda h}$. The α satisfies :

$$\boldsymbol{b}^{\mathrm{T}}(I - \alpha h A)^{-1}\mathbf{1}\alpha h - \mathrm{e}^{\lambda h} + 1 = 0, \quad ⑤$$

where $\boldsymbol{b}$ and A are constant vector and matrix that specify p-stage Runge-Kutta methods.

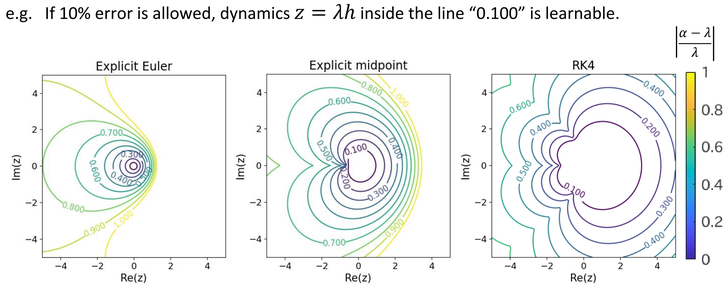
→ α and the learnability can be calculated

Example

Visualization of learnability

Learnability regions for some Runge-Kutta methods

e.g. If 10% error is allowed, dynamics $z = \lambda h$ inside the line “0.100” is learnable.

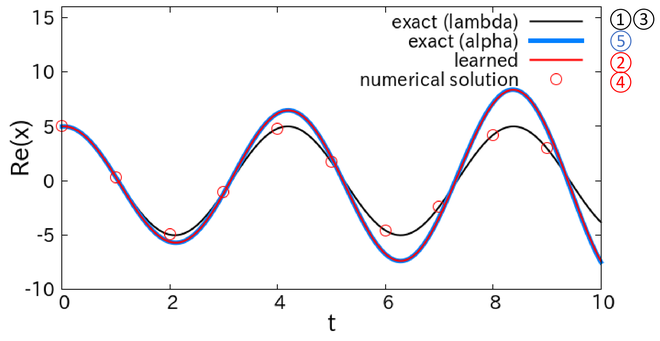


■ $\left|\frac{\alpha-\lambda}{\lambda}\right|$ is a function of $z = \lambda h$
■ h is usually fixed, so the modeling error can be controlled by the choice of discretization method

Experiment

The result of learning $\lambda = 1.5i$
with the classical 4th order Runge-Kutta ($h = 1.0$).

Learned model and prediction for $\lambda = 1.5i$



Learning is successful: ③=④
”∘”, the numerical solution of f_{NN} with the method, is on the exact solution “—”

But the learned dynamics differs from the target: ①≠②
— : the accurately integrated solution of f_{NN}
— : the target dynamics

The difference is predicted: ②=⑤
— : the learned dynamics f_{NN}
— : the theoretical prediction