Using what you know: 
Learning dynamics from partial observations with structured neural ODEs

Mona Buisson-Fenet 1 2 3  Valery Morgenthaler 3  Sebastian Trimpe 2  Florent Di Meglio 1

Abstract

Identifying dynamical systems from experimental data is a notably difficult task. Prior knowledge generally helps, but the extent of this knowledge varies with the application, and customized models are often needed. We propose a flexible framework to incorporate a broad spectrum of physical insight into neural ODE-based system identification, giving physical interpretability to the resulting latent space. This insight is either enforced through hard constraints in the optimization problem or added in its cost function. In order to link the partial and possibly noisy observations to the latent state, we rely on tools from nonlinear observer theory to build a recognition model. We demonstrate the performance of the proposed approach on numerical simulations and on an experimental dataset from a robotic exoskeleton.

1. Introduction

Predicting the behavior of complex systems is of great importance in many fields. In engineering for instance, designing controllers for robotic systems requires accurate predictions of their evolution. The behavior of such systems often follows a certain structure, which can be inferred, for example from the laws of physics. Mathematically, this structure is often captured by differential equations. However, even an accurate model cannot account for all aspects and physical parameters can only be measured with uncertainty. Data-driven methods promise to enhance our predictive capabilities for ever more complex systems based on experimental data.

In the case of dynamical systems, not all system states can usually be measured, so this experimental data is only partial and also noisy. In general, learning the dynamics is an ill-posed problem: given observations, many different state-space representations can explain them. Physical knowledge can help reduce the number of possible models and improve the performance of data-driven approaches.

Learning latent representations of the available data is an active research area in machine learning. In particular, neural ordinary differential equations (NODEs) were introduced by Chen et al. (2018) and have since sparked significant interest, e.g., Zhong et al. (2020); Rubanova et al. (2019). The aim is to approximate a vector field that generates the observed data following a continuous-time ODE with a neural network. However, as for most machine learning methods, little insight on the desired latent representation is usually provided. This leads to difficulties with the interpretability of the obtained models, and their capability to generalize.

In this paper, we show that the NODE formulation is well-suited for learning dynamical systems from partial measurements. It is both general enough to avoid needing a new design for each new system, but can also enforce a wide range of physical insight that may be available, allowing for a physically meaningful and interpretable model. This is illustrated in Fig. 1: the NODE optimization problem can directly include physical knowledge in the form of “soft” priors (extra cost terms) or “hard” priors (constraints). Our main contributions can be summarized as follows:

- We formulate NODEs as a flexible framework for learning dynamics, that enables enforcing a broad spectrum of physical knowledge;
- We introduce recognition models to link observations and latent state, then propose several forms based on nonlinear observer design;
- We demonstrate the ability of structured NODEs to enforce increasing physical priors in a simulation study;
- We apply the proposed approach to an experimental dataset obtained on a robotic exoskeleton, illustrating the possibility of learning a physically sound model of complex dynamics from real-world data.
2. Related work

The proposed method is based on two active research areas: nonlinear observer design and machine learning for dynamical systems. In this section, we give an overview of the main trends and the most related methods on these topics.

2.1. System theory

System identification The field of system identification aims at finding a possible dynamics model given a finite amount of partial measurements (Ljung, 1987; Nelles, 2001; Schoukens & Ljung, 2019). For linear systems, a suitable set of system matrices can be identified using subspace methods (Viberg, 1995). For nonlinear systems, most state-of-the-art techniques aim at estimating the variables of a given parametric model using Bayesian parameter estimation (Galioto & Gorodetsky, 2020) or optimization-based methods (Schittkowski, 2002; Raue et al., 2013; Villaverde et al., 2021), or a decomposition of its dynamics on a suitable basis of functions (Sjöberg et al., 1995). These classical methods tend to be system-specific: they require expert knowledge to construct a parametric model or precisely pick the hypothesis class in which it will be approximated. In this paper, we focus on the case where no parametric model is available and show that NODEs are a general tool for system identification, in which a broad range of physical knowledge can be included by adapting the formulation to the use case.

Observer design When identifying a state-space model from partial observations, the unknown latent state must be estimated. This is related to state observers or estimators, which infer the state from observations by designing an auxiliary observer system driven by the measurement. Observers often assume a good dynamics model, but designs that can deal with imperfect models are also available. In that case, the unknown parts of the dynamics can be overridden through high-gain or sliding-mode designs to enable convergence (Buisson-Fenet et al., 2021; Shtessel et al., 2016). Otherwise, the unknown parameters can be seen as extra states with constant dynamics, and extended state observers can be designed, such that the estimated state and parameters converge asymptotically (Praly et al., 2006).

2.2. Learning dynamical systems

Learning dynamical systems from data is also investigated in machine learning (Legaard et al., 2021; Nguyen-Tuong & Peters, 2011). We focus on settings considered realistic in system theory, i.e., methods that allow for control and partial observations, and can ensure certain physical properties.

