CONTINUOUS-TIME IDENTIFICATION OF DYNAMIC STATE-SPACE MODELS BY DEEP SUBSPACE ENCODING

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ABSTRACT

Continuous-time (CT) modeling has proven to provide improved sample efficiency and interpretability in learning the dynamical behavior of physical systems compared to discrete-time (DT) models. However, even with numerous recent developments, the CT nonlinear state-space (NL-SS) model identification problem remains to be solved in full, considering common experimental aspects such as the presence of external inputs, measurement noise, latent states, and general robustness. This paper presents a novel estimation method that addresses all these aspects and that can obtain state-of-the-art results on multiple benchmarks with compact fully connected neural networks capturing the CT dynamics. The proposed estimation method called the subspace encoder approach (SUBNET) ascertains these results by efficiently approximating the complete simulation loss by evaluating short simulations on subsections of the data, by using an encoder function to estimate the initial state for each subsection and a novel state-derivative normalization to ensure stability and good numerical conditioning of the training process. We prove that the use of subsections increases cost function smoothness together with the necessary requirements for the existence of the encoder function and we show that the proposed state-derivative normalization is essential for reliable estimation of CT NL-SS models.

1 INTRODUCTION

Dynamical systems described by nonlinear state-space models with a state vector $x(t) \in \mathbb{R}^{n_x}$ are powerful tool of many modern sciences and engineering disciplines to understand potentially complex dynamical systems. One can distinguish between Discrete-Time (DT) $x_{n+1} = f(x_n)$ and Continuous-Time (CT) $\frac{dx(t)}{dt} = f(x(t))$ state-space models. In general, obtaining DT dynamical models from data is easier than CT models since data and computers are inherently discrete. However, the additional implementation complexity and computational costs associated with identifying CT models can be justified in many cases. First and foremost, from the natural sciences, we know that many systems are compactly described by CT dynamics which makes the continuity prior of CT models a well-motivated regularization/prior (De Brouwer et al., 2019). It has been observed that this regularization can be beneficial for sample efficiency (De Brouwer et al., 2019) which is a common observation when "including physics" in learning approaches (Karniadakis et al., 2021). Furthermore, the analysis of ODE equations is a well-regarded field of study with many powerful results and methods which could further improve model interpretability (Fan et al., 2021), such as applied in Bai et al. (2019). Another inherent advantage is that these models can be used with irregular sampled or missing data (Rudy et al., 2019). Lastly, in the control community, CT models are generally regarded desirable for control synthesis tasks as shaping the behavior of controller is much more intuitive in CT (Garcia et al., 1989). Hence, developing robust and general CT models and estimation methods would be greatly beneficial.

In the identification of physical CT systems it is common to encounter aspects with challenges such as: external inputs ($u(t)$), noisy measurements, latent states, unknown measurement function/distribution (e.g. $y(t) = h(x(t))$), the need for accurate long-term predictions and a need for a sufficiently low computational cost. For instance, all these aspects need to be considered for the cascade tank benchmark problem (Schoukens & Noël, 2017). These aspects and the considered CT state-space model is summarized in Figure 1. Many of these aspects have been studied independently, for instance, Brajard et al. (2020); Rudy et al. (2019) explicitly addressed the presence

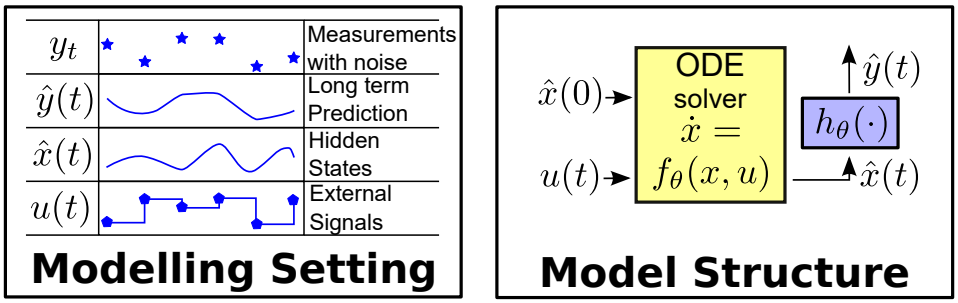

Figure 1: In this work we consider the problem of estimating continuous-time (CT) state-space models from noisy observation (additive noise) with long-term prediction capabilities, hidden states and external signals in a computationally efficient and robust manner.

of noise on the measurement data, Maulik et al. (2020); Chen et al. (2018) provided methods for modeling dynamics with latent states, Zhong et al. (2020) considers the presence of known external inputs, Zhou et al. (2021a) provides a computationally tractable method for accurate long-term sequence modeling. However, formulating models and estimation methods for the combination of multiple or all aspects is in comparison underdeveloped with only a few attempts (Forgione & Piga, 2021).

In contrast to previous work, we present the CT encoder method which is a general, robust and well-performing estimation method for CT state-space model identification. That is, the formulation addresses noise assumptions, external inputs, latent states, an unknown output function, and provides state-of-the-art results on multiple benchmarks of real systems. The presented subspace encoder method is summarized in Figure 2. The proposed method considers a cost function evaluating only short subsections of the available dataset which reduces the computational complexity. Furthermore, we show theoretically that considering subsections enhances cost function smoothness and thus optimization stability. The initial states of these subsections are estimated using the encoder function for which we present necessary requirements for its existence. Lastly, we introduce a normalization of the state and state-derivative and we show that it is required for proper CT estimation. Moreover, we attain additional novelty as these results are obtained without needing to impose a specific structure on the state-space (e.g. Greydanus et al. (2019); Cranmer et al. (2020)) obtaining a widely applicable method.