Physics-aware models The dynamics models obtained from machine learning often struggle with generalization and generally do not verify important physical principles such as conservation laws. Therefore, there have been efforts to bring together machine learning and first principles to learn physics-aware models; see Wang & Yu (2021) for an overview on this approach in deep learning. In general, there are two takes on including physical knowledge in data-driven models. On the one hand, terms can be added to the cost function to penalize certain aspects. For example, if a prior model is known from first principles, it is possible to learn a residual model of minimal norm. For NODEs, this is investigated by (Yin et al., 2021) for full state observations. On the other hand, structural constraints can be added to the optimization problem to enforce physical properties. For NODEs, this has been investigated for Hamiltonian (Zhong et al., 2020) or port-Hamiltonian models (Massaroli et al., 2020a). However, little previous work on NODEs assumes partial and noisy measurements of system trajectories. Various methods have been proposed for learning physics-aware dynamics models, such as Bayesian approaches, in which prior knowledge can be enforced in the form of the kernel (Wu et al., 2019), by structural constraints (Rath et al., 2021; Ensinger et al., 2022), or by directly estimating the variables of a parametric model (Galioto & Gorodetsky, 2020). In this paper, we focus on NODEs, which leverage the predictive
power of deep learning while enforcing that the obtained trajectory be the solution of an ODE.

**Partial observations** Most NODE frameworks for dynamical systems assume full state measurements. Partial observations greatly increase the complexity of the problem: the latent state is unknown, leading to a large number of possible state-space representations. In this case, the question of linking the observations with the latent state needs to be tackled. In Bayesian approaches, the distribution over the initial state can be conditioned on the first observations then approximated by a so-called recognition model (Eleftheriadis et al., 2017; Doerr et al., 2017; 2018). In deep learning, an encoder can be trained to map the observations to the latent state that follows an ODE (Rubanova et al., 2019; Doyeon et al., 2021; de Brouwer et al., 2019). The particular case in which this ODE is linear and evolves according to the Koopman operator (that can be jointly approximated) is investigated in Lusch et al. (2018); Bevanda et al. (2021). However, little insight on the desired latent representation is usually provided. This leads to difficulties for the obtained models to generalize, but also with their interpretability: often in a control environment, the states should have a physical meaning. Therefore, we propose to learn a recognition model that maps the observations to the latent state, while enforcing physical knowledge in the latent space.

### 2.3. Structure of the paper

We introduce neural ODEs for dynamical systems with partial observations and control inputs in Sec. 3. In Sec. 4, we present recognition models to link the observations to the latent state. We then show how physical knowledge can be included in Sec. 5. In Sec. 6, we demonstrate the proposed framework on a simulation case study and an experimental use case, before concluding in Sec. 7.

### 3. Problem statement

Consider a general continuous-time nonlinear system

\[
\begin{align*}
\dot{x}(t) &= f(x(t), u(t)) \quad x(0) = x_0 \\
y(t) &= h(x(t), u(t)) + \epsilon(t),
\end{align*}
\]

where \( x(t) \in \mathbb{R}^{d_x} \) is the state, \( u(t) \in \mathbb{R}^{d_u} \) is the control input, \( y(t) \in \mathbb{R}^{d_y} \) is the measured output, and \( f, h \) are the true dynamics and measurement functions, assumed continuously differentiable. We denote \( \dot{x}(t) \) the derivative of \( x \) w.r.t. time \( t \), and generally omit the time dependency for simplicity of notation. We only have access to partial measurements \( y \) corrupted by noise \( \epsilon \), the control input \( u \), and the measurement function \( h \). This setting is considered realistic in system identification, since \( y \) is measured by sensors, \( u \) is chosen by the user, and \( h \) reflects their prior knowledge: if the structure of the model is known, then the user knows \( d_x \) and which states are measured; if not, then \( d_x \) can be chosen large enough and \( h \) measures the first \( d_y \) states. We assume that the solutions to (1) are well-defined and that there exists a compact set \( \mathcal{X} \) such that \( x(t) \in \mathcal{X} \) \( \forall t \geq 0 \). We aim to estimate \( f \) the dynamics of the system.

The objective of NODEs (Chen et al., 2018) is to learn a vector field that generates the data through an ODE, possibly up to an input and output transformation; see Massaroli et al. (2020b) for an overview. While the interpretation of this formulation for general machine learning tasks remains open, it is very natural for dynamical systems, which are generally modeled by ordinary or partial differential equations: learning the NODE boils down to approximating the dynamics with a neural network (NN). However, there is no unifying framework for applying NODEs to dynamical systems in realistic settings, i.e., with partial and noisy trajectory data, with a control input, and using all available physical knowledge. In the following, we present a general formulation of NODEs for dynamical systems, then propose recognition models and including physical knowledge to make it practically applicable. The proposed approach can then cover the whole spectrum presented in Fig. 1.