Our main contributions are the following;

- We formally derive the problem of CT state-space model estimation with latent states, external inputs, and measurement noise.
- We reduce the computational loads by proposing the subspace encoder identification algorithm that employs short subsections, an encoder function that estimates the initial latent states of these subsections, and a state-derivative normalization term for robustness.
- We make multiple theoretical derivations; *(i)* we prove that the use of short subsections increases cost function smoothness by Lipschitz continuity analysis, *(ii)* we derive necessary conditions for the encoder function to exist and *(iii)* we show that a state-derivative normalization term is required for proper CT models estimation.
- We demonstrate that the proposed estimation method obtains state-of-the-art results on multiple benchmarks.

2 Related work

One of the most influential papers in CT model estimation is the neural ODE contribution (Chen et al., 2018) which showed that residual networks can be viewed as an Euler discretization of a continuous in-depth neural network. Moreover, they also show that one can employ numerical integrators to integrate through depth in a computationally efficient manner. This depth can be interpreted as the time direction to be able to model dynamical systems. However, the neural ODE does not

scale well for long sequences, nor does it consider external inputs or noise, and the optimization process is often unstable. The ideas in the neural ODE contribution have been extended to/used in, for instance, normalizing flows to efficiently model arbitrary probability distributions (Papamakarios et al., 2021; Grathwohl et al., 2019), and enhance the understanding and interpretability of neural networks (Fan et al., 2021).

An adjacent research direction is the method/models which consider CT dynamics and directly use the state derivatives and often the noiseless states to formulate structured and interpretable models such as Hamiltonian Neural Networks (HNN) (Greydanus et al., 2019), Lagrangian Neural Networks (LNN) (Cranmer et al., 2020) and Sparse Identification of Nonlinear Dynamics (SINDy) (Brunton et al., 2016). In contrast, the proposed method is formulated for an unstructured state-space and does not require the system state or the state derivatives to be known.

Our method is in part related to (Ayed et al., 2019) which concerns the estimation of CT models with latent variables. They also employ an encoder function to estimate initial states, however it is only dependent on the past outputs, contains a partially known state and do not provide theoretical insight into it. However, they only consider a fixed output function and solve their optimization problem as an optimal control problem whereas our formulation alters the simulation loss function to obtain the computationally desirable form. Furthermore, (Forgione & Piga, 2021), to which we compare in this work, considers a CT model with latent variables, subsections, and an additional loss term for the integration error. However, they include the initial states of these subsections as free optimization parameters. This increases the model complexity with the number of subsections. In contrast, our proposed method uses an encoder to estimate the initial states. This results in fixed model complexity. Furthermore, we only employ a single loss function and a novel state-derivative normalization term.

3 PROBLEM STATEMENT

Consider a system represented by a continuous-time nonlinear state-space (CT NL-SS) description sampled at a fixed interval Δt for simplicity:

$$\begin{aligned} \dot{x}_s(t) &= f(x_s(t), u(t)), \\ y_k &= h(x_{s,k}, u_k) + w_k, \end{aligned} \tag{1}$$

where the subscript notation denotes sampling as $x_{s,k} = x_s(k\Delta t)$, $x_s(t) \in \mathbb{R}^{n_{x_s}}$ is the system state variable, $u(t) \in \mathbb{R}^{n_u}$ the input, $y_k \in \mathbb{R}^{n_y}$ the output, f represents the system dynamics and h the output function and $w_k \in \mathbb{R}^{n_y}$ is a zero-mean white noise with finite variance Σ_w.

For this system, the CT model estimation problem can be expressed for a given dataset of measurements:

$$D_N = \{(u_0, y_0), (u_1, y_1), ..., (u_{N-1}, y_{N-1})\},$$

with unknown w_k, $x_s(t)$, $\dot{x}_s(t)$, $\dot{y}_k$ and initial state $x_s(0)$, as the following optimization problem (a.k.a. simulation loss minimization):

$$\begin{aligned} \min_{\theta, x(0)} \quad & \frac{1}{N} \sum_{k=0}^{N-1} \|y(k\Delta t) - \hat{y}(k\Delta t)\|_2^2, \\ \text{s.t.} \quad & \hat{y}(t) = h_\theta(x(t)), \\ & \dot{x}(t) = f_\theta(x(t), u(t)), \end{aligned} \tag{2}$$

where $x(t) \in \mathbb{R}^{n_x}$ is the model state, h_θ and f_θ are the output and state-derivative functions parameterized by θ and being Lipschitz continuous in their inputs and parameterization.

To obtain the simulation output $\hat{y}(k\Delta t)$ one can integrate $\dot{x}(t) = f_\theta(x(t), u(t))$ starting from the initial state $x(0)$. This integration can be performed with any ODE solver that allows for back-propagation such as Euler ($x(t + \Delta t) = x(t) + \Delta t f_\theta(x(t), u(t))$), RK4, or numerous adaptive step methods (Chen et al., 2018; Ribeiro et al., 2020).[1] To make this a well-posed optimization problem, additional information or an assumption on the inter-sample behavior of $u(t)$ is required, since,

[1] The adjoint methods for gradient computation is not within the scope of this research.

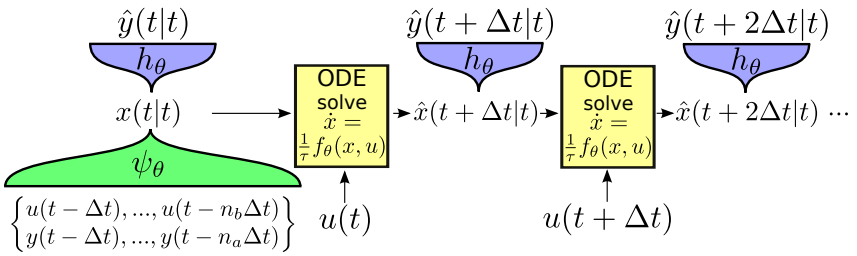

Figure 2: The CT subspace encoder (SUBNET) method applied on a subsection of the data of length $T\Delta t$ starting from time t. The encoder ψ_θ estimates the initial state, h_θ provides the output predictions while $\frac{1}{\tau} f_\theta$ governs the state dynamics. All three functions are parameterized by fully connected neural networks. Lastly, the $\frac{1}{\tau}$ factor is the novel state-derivative normalization factor.

for example, $u(\Delta t/2)$ is not present in D_N. This behavior is often chosen to be Zero-Order Hold (ZOH) (Forgione & Piga, 2021) as seen an example of in Figure 1.

Multiple major issues are encountered when solving the optimization Problem (2) with a gradient-descent-based method. A first issue is that computing the value of the loss function requires a forward pass on the whole length of the dataset (Ayed et al., 2019). Hence, the computational complexity grows linearly with the length of the dataset. Furthermore, a common occurrence is that the values of $x(t)$ or its gradient grows exponentially which results in non-smooth loss functions or gradients. This causes gradient-based optimization algorithms to become unreliable since the optimization process might be unstable or converge to a local minima (Ribeiro et al., 2020). All these issues are addressed in the proposed method.

4 Proposed method

We propose to consider multiple overlapping short subsections of length $T\Delta t$ to form a truncated simulation loss instead of simulating over the entire length of the dataset. We express this in the following optimization problem (note that we express the optimization problem with discrete-time notation ($u_k := u(k\Delta t)$) for brevity):

$$\begin{aligned} \min_{\theta} \quad & \frac{1}{N-T-\max(n_a,n_b)+1} \sum_{n=\max(n_a,n_b)}^{N-T} \frac{1}{T} \sum_{k=0}^{T-1} \|y_{n+k} - \hat{y}_{n+k|n}\|_2^2, \\ \text{s.t.} \quad & \hat{y}_{n+k|n} = h_\theta(x_{n+k|n}), \\ & x_{n+k+1|n} = \text{ODEsolve}[\frac{1}{\tau} f_\theta, x_{n+k|n}, u_{n+k}, \Delta t], \\ & x_{n|n} = \psi_\theta(u_{n-1}, ..., u_{n-n_b}, y_{n-1}, ..., y_{n-n_a}). \end{aligned} \tag{3}$$

Here, the pipe (|) notation indicates the current index and the starting index as (current index | start index) to differentiate between different subsections. Furthermore, ODEsolve indicates a numerical scheme which integrates $1/\tau\ f_\theta(x, u)$ from the initial state $x_{n+k|n}$ for a length of Δt given the input u_{n+k}. Lastly, we introduced an encoder function ψ_θ with encoder lengths n_a and n_b, for the past output and input samples respectively, which estimates the initial states of the considered subsection. A graphical summary of the proposed method called the CT subspace encoder (abbreviated as SUBNET) can be viewed in Figure 2.

The first observation is that optimization Problem (3) is a generalisation of (2) since if $T = N$ and $n_a = n_b = 0$, the original optimization Problem (2) is recovered. However, as one might observe, this optimization problem is less computationally challenging to solve if $T < N$ since the first sum can be computed in parallel. Moreover, the smoothness of the encoder cost function is also enhanced since the associated Lipschitz constant $L_{V^{(\text{enc})}}$ can scale exponentially with the subsection length ($T\Delta t$) as shown in Theorem 1. The enhanced smoothness is reflected in the ease of optimization (Ribeiro et al., 2020).

Theorem 1. *The Lipschitz constant $L_{V^{(enc)}}$ of the cost function* (3)

$$\|V^{(enc)}(\theta_1) - V^{(enc)}(\theta_2)\|_2 \leq L_{V^{(enc)}}\|\theta_1 - \theta_2\|_2 \tag{4}$$

scales as

$$L_{V^{(enc)}} = \mathcal{O}(\exp(2T\Delta t L_f/\tau)) \tag{5}$$

where L_f is the Lipschitz constant of f_θ.

Proof. See Appendix 8.1 □

An error in the initial state of $x_{n|n}$ can significantly bias the estimate due to the short nature of the subsections. To counter this, we formulated an encoder function ψ_θ which estimates the initial state of each subsection. We do not add any additional loss term since an improved initial state error estimate also minimizes the transient error (Forgione & Piga, 2021) which is present in the encoder loss.

A natural question to ask is under which conditions there exists an encoder function that can map from the past inputs and outputs to this initial state. In Appendix 8.2, we formally derive necessary conditions for the existence. These necessary conditions are that, state derivative f_θ requires to be Lipschitz continuous in x, and if the number of considered past outputs n_a and inputs n_b are equal then $n_a \geq n_x/n_y$ needs to be satisfied, among other conditions.

It is widely known that input and output normalization is essential for obtaining competitive models throughout deep learning. Input and output normalization is insufficient when considering CT state-space model due to the presents of the hidden state $x(t)$ and the state-derivative $f(x, u)$. However, as shown in Theorem 2, any CT system can be transformed to become normalized by the introduction of a state transform and a positive $1/\tau$ normalization factor.