For estimating the unknown state and dynamics, we assume we have access to \( N \) measured trajectories indexed by \( j \), denoted \( y^j \) and sampled at times \( t_i \), \( i \in \{1, \ldots, n\} \). We approximate the true dynamics \( f \) with a NN with weights \( \theta \) denoted \( f_\theta \). If the initial conditions \( x_0^j \) are known, learning \( f_\theta \) can be formulated as the following optimization problem:

\[
\begin{align*}
\min_{\theta} \frac{1}{2d_y nN} \sum_{j=1}^{N} \sum_{i=1}^{n} \|y^j(t_i) - y^j(t_i)\|^2_{L_2} := L(\theta) \\
\text{s.t.} \quad \dot{x}^j &= f_\theta(x^j, u^j), \quad y^j = h(x^j, u^j), \\
x^j(0) &= x_0^j
\end{align*}
\]

where the constraint is valid for all \( j \in \{1, \ldots, N\} \). Several methods have been proposed to compute the gradient of \( L(\theta) \); see Schittkowski (2002); Alexe & Sandu (2009); Massaroli et al. (2020b) for more details. We opt for automatic differentiation through the numerical solver used to solve the ODE (torchdiffeq by Chen et al. (2018)), then apply gradient-based methods such as Adam (Kingma & Ba, 2015) to find a local optimum of this nonconvex problem.

In (2), we assume the user has no physical knowledge about the dynamics \( f \). In this case, the problem of learning the dynamics from data is not well-posed: for a given state trajectory, there exist several state-space representations \( f \) that can generate this data, even more so when we only observe \( y = h(x, u) \). This is known as the unidentifiability problem (Aliee et al., 2021). Therefore, without additional costs and constraints, we cannot expect the obtained dynamics model to be unique. Solving (2) then yields a latent state-space representation that explains the data, but not necessarily one
that is physically meaningful. This is problematic when the learned dynamics model is used for downstream control or monitoring tasks, for which physically interpretable states are often needed. In this work, we show that the NODE problem formulation enables estimating \( f \) while including all available physical knowledge, as discussed in Sec. 5.

**Remark 1** The length and sampling times of the training trajectories need not be fixed. As long as they are known, we can interpolate the signals, compute the loss and perform optimization. However, if all trajectories have the same sampling times, then all simulations can be run in parallel, which is computationally more efficient. Also, it would be beneficial to optimize all model parameters hierarchically: learn a first model on short training trajectories, which lead to a simpler optimization problem (Ribeiro et al., 2020), then fine-tune it on increasingly long trajectories. However, this and other procedures for increasing final accuracy necessitate extra implementation efforts and are not directly relevant for this work. In the following, we consider that the sampling times are the same for all trajectories.

### 4. Recognition models

In the case of partial observations, the initial condition \( x_0 \) in (2) is unknown and needs to be estimated jointly with \( f_\theta \). In standard system identification, the unknown initial condition is usually optimized directly as a free variable; in this case, it needs to be optimized again with each new trajectory and cannot be used as such for prediction. We propose to estimate it from the observations by learning a recognition model \( \psi \) that links the output to the initial state. The term recognition model has been used to designate approximating the initial latent state from partial observations (Eleftheriadis et al., 2017; Doerr et al., 2017; 2018; Rubanova et al., 2019). For NODEs, recognition models have also been called augmentation strategies (Massaroli et al., 2020b; Chalvidal et al., 2021; Norcliffe et al., 2021).

Whether the state can be estimated from the output is a precise notion in system theory, called observability. There is no simple criterion to determine if a nonlinear system is observable. However, notions of observability are often assumed to render the problem feasible, otherwise there is no hope of learning \( f_\theta \) from the observations only. We use the following definition from Bernard (2019):

**Definition 1** System (1) is uniformly distinguishable in time \( t_c \) if for any input \( u : \mathbb{R} \mapsto \mathbb{R}^{d_u} \) and for any given initial conditions \( x_a, x_b \in X \) at \( t_0 = 0 \), we have

\[
y_{a,u}(t) = y_{b,u}(t) \quad \forall t \in [0, t_c] \Rightarrow x_a = x_b,
\]

where \( y_{a,u} \) (resp. \( y_{b,u} \)) is the output of (1) given input \( u \) and initial condition \( x_a \) (resp. \( x_b \)).

Hence, if (2) is observable, then \( x(0) \) is uniquely determined by \( y([0, t_c]) \) and \( u([0, t_c]) \) for \( t_c \) large enough.