Theorem 2. *For any system of the form $\dot{x}(t) = f(x(t), u(t))$ with finite $x(t)$ and $\dot{x}(t)$ there exists a τ and a state transformation $\gamma\tilde{x}(t) = x(t)$ such that both the state $\tilde{x}$ and state-derivative $\tilde{f}$ of the transformed system $\dot{\tilde{x}} = \frac{1}{\tau}\tilde{f}(\tilde{x}(t), u(t))$ are normalized as in*

$$\textit{RMS}(\tilde{x}) = \sqrt{\frac{1}{L}\int_0^L \frac{1}{n_x}\|\tilde{x}(t)\|_2^2 dt} = 1 \qquad \& \qquad \textit{RMS}(\tilde{f}) = 1. \tag{6}$$

Proof. With

$$\gamma = \text{RMS}(x) \qquad \& \qquad \frac{1}{\tau} = \frac{\text{RMS}(\dot{x})}{\text{RMS}(x)} \tag{7}$$

the normalization conditions are satisfied, as shown below

$$\text{RMS}(\tilde{x}) = \text{RMS}(x)/\gamma = 1 \tag{8a}$$

$$\text{RMS}(\tilde{f}) = \tau\text{RMS}(\dot{\tilde{x}}) = \tau\text{RMS}(\dot{x})/\gamma = \tau\text{RMS}(\dot{x})/\text{RMS}(x) = 1 \tag{8b}$$

□

Hence, considering only state normalization $\tau = 1$, one cannot obtain models where both the state-derivative $\tilde{f}$ function and state $\tilde{x}$ are normalized for most systems. Thus, including state-derivative normalization is essential for proper normalization in CT model estimation. Furthermore, this proof also guides the choice of τ since the amplitude of $\text{RMS}(x)/\text{RMS}(\dot{x})$ might be known from physical insight or by an approximate model.

5 Experiments

5.1 Benchmark descriptions

The **Cascade Tank with overflow (CCT)** benchmark (Schoukens & Noël, 2017; Schoukens et al., 2017) consists of measurements taken from a two-tank fluid system with a pump. The input signal controls a water pump that delivers water from the reservoir to the upper tank. Through a small

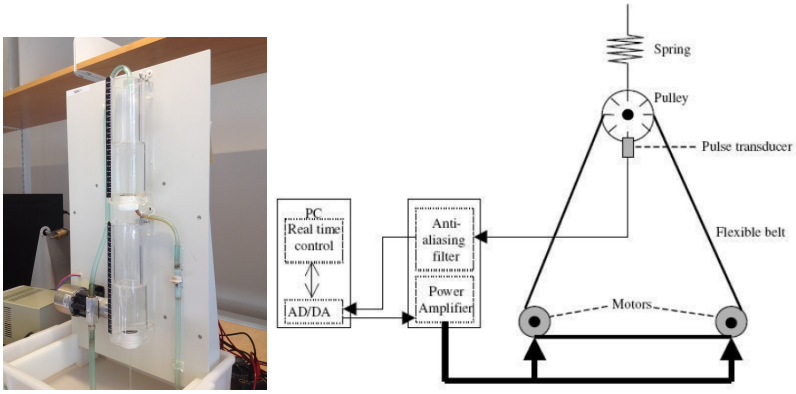

Figure 3: A photo of the **Cascade Tank with overflow (CCT)** system (Schoukens & Noël, 2017) and a graphical depiction of the **Coupled Electric Drive (CED)** system (Wigren & Schoukens, 2017). These two systems are the basis of the benchmarks used in the analysis and comparison of the SUBNET method.

opening in the upper tank, the water enters the lower tank where the water level is recorded. Lastly, through a small opening in the lower tank, the water re-enters the reservoir. This benchmark is nonlinear as the flow rates are governed by square root relations and the water can overflow either tank which is a hard nonlinearity. The benchmark consists of two datasets with measurements of 1024 samples each at a sample rate of $\Delta t = 4\text{s}$. The first dataset is be used for training, the first 512 samples of the second set are used for validation (used only for early stopping) and the entire second set for testing. Most of the other methods to which we compare use the entire second set as validation and test set, as no explicit test set is provided in this benchmark description.

The **Coupled Electric Drive (CED)** benchmark (Wigren & Schoukens, 2017) consists of measurements from a belt and pulley with two motors where both clockwise and counter-clockwise movement is permitted. The motors are actuated by the given inputs and the measured output is a pulse transducer that only measures the absolute velocity (i.e. insensitive to the sign of the velocity) of the belt. The system approximately has three states; the velocity of the belt, the position of the pulley, and the velocity of the pulley. The benchmark consists of two datasets of 500 samples each at a sample rate of $\Delta t = 20\text{ms}$. The first 300 samples are used for training and the other 200 samples are for testing, of those samples the first 100 samples are also used for validation with both datasets. Similar to the last benchmark, even with this overlap, it is still a fair comparison as most of the other methods to which we compare use the entire second set as validation and test.

5.2 Results

Using the SUBNET method Eq. (3) we estimate models where the three functions h_θ, f_θ and ψ_θ are implemented as 2 hidden layer neural networks with 64 hidden nodes per layer, tanh activation and a linear bypass from the input to the output for both benchmarks. As an ODE solver, we use a single RK4 step between samples and assume that the input signal is zero-order hold. As for the implementation of the CT subspace encoder method, the following hyper-parameters are considered; $n_x = 2$, $n_a = n_b = 5$ and $T = 30$ for CCT and $n_x = 3$, $n_a = n_b = 4$ and $T = 60$ for CED. These hyperparameters are chosen based on few-step prediction-error figures as was shown in (Beintema et al., 2021). The training is done by using the Adam optimizer with default settings (Kingma & Ba, 2015) with a batch size of 32 for CED and 64 for CCT and using a simulation on the validation dataset for early stopping to reduce overfitting.

We also directly compare with a reproduction of neural ODE on both benchmarks. We adapt the code and the example ("`latent_ODE.py`") available online (Chen et al., 2018) to include ZOH inputs, leaving the neural network unaltered and an RK4 integrator. We observed that the initial model was unstable for CCT and under performing for CED and, hence, the neural ODE method alone was unable to provide state-of-the-art results. To stabilize and improve the neural ODE method we also introduce a state-derivative normalization term $1/\tau$ motivated by Theorem 2. The value of

Table 1: The test RMSE simulation on two benchmarks for the CT SUBNET method using an ensemble of models. The value given is the best RMSE simulation of all estimated models and the value between parentheses is the mean performance of the models. Note that we are unable to report the results for the neural ODE without state-derivative normalization $1/\tau$ for CCT since the optimization was unstable.

(a) CCT benchmark

Method	**RMSE**
BLA (Relan et al., 2017)	0.75
Volterra model (Birpoutsoukis et al., 2018)	0.54
State-space with GP-inspired prior (Svensson & Schön, 2017)	0.45
SCI (Forgione & Piga, 2021)	0.40
NL-SS + NLSS2 (Relan et al., 2017)	0.34
TSEM (Forgione & Piga, 2021)	0.33
Tensor B-splines (Karagoz & Batselier, 2020)	0.30
Vanilla neural ODE (Chen et al., 2018)	NaN
neural ODE with normalization ($\Delta t/\tau = 0.03$)	0.18 (0.33)
Grey-Box with physical overflow model (Rogers et al., 2017)	0.18
DT subspace encoder	0.37 (0.97)
CT subspace encoder ($\Delta t/\tau = 0.032$)	**0.22 (0.30)**

(b) CED benchmark

Method	**RMSE [ticks/s]**	
	Set 1	**Set 2**
RBFNN - FSDE (Ayala et al., 2014)	0.130	0.185
GP with rational quadratic kernel (Zhou et al., 2021b)	0.150	0.167
GP with squared exponential kernel (Zhou et al., 2021b)	0.153	0.132
Sparse Bayesian MLP (Zhou et al., 2021b)	0.149 (0.187)	0.120 (0.134)
Cascaded Splines (Scarpiniti et al., 2015)	0.216	0.110
Sparse Bayesian LSTM (Zhou et al., 2021b)	0.121 (0.155)	0.097 (0.126)
Extended Fuzzy Logic (Sabahi & Akbarzadeh-T, 2015)	0.150	0.092
Vanilla neural ODE (Chen et al., 2018)	0.141 (0.362)	0.098 (0.370)
neural ODE with normalization ($\Delta t/\tau = 0.12$)	0.131 (0.198)	0.086 (0.158)
DT subspace encoder	0.169 (0.187)	0.117 (0.1557)
CT subspace encoder ($\Delta t/\tau = 0.3$)	**0.115 (0.143)**	**0.074 (0.100)**

$1/\tau$ for CCT and CED for neural ODE was initially chosen to be the optimal value found in the SUBNET approach, however, in the CED case, it was lowered due to optimization instabilities. [2]

We compared our obtained model to the literature in Table 1. We report both the mean and the minimum of an ensemble of models estimated only differing in parameter initialization. This ensemble consists of 17 SUBNET models for both CCT and CED and 24 and 8 neuralODE models for CCT and CED respectively. The table shows that the obtained models with the CT subspace encoder method are state-of-the-art. The obtained models are the best known models with a black-box approach on both benchmarks. Furthermore, we use an unrestricted state-space and fully connected neural networks as model elements. Remarkably, the resulting performance is close to the performance of a grey-box model. Furthermore, Figure 4 illustrates that the resulting models have been able to model the nonlinear behavior present in both benchmarks.

Table 1 also contains neural ODE with normalization. One observation is that the best and mean performance difference is significantly larger than of SUBNET. We think that this is due to the availability of only a single sequence in the training set for the CCT benchmark (and two sequences for CED) which results in extensive overfitting. In comparison, the subspace encoder method is less prone to overfitting since it uses many subsections of the available sequence(s). Moreover, the subspace encoder method only requires about 20 minutes to train a model to the lowest validation loss, whereas, neural ODE requires about 2 hours for CED and 5 hours for CCT.

When we introduced the state-derivative normalization factor $1/\tau$, we argued that it would normalize f_θ and that it would increase optimization stability and, hence, the quality of the obtained models. We provide experimental insight for these two statements by providing a parameter sweep over $\Delta t/\tau$. Moreover, to eliminate variations due to different initial parameters we trained an ensemble of models which creates box-plots with $\text{RMS}(x) = \sqrt{1/N n_x \sum_k \|x(k\Delta t)\|_2^2}$, $\text{RMS}(f)$, and the RMSE simulation. These box-plots as shown in Figure 5 indeed illustrate that there exists an $1/\tau$ such that both $RMS(f) \approx RMS(x) \approx 1$ and that the best performing models are close to that value of $1/\tau$. Moreover, to illustrate that improper normalization (i.e. $\tau = 1$) can diminish the performance for both CCT and CED, observe that the RMSE simulation is 2.0 and 0.3 ticks/s for $\Delta t/\tau = \Delta t = 4$ s and $\Delta t/\tau = \Delta t = 0.02$ s respectively.

[2]The code used for both SUBNET and neural ODE experiments is available at *"Github link removed for double-blind reviews, see zip file from supplementary materials until de-anonymization"*