We propose to learn a recognition model \( \psi \) with some input \( \bar{z}(t_c) \), whose definition depends on the chosen method as described in the following. This model is designed as a NN with weights \( \theta_\psi \), which are optimized jointly with \( \theta \). This leads to the modified problem formulation:

\[
\min_{\theta, \theta_\psi} \frac{1}{2d_y n N} \sum_{j=1}^N \sum_{i=1}^n \| y_j'(t_i) - \psi_j'(t_i) \|_2^2 := L(\theta, \theta_\psi)
\]

\[
s.t. \quad \ddot{x}_j = f_\theta(x_j, u_j), \quad y_j = h(x_j, u_j),
\]

\[
x_j(0) = \psi(\bar{z}(t_c)).
\]

The most straightforward approach is to learn a recognition model directly from \( y_{0:t_c} = (y(0), \ldots, y(t_c)) \) to the latent state. For nonautonomous systems, the first inputs should also be taken into account, which yields \( \bar{z}(t_c) = (y_{0:t_c}, u_{0:t_c}) \). It has been used for approximating the distribution over the initial state conditioned on \( y_{0:t_c} \) (Eleftheriadis et al., 2017; Doerr et al., 2017; 2018; Rubanova et al., 2019), e.g., for joint inference and learning of Gaussian process state-space models. Augmentation strategies for NODEs (Massaroli et al., 2020b; Chalvidal et al., 2021; Norcliffe et al., 2021) are often particular cases with \( t_c = 0 \): for many nonlinear systems, this is too little information and does not enable the estimation of \( x(0) \) as per Definition 1. There are few works on NODE-based system identification from partial observations, which either train a recognition model from \( y_{-t_c,0} \) (Ayed et al., 2020) or learn the dynamics of \( y_{0:t_c} \) (Schlaginhaufen et al., 2021). No physical knowledge is then embedded in the latent space.

This approach \( \bar{z}(t_c) = (y_{0:t_c}, u_{0:t_c}) \), further denoted direct, is justified by the observability assumption: for \( t_c \) large enough, this is all the information needed to estimate \( x(0) \). However, for large \( t_c \), the input dimension becomes arbitrarily high, so that optimizing \( \psi \) is more difficult. Therefore, we propose a new type of recognition model based on nonlinear observer design, leading to different choices of \( \bar{z}(t_c) \).

### 4.1. Background on KKL observers

The field of nonlinear observer design is concerned with the estimation of the state of nonlinear dynamical systems from partial observations; see e.g., (Bernard, 2019) for an overview. A particular method that has recently gained interest is the Kazantzis-Kravaris/Luenberger (KKL) observer (Andrieu & Praly, 2006). It relies on building a contracting linear system of state \( z \):

\[
\dot{z} = Dz + Fy, \quad z(0) = z_0
\]

where \( z \in \mathbb{R}^{d_z} \) with \( d_z = d_y(d_x + 1) \), \( z_0 \) is an arbitrary initial condition, \( y \) is the output of (1), \( D \) is Hurwitz, and
We propose to train a recognition model $x(t)$ of $(D, F)$ is a controllable pair (Kailath, 1980). Under mild assumptions, mainly $x(t) \in \mathcal{X}$ compact $\forall t \geq 0$ and (1) is backward distinguishable, the existence of an injective transformation from the original state-space (1) to the form (5) is studied. For autonomous systems, it is shown by Andrieu & Praly (2006) that if the eigenvalues of $D$ have sufficiently large negative real parts, there exists an injective transformation $T$ and its pseudo-inverse $T^*$ such that

$$\|x(t) - T^*(z(t))\| \to 0, \quad t \to \infty$$  \hspace{1cm} (6)

meaning that $T^*(z(t))$ with $z(t)$ from (5) is an observer for $x(t)$. However, $T$ and $T^*$ cannot be computed analytically in general. Therefore, it has been proposed to learn them from full-state simulations (da Costa Ramos et al., 2020) or to directly learn $h \circ T^*$ from partial observations to build an output predictor (Janny et al., 2021).

These results are extended to nonautonomous systems by Bernard & Andrieu (2019). The main differences are that the eigenvalues no longer need to be sufficiently large and that $T$ is time-dependent. In particular, it depends on the past values $u([0, t])$ and becomes injective for $t \geq t_c$ with $t_c$ from the backward distinguishability assumption. If a generating system for the input $u$ is known, we can also consider the extended system

$$\dot{x} = f(x, u), \quad y = h(x, u),$$

$$\dot{\omega} = s(\omega), \quad u = l(\omega)$$  \hspace{1cm} (7)

where $\omega$ generates $u$. Then, given

$$\dot{z} = Dz + F \begin{pmatrix} y \\ u \end{pmatrix}, \quad z(0) = z_0,$$  \hspace{1cm} (8)

a static observer can again be built to estimate $x$. Hence, the time dependency in $T$ disappears at the cost of a higher dimension $d_z = (d_y + d_u)(d_x + d_\omega + 1)$.

To sum up, these results guarantee the existence of $T^*$ such that for $t$ large enough, we have $x(t) \approx T^*(z(t))$ for autonomous systems. For nonautonomous systems, $x(t)$ also depends on $u_{0:t}$, directly or indirectly through (8). This $z(t)$ can then be used as input to a recognition model. Contrarily the direct approach where the input to $\psi$ is a potentially large stack of observations, $z(t)$ has a fixed dimension, and contains a compressed version of the information in $y_{0:t}$.