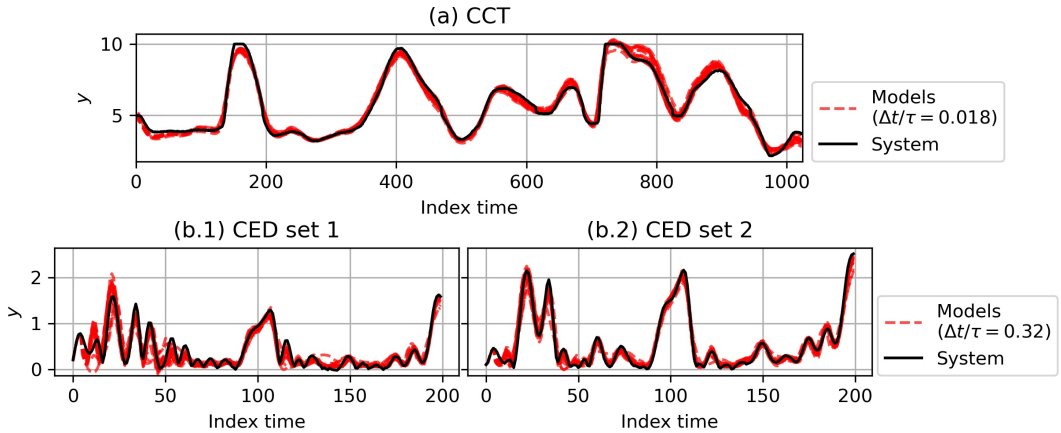

Figure 4: The time-domain simulation using the obtained models for the CT encoder method with a given $\Delta t/\tau$ (3) can make accurate long-term predictions. The CED benchmark is split since it contains two test sequences.

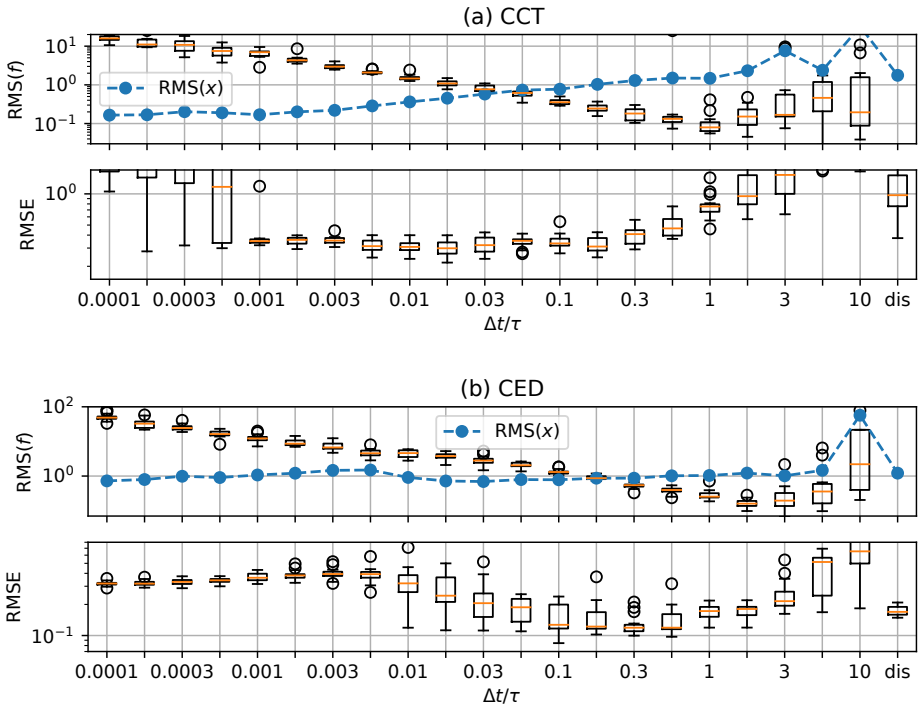

Figure 5: On the CCT and CED benchmarks the state amplitude $RMS(x)$, state-derivative amplitude $RMS(f)$ and RMSE simulation as function of the state-derivative normalization parameter $\Delta t/\tau$ as in $\dot{x} = \frac{1}{\tau} f_\theta(x, u)$ and the discrete-time case (dis). These two figures show that there exists a range of state-derivative normalization factors $\Delta t/\tau$ such where $RMS(f) \approx RMS(x) \approx 1$. Furthermore, this normalization factor is in the range where the RMSE simulation is significantly lowered.

6 Conclusion

In this paper, we introduced the CT subspace encoder approach to identify nonlinear dynamical systems in the presents of latent states, external inputs, and measurement noise. We showed that the proposed method can obtain state-of-the-art CT models only consisting of fully connected neural

networks. The approach improved computational cost and stability by considering multiple subsections where the initial state is estimated with an encoder function to reduce bias and a state-derivative normalization term to improve optimization stability. On this structure we make multiple theoretical derivations; increased cost function smoothness, necessary conditions for the existence of the encoder function and that for proper normalization in CT modelling one requires the state-derivative normalization term. Furthermore, we obtain state-of-the-art results on two benchmark examples.

7 Reproducibility Statement

- **Datasets:** *(i)* The CCT dataset is described in Schoukens & Noël (2017); Schoukens et al. (2017) and is available for download at `https://data.4tu.nl/articles/dataset/Cascaded_Tanks_Benchmark_Combining_Soft_and_Hard_Nonlinearities/12960104`, *(ii)* The CED dataset is described in Wigren & Schoukens (2017) and is available for download at `http://www.it.uu.se/research/publications/reports/2017-024/`.
- **Code:** Both the implementation and experiments of CT SUBNET and neural ODE are available at *"Github link removed for double-blind reviews, see zip file from supplementary materials until de-anonymization"*.
- **Hardware:** It takes about 15 minutes to estimate a single CT SUBNET model and 2 hours for a single neural ODE model on a consumer laptop.

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8 Appendix

8.1 Proof of theorem 1

Recall that the subspace encoder loss function as in Eq. 3 can be expressed in the following form

$$\begin{aligned} V^{\text{enc}}(\theta) = \quad & \frac{1}{N-T-\max(n_a,n_b)+1} \sum_{n=\max(n_a,n_b)}^{N-T} \frac{1}{T} \sum_{k=0}^{T-1} \|y_{n+k} - \hat{y}_{n+k|n}\|_2^2, \\ \text{with} \quad & \hat{y}_{n+k|n} = h_\theta(x_{n+k|n}) = h_\theta(x((n+k)\Delta t|n\Delta t)), \\ & \dot{x}(t|n\Delta t) = \frac{1}{\tau} f_\theta(x(t|n\Delta t), u(t)) \\ & x(n\Delta t|n\Delta t) = \psi_\theta(u_{n-1}, ..., u_{n-n_b}, y_{n-1}, ..., y_{n-n_a}). \end{aligned} \tag{9}$$

Our aim is to derive the scaling in T of the Lipschitz constant L_{enc} as defined in

$$|V^{\text{enc}}(\theta_1) - V^{\text{enc}}(\theta_2)|^2 \leq L_{\text{enc}}^2 \|\theta_1 - \theta_2\|_2^2. \tag{10}$$

We aim to express L_{enc} in terms of the following Lipschitz constants

$$\|h_{\theta_1}(x_1) - h_{\theta_2}(x_2)\|_2^2 \leq L_h^2(\|x_1 - x_2\|_2^2 + \|\theta_1 - \theta_2\|_2^2). \tag{11a}$$

$$\|f_{\theta_1}(x_1, u) - f_{\theta_2}(x_2, u)\|_2^2 \leq L_f^2(\|x_1 - x_2\|_2^2 + \|\theta_1 - \theta_2\|_2^2), \tag{11b}$$

$$\|\psi_{\theta_1}(u_{\text{past}}, y_{\text{past}}) - \psi_{\theta_2}(u_{\text{past}}, y_{\text{past}})\|_2^2 \leq L_\psi^2 \|\theta_1 - \theta_2\|_2^2. \tag{11c}$$

Furthermore, to derive the scaling of L_{enc} we use known properties of the Lipschitz constant that being;

- The sum property: $c(x) = a(x) + b(x)$ has a Lipschitz constant of $L_c = L_a + L_b$.
- The multiplication property: $c(x) = a(x)b(x)$ has a Lipschitz $L_c = M_a L_b + M_b L_a$ where M_a is the maximal value of a on a closed set of inputs $x \in X$ and M_b similarly defined.

Since the encoder loss function as in Eq. 3 can be written as a sum as

$$V^{\text{enc}}(\theta) = \frac{1}{N-T-\max(n_a,n_b)+1} \sum_{n=\max(n_a,n_b)}^{N-T} V^{\text{sec}}(n, \theta_1) \tag{12a}$$

$$V^{\text{sec}}(n, \theta_1) = \frac{1}{T} \sum_{k=0}^{T-1} \|y_{n+k} - \hat{y}_{n+k|n}\|_2^2 \tag{12b}$$

$$|V^{\text{sec}}(n, \theta_1) - V^{\text{sec}}(n, \theta_2)|^2 \leq L_{\text{sec}}^2 \|\theta_1 - \theta_2\|_2^2, \tag{12c}$$

this implies that $L_{\text{enc}} = L_{\text{sec}}$ by the sum property since

$$L_{\text{enc}} = \frac{1}{N-T-\max(n_a,n_b)+1} \sum_{n=\max(n_a,n_b)}^{N-T} L_{\text{sec}}. \tag{13}$$

Hence, it is sufficient to consider only a single subsection, take $n = 0$ and drop the bar notation for simplicity of notation.

By the sum and multiplication properties we derive that

$$|V^{\text{sec}}(\theta_1) - V^{\text{sec}}(\theta_2)| \leq 2/T \sum_{k=0}^{T-1} (M_y + M_k) \|\hat{y}_{1,k} - \hat{y}_{2,k}\|_2, \tag{14}$$

where M_y is the bound on $\|y(t)\|_2$ and M_k the bound on $\|\hat{y}_k\|_2$. The M_k bound scales the same as $\|\hat{y}_{1,k} - \hat{y}_{2,k}\|_2$ as shown in Ribeiro et al. (2020). The $\|\hat{y}_{1,k} - \hat{y}_{2,k}\|_2$ expression can be expanded by using Eq. 11a as

$$\|\hat{y}_{1,k} - \hat{y}_{2,k}\|_2^2 \leq L_h^2 (\|x_1(k\Delta t) - x_2(k\Delta t)\|_2^2 + \|\theta_1 - \theta_2\|_2^2). \tag{15}$$

Next, we aim to derive an expression for the Lipschitz constant $L_x(t)$ given in terms of

$$\|x_1(t) - x_2(t)\|_2^2 \leq L_x(t)^2 \|\theta_1 - \theta_2\|_2^2. \tag{16}$$

where by Eq. (11c)

$$L_x(0) = L_\psi. \tag{17}$$

By considering a small increment in time of length h we can express $L_x(t+h)$ in terms of $L_x(t)$. Using the fact that h is small we can use an Eurler step and discard higher order terms of h as;

$$\begin{aligned}
\|x_1(t+h) - x_2(t+h)\|_2^2 &= \|(x_1(t) - x_2(t)) + h/\tau(f_{\theta_1}(x_1(t), u(t)) - f_{\theta_2}(x_2(t), u(t)))\|_2^2 \\
&\leq \|x_1(t) - x_2(t)\|_2^2 + 2h/\tau \|x_1(t) - x_2(t)\|_2 \|f_{\theta_1}(x_1(t), u(t)) - f_{\theta_2}(x_2(t), u(t))\|_2
\end{aligned}$$

by the triangle inequality. Next, we can replace all the f terms by Eq. (11b) and x terms by Eq. (16) to derive an expression for $L_x(t+h)$ as

$$\begin{aligned}
&\leq \|x_1(t) - x_2(t)\|_2^2 + 2h/\tau \|x_1(t) - x_2(t)\|_2 L_f \sqrt{\|x_1(t) - x_2(t)\|_2^2 + \|\theta_1 - \theta_2\|_2^2} \\
&\leq \left(L_x(t)^2 + 2h/\tau L_x(t) L_f \sqrt{L_x(t)^2 + 1} \right) \|\theta_1(t) - \theta_2(t)\|_2^2 \\
&L_x(t+h) = \sqrt{L_x(t)^2 + 2h L_x(t) \sqrt{L_x(t)^2 + 1} L_f/\tau}.
\end{aligned}$$

This expression allows us to derive that the derivative of $L_x(t)$ is given by

$$\dot{L}_x(t) = \lim_{h \to 0} \frac{L_x(t+h) - L_x(t)}{h}, \tag{18}$$

$$= \sqrt{1 + L_x(t)^2} L_f/\tau. \tag{19}$$

which suggests that $\dot{L}_x(t)$ is continuous in t and has the closed form solution as

$$L_x(t) = L_x(0) + \int_0^t \dot{L}_x(t') dt' \tag{20}$$

$$= \sinh(t L_f/\tau + \text{arcsinh}(L_\psi)) \tag{21}$$

Now by substituting Eq. (21) into, (16), (15), (14) and using (13) we arrive at the following expression for L_{enc} as

$$L_{\text{enc}} = 2/T \sum_k (M_y + M_k) L_h (\sinh(k\Delta t L_f/\tau + \text{arcsinh}(L_\psi)) + 1) \tag{22a}$$

which scales in the limit of large T as

$$L_{\text{enc}} = \mathcal{O}(\exp(2T\Delta t L_f/\tau)), \tag{23a}$$

since $L_f > 0$ and $\Delta t > 0$. Note that the 2 in the exponent is from the multiplication with M_k which also scales as the y term as previously mentioned.

8.2 RECONSTRUBABILITY OF THE INITIAL STATE FROM PAST INPUT AND OUTPUTS

To derive the conditions on the existence of the encoder function suppose that we have a system given by

$$\dot{x}(t) = f(x(t), u(t)) \tag{24a}$$
$$y_n = h(x_n) + w_n \tag{24b}$$

where $x_n = x(n\Delta t)$. For this system if a state is given $x(t_0)$ along the input trajectory $u(t)$ one would in principle be able to compute $x(t)$ for all $t > t_0$. However, since we aim to construct the state given past outputs we need $x(t)$ for $t < t_0$ which requires backwards in time integration. This backwards integration on f is guaranteed to be unique if f is Lipschitz continuous in x for all u as by the Picard–Lindelöf theorem (Murray & Miller, 2013). Hence, since f is assumed to be Lipschitz continuous we can construct an operator f_d which can integrate backwards or forwards as

$$x_{n+1} = f_d(x_n, u_n) \rightarrow x_{n-1} = f_d^{-1}(x_n, u_{n-1}) \tag{25}$$

where u is subject to ZOH.

This operator allows us to construct past outputs as

$$\begin{aligned}
y_{n-1} &= (h \circ f_d^{-1})(x_n, u_{n-1}) + w_{n-1} \\
y_{n-2} &= (h \circ f_d^{-2})(x_n, u_{n-1}, u_{n-2}) + w_{n-2} \\
&\vdots \\
y_{n-z} &= (h \circ f_d^{-z})(x_n, u_{n-1}, u_{n-2}, ..., u_{n-z}) + w_{n-z} \\
Y_n^{-z} &= (H \circ F_d^{-z})(x_n, U_n^{-z}) + W_n^{-z}
\end{aligned} \tag{26}$$

where

$$f_d^{-p}(x_n, u_{n-1}, ..., u_{n-p}) = f_d^{-p+1}(f_d^{-1}(x_n, u_{n-1}), u_{n-2}, ..., u_{n-p})$$

is the application of f_d^{-1}, p times to obtain x_{n-p}. Furthermore, $Y_n^{-z} = [y_{n-1}^\top, y_{n-2}^\top, ..., y_{n-z}^\top]^\top$ and, $(H \circ F_d^{-z})$ and W_n^{-z} are similarly defined. To construct the initial state x_n we need to invert Eq. (26). This inverse is also known as a reconstructability map (Katayama, 2005). However, for the inverse to exist, several necessary requirements can be derived. One such necessary requirement is that a small perturbation to a solution x_n should change $(H \circ F_d^{-z})$, otherwise these solutions are indistinguishable from the output. This is formalized stating by that the matrix $\frac{\partial (H \circ F_d^{-z})(x_n, U_n^{-z})}{\partial x_n}$ has a null-space of rank zero which is also known as the local observability condition. This is the same as the condition that the column rank $\geq n_x$. A necessary requirement for this column rank condition is that the number of columns is equal to or greater than the number of rows i.e. $zn_y \geq n_x$.

Hence, under the right conditions, it might be possible to solve Eq. (26) for a singular x_n since this equation is a nonlinear fixed point problem if W_n^{-z} is known. For the case that W_n^{-z} is unknown one can estimate the state $\hat{x}_n \approx x_n$ by solving the nonlinear regression problem;

$$\hat{x}_n = \arg\min_{\hat{x}_n} \|Y_n^{-z} - (H \circ F_d^{-z})(\hat{x}_n, U_n^{-z})\|_2, \tag{27a}$$
$$= \arg\min_{\hat{x}_n} \|L(\hat{x}_n, Y_n^{-z}, U_n^{-z})\|_2. \tag{27b}$$

Hence, both f uniformly Lipschitz continuous and $(\nabla_x L)^T \nabla_x L$ being full rank in $\hat{x}_n$ are necessary conditions for the existence of a unique reconstrubability map.

Computing the reconstructability map for our model thus requires solving an optimization problem that becomes computationally infeasible during training. Hence, the encoder function aims to approximate the solution to Problem (27).