### 4.2. KKL-based recognition

We propose to train a recognition model $x(0) = \psi(\tilde{z}(t_e))$ based on KKL observers. Running the observer in forward time for $t_e$ gives $x(0) \approx T(z(t_e))$, then only the samples $y(t_i)$ for $t_i > t_e$ are used for data fitting in (4). It is also possible to run it in backward time by simulating (5) - resp. (8) - from $t_s$ to 0, such that $x(0) \approx T(z(0))$ for $t_e$ large enough. Then, the whole training trajectory can be used for data fitting. We propose several options:

- **direct**: $\tilde{z}(t_e) = (y_{0:t_s}, u_{0:t_s})$,
- **KKL**: $\tilde{z}(t_e) = (z(t_e), u_{0:t_s})$ where $z$ is solution of (5) simulated forward or backward in time,  
- **KKLu**: $\tilde{z}(t_e) = z(t_e)$ where $z$ is solution of (8) simulated forward or backward.

These forms of recognition models are all justified for $t_e$ large enough by the observability assumption, but contain a filtered and increasingly compressed version of the information in $(y_{0:t_s}, u_{0:t_s})$. This allows for a low-dimensional input to $\psi$, which is expected to be easier to train.

### Optimizing D jointly

With any KKL-based recognition model, the choice of $D$ in (5) - resp. (8) - is critical since it controls the convergence rate of $z$. Hence, we propose to optimize $D$ jointly with $\theta, \theta_\psi$ by including the ODE on $z$ in the optimization problem, as in Janny et al. (2021). This leads to a computational overhead but improves the performance. More details are provided in the supplementary material.

### 5. Enforcing physical knowledge

The aim of learning dynamical systems is generally to monitor, predict or control their behavior, tasks for which physically meaningful states are often necessary. One of the main advantages of the NODE formulation is that it is general: it can conceptually be applied to any observable system, contrarily to many classical, system-specific identification methods. However, it is also very straightforward to include physical knowledge in the optimization problem (4), which eases the generalization but also the interpretation of the obtained models. The extent of this physical knowledge varies depending on the use case, forming a broad spectrum of possible insight illustrated in Fig. 1. As we shall show, NODEs can easily be adapted to move from one end of the spectrum to the other by changing (4): no knowledge at all will lead to one of infinitely many possible state-space representations, while for very strong priors, only one representation may remain feasible. Some forms of prior knowledge have been proposed in the literature and are categorized below. Our contribution is to show that the NODE formulation can cover the whole spectrum of system identification illustrated in Fig. 1, on which these works can be situated. Further, we combine this with partial observations, which have rarely been considered in the literature.
5.1. Soft priors

The first approach to include physical knowledge in NODEs is to add “soft” priors to the optimization problem. The most common case is when a prior model of the system, denoted $f_0$, is available from first principles. We can then learn a residual NODE on top of $f_0$, while penalizing the norm of $f_0$ to correct the prior only as much as necessary to fit the observations. This is investigated in Yin et al. (2021); Mehta et al. (2020) for full state observations. It yields the modified optimization problem:

$$\min_{\theta, \psi} L(\theta, \psi) + \frac{\lambda}{2d_y n N} \sum_{j=1}^{N} \sum_{i=1}^{n} \left\| f_\theta(x_j^i(t), u_j^i(t)) \right\|_2$$

s.t.  

$$\dot{x}^j = f_\theta(x^j, u^j) + f_0(x^j, u^j),$$

$$x^j(0) = \psi(z^j(t_c)), \quad y^j = h(x^j, u^j), \quad (9)$$

where $\lambda$ is a scaling factor set by the user. Other quantities can be known a priori and enforced similarly to (9), such as the total energy of the system (Eichelsdörfer et al., 2021) or stability through a Lyapunov-inspired cost function (Manek & Kolter, 2019; Schlaginhaufen et al., 2021).

5.2. Hard constraints

Structural knowledge about the considered system can also be available. In that case, it can be enforced by “hard” constraints in the optimization problem. As an example, if the system is known to be Hamiltonian, we can write:

$$\min_{\theta, \psi} L(\theta, \psi)$$

s.t.  

$$\dot{q}^j = \frac{\partial H_\theta}{\partial p}(x^j, u^j), \quad \dot{p}^j = -\frac{\partial H_\theta}{\partial q}(x^j, u^j)$$

$$x^j(0) = \psi(z^j(t_c)), \quad y^j = h(x^j, u^j), \quad (10)$$

where $x = (q, p)$ are the generalized coordinates and $H_\theta$ is the approximate Hamiltonian. This yields a harder optimization problem, but improves performance and interpretability of the model. This line of work originates from Greydanus et al. (2019); Crammer et al. (2020) and has been extended to NODEs for Hamiltonian and port-Hamiltonian systems (Zhong et al., 2020; Massaroli et al., 2020a). However, these studies consider full state or even acceleration measurements to directly approximate the function of interest.

The above describes a family of optimization problems for dynamics learning: without prior knowledge (4), with “soft” priors (here a residual model) (9), and with “hard” priors (here a Hamiltonian structure) (10). While individual instances have been proposed in prior work, we regard the NODE formulation as a flexible framework for system identification: the whole spectrum of prior knowledge in Fig. 1 can be covered by mixing and matching such instances. We combine this view with recognition models for dealing with partial observations, and apply this empirically.

6. Experiments

We demonstrate the ability of the proposed approach to learn dynamics from partial observations with varying degrees of prior knowledge, as illustrated in Fig. 1. As discussed above, previous works on enforcing physical knowledge in NODEs consider full state measurements (Yin et al., 2021; Massaroli et al., 2020a; Zhong et al., 2020). On the other hand, few works do consider partial observations (Schlaginhaufen et al., 2021; Rubanova et al., 2019; Ayed et al., 2020), but they do not enforce physical priors. Therefore, we cannot directly compare our approach that combines partial observations and physical knowledge to existing baselines. Instead, we provide an extensive case study on the harmonic oscillator, which is often used in the literature, and demonstrate the ability of structured NODEs to learn dynamics from partial measurements with increasing priors. We also investigate the performance of the proposed recognition methods on simulations of two nonlinear systems. Finally, we apply our approach to a real-world, complex use case obtained on a robotic exoskeleton.

6.1. Benchmark of recognition models

We demonstrate that the proposed recognition models can estimate the initial condition of a system from partial and noisy observations of two systems. The first is a simplified model of the dynamics of a two-story building during an earthquake (Winkel, 2017; Karlsson & Svanström, 2019) with $d_x = 4$, $d_y = 1$. The second is the FitzHugh-Nagumo model, a simplified representation of a spiking neuron subject to a constant stimulus (Clairon & Samson, 2020) with $d_x = 2$, $d_y = 1$. The dynamics models are considered known, including the perturbation caused by the earthquake, up to a few parameters optimized jointly with $\psi$. This ensures that while dynamical parameters and recognition model are learned together, $x(0)$ is estimated in the physical coordinates, such that we can compare it to the ground truth.

2Implementation details are provided in the supplementary material and code to reproduce the experiments is available.
We train ten direct, forward KKL and backward KKL recognition models on a synthetic dataset obtained from simulations of an autonomous harmonic oscillator with unknown frequency. The system is as follows:

\[ \dot{x}_1 = x_2, \quad \dot{x}_2 = -\omega^2 x_1, \] (11)

where \( \omega^2 > 0 \) is the unknown frequency of the oscillator and \( y = x_1 \) is measured, corrupted by Gaussian noise of standard deviation \( \sigma = 0.01 \) (resp. \( \sigma = 0.02 \)), \( t_c = 1.2 \) s, and we compute the RMSE on the predictions of hundred test trajectories. The results are presented in Fig. 2. They indicate that the more compressed structure from observer design helps build a more effective recognition model. The direct method with \( t_c = 0 \) was also trained but is not shown here, since it leads to much higher error as it does not verify the observability assumption.

### 6.2. Harmonic oscillator with increasing priors

We now illustrate structured NODEs with KKL-based recognition models on a synthetic dataset obtained from simulations of an autonomous harmonic oscillator with unknown frequency. The system is as follows:

\[ \dot{x}_1 = x_2, \quad \dot{x}_2 = -\omega^2 x_1, \] (11)

where \( \omega^2 > 0 \) is the unknown frequency of the oscillator and \( y = x_1 \) is measured, corrupted by Gaussian noise of standard deviation \( \sigma = 0.01 \). Various designs have been proposed to identify both the state and the model, i.e., the frequency, for example subspace methods, or an extended state-space model with a nonlinear observer; see Praly et al. (2006) and references therein. We demonstrate that structured NODEs can solve this problem while enforcing increasing physical knowledge. The results are illustrated in Fig. 3 with a backward KKL recognition model, \( \omega = 1 \), \( N = 20 \) trajectories of 3 s for training and 30 s for testing.

First, the NODE is trained without any structure (a) as in (4), which leads to one of many possible state-space models: it fits the observations in \( x_1 \) but finds another coordinate system for the unmeasured state, as expected for general latent NODEs. It also does not conserve energy. Then, we enforce a Hamiltonian structure (b) as in (10) with \( x_1 = q \), \( x_2 = p \). This leads to a dynamics model again in another coordinate system, but that conserves energy: we learn the dynamics up to a symplectomorphism (Bertalan et al., 2019). We then impose \( \dot{x}_1 = x_2 \) and only learn \( \dot{x}_2 = -\nabla H(x_1) \) (c) in (10). This enforces a particular choice of Hamiltonian dynamics, such that the obtained model conserves energy and stays in the physical coordinate system \( (x_1 \text{ position}, x_2 \text{ velocity}) \). Imposing even more structure, we only optimize the unknown frequency \( \omega^2 \) jointly with the recognition model, while the rest of the dynamics are considered known (d). Another possibility is to consider the extended state-space model where \( x_3 = \omega^2 \) has constant dynamics (e). In that case, only a recognition model needs to be trained; however, \( x(0) \in \mathbb{R}^3 \) including the frequency is estimated for each trajectory, such that this formulation is much more open. Both (d) and (e), which correspond to the right end of the spectrum in Fig. 1, also lead to energy conserving trajectories in the physical coordinates.

These results illustrate that structured NODEs can flexibly incorporate gradual priors for learning dynamics from partial and noisy observations. Note that standard methods tailored to the harmonic oscillator may perform better, however, they are usually not as general nor as flexible.

### 6.3. Experimental dataset from robotic exoskeleton

We demonstrate the performance of the proposed framework on a real-world dataset. We use a set of measurements collected from a robotic exoskeleton at Wandercraft, presented in Vigne (2021) and Fig. 5. This robot features mechanical deformations at weak points of the structure that are neither captured by Computer-Assisted Design modelling nor measured by encoders. These deformations, when measured by a motion capture device, can be shown to account for significant errors in foot placement. Further, they exhibit nonlinear spring-like dynamics that complicate control...
design. The dataset is obtained by fixing the robot basin to a wall and sending a sinusoidal excitation to the front hip motor at different frequencies. The sagittal hip angle is measured by an encoder, while the angular velocity of the thigh is measured by a gyroscope. In Vigne (2021), first results are obtained using linear system identification: the observed deformation is modeled as a linear spring in the hip, and this model is linearized around an equilibrium point, then its parameters are estimated. These estimates are sufficient for tuning a robust controller to compensate for the deformation. We aim to learn a more accurate model of this dynamical system of dimension $d_z = 4$, where $y = (x_1, x_4)$, by identifying the nonlinear deformation terms.

We investigate three settings: no structure, imposing $\dot{x}_1 = x_2$ and $\dot{x}_3 = x_4$, and learning the residual of the prior linear model on top of this structure. In each setting, we learn from $N = 265$ trajectories of length 0.2 s in a subset of input frequencies. One test trajectory in the trained regime is shown in Fig. 11 and illustrates the data fitting capabilities.

These experiments demonstrate that structured NODEs combined with recognition models can identify real-world nonlinear systems from partial and noisy observations. The obtained models can fit data from a complex nonlinear system excited with different input frequencies, and somewhat generalize to unseen frequencies. The predictions are not perfect, but much more accurate than those of the prior model, as seen in Fig. 11; this is enough to be used in closed-loop tasks such as control or monitoring. Imposing $\dot{x}_{1/3} = x_{2/4}$ leads to similar performance as without structure, but a physically meaningful state-space representation that can be interpreted in terms of position and velocity. Due to the inaccurate predictions of the prior model, learning its residuals leads to lower performance.

7. Conclusion

The general formulation of NODEs makes them well-suited for nonlinear system identification. However, learning physically sound dynamics in realistic settings, i.e., with control inputs and partial, noisy observations, remains challenging. We view the NODE problem formulation as a flexible framework in which a wide spectrum of physical priors can be embedded, by combining the literature or other insights to match all available knowledge. We propose novel recognition models based on nonlinear observer design to efficiently link the observations to the latent state. Such structured NODEs can learn physically interpretable models in realistic settings, as illustrated on a real-world dataset.

For any of the proposed recognition methods, the model $\psi$ could be designed as a more complex encoder than a feed-forward NN (Shankar et al., 2021; Chalvidal et al., 2021; Rubanova et al., 2019). This does not change the approach itself, but modifies the design and adds terms to the cost function. In that case, we expect $\psi$ to be harder to learn; hence, we focus on simpler models in this paper.
Also, NODEs can be combined with Convolutional Neural Networks to capture spatial dependencies and learn Partial Differential Equations (PDEs) instead of ODEs, as investigated in Dulny et al. (2021); Xu et al. (2021). We only consider dynamical systems that can be modeled by ODEs, but expect the proposed approach to extend to PDEs.

Software and Data

Implementation details are provided in the supplementary material. Code to reproduce all of the results is available at https://anonymous.4open.science/r/structured_NODEs-7C23.

References

Alexe, M. and Sandu, A. Forward and adjoint sensitivity analysis with continuous explicit Runge-Kutta schemes. *Applied Mathematics and Computation*, 208(2):328–346, 2009.

Aliee, H., Theis, F. J., and Kilbertus, N. Beyond Predictions in Neural ODEs: Identification and Interventions. *arXiv preprint arXiv:2106.12430*, 2021.

Andrieu, V. and Praly, L. On the existence of a Kazantzis-Kravaris/Luenberger observer. *SIAM Journal on Control and Optimization*, 45(2):422–456, 2006.

Ayed, I., Bezenac, E. D., Pajot, A., and Gallinari, P. Learning the Spatio-Temporal Dynamics of Physical Processes from Partial Observations. In *Proceedings of the IEEE International Conference on Acoustics, Speech and Signal Processing*, pp. 3232–3236, 2020.

Bernard, P. Observer Design for Nonlinear Systems. In *Lecture Notes in Control and Information Sciences*, volume 479. Springer International Publishing, 2019.

Bernard, P. and Andrieu, V. Luenberger Observers for Nonautonomous Nonlinear Systems. *IEEE Transactions on Automatic Control*, 64(1):270–281, 2019.

Bertalan, T., Dietrich, F., Mezić, I., and Kevrekidis, I. G. On learning Hamiltonian systems from data. *Chaos*, 29(12), 2019.

Bevanda, P., Beier, M., Kerz, S., Lederer, A., Sosnowski, S., and Hirche, S. KoopmanizingFlows: Diffeomorphically Learning Stable Koopman Operators. *arXiv preprint arXiv:2112.04085*, 2021.

Buisson-Fenet, M., Morgenthaler, V., Trimpe, S., and Di Meglio, F. Joint state and dynamics estimation with high-gain observers and Gaussian process models. *IEEE Control Systems Letters*, 5(5):1627–1632, 2021.

Chalvidal, M., Ricci, M., VanRullen, R., and Serre, T. Go with the Flow: Adaptive Control for Neural ODEs. In *Proceedings of the International Conference on Learning Representations*, 2021.

Chen, R. T., Rubanova, Y., Bettencourt, J., and Duvenaud, D. Neural Ordinary Differential Equations. In *Advances in Neural Information Processing Systems 32*, pp. 6572–6583, 2018.

Clairon, Q. and Samson, A. Optimal control for estimation in partially observed elliptic and hypoelliptic linear stochastic differential equations. *Statistical Inference for Stochastic Processes*, 23:105–127, 2020.

Cranmer, M., Greydanus, S., Hoyer, S., Battaglia, P., Spergel, D., and Ho, S. Lagrangian Neural Networks. In *ICLR 2020 Workshop on Integration of Deep Neural Models and Differential Equations*, 2020.

da Costa Ramos, L., Di Meglio, F., Figuiera da Silva, L. F., Bernard, P., and Morgenthaler, V. Numerical design of Luenberger observers for nonlinear systems. In *Proceedings of the 59th Conference on Decision and Control*, pp. 5435–5442, 2020.

de Brouwer, E., Simm, J., Arany, A., and Moreau, Y. GRU-ODE-Bayes: Continuous modeling of sporadically-observed time series. In *Advances in Neural Information Processing Systems 33*, 2019.

Doerr, A., Daniel, C., Nguyen-Tuong, D., Marco, A., Schaal, S., Toussaint, M., and Trimpe, S. Optimizing long-term predictions for model-based policy search. *Proceedings of the 1st Conference on Robot Learning*, 78:227–238, 2017.

Doerr, A., Daniel, C., Schiegg, M., Nguyen-Tuong, D., Schaal, S., Toussaint, M., and Trimpe, S. Probabilistic recurrent state-space models. *Proceedings of the 35th International Conference on Machine Learning*, pp. 1280–1289, 2018.

Doyeon, T., Thomas, K., Luo, Z., Pillow, J. W., and Brody, C. D. Inferring Latent Dynamics Underlying Neural Population Activity via Neural Differential Equations. In *Proceedings of the 38th International Conference on Machine Learning*, pp. 5551–5561, 2021.

Dulny, A., Hotho, A., and Krause, A. NeuralPDE: Modelling Dynamical Systems from Data. 2021.

Eichelsdörfer, J., Kaltenbach, S., and Koutsourelakis, P.-S. Physics-enhanced Neural Networks in the Small Data Regime. *Workshop on Machine Learning and the Physical Sciences (NeurIPS 2021)*, 2021.
Eleftheriadis, S., Nicholson, T. F., Deisenroth, M. P., and Hensman, J. Identification of Gaussian process state space models. In Advances in Neural Information Processing Systems 31, pp. 5310–5320, Long Beach, California, 2017.

Ensinger, K., Solowjow, F., Tiemann, M., and Trimpe, S. Structure-preserving Gaussian Process Dynamics. arXiv preprint arXiv:2102.01606, 2022.

Galioto, N. and Gorodetsky, A. A. Bayesian system ID: optimal management of parameter, model, and measurement uncertainty. Nonlinear Dynamics, 102:241–267, 2020.

Greydanus, S., Dzamba, M., and Yosinski, J. Hamiltonian Neural Networks. In Advances in Neural Information Processing Systems 33, 2019.

Janny, S., Andrieu, V., Nadri, M., and Wolf, C. 2021.

Kailath, T. Linear Systems. Prentice Hall PTR, Englewood Cliffs, New Jersey, 1980.

Karlsson, D. and Svanström, O. Modelling Dynamical Systems Using Neural Ordinary Differential Equations, Master’s thesis in Complex Adaptive Systems, Department of Physics, Chalmers University of Technology, 2019.

Kingma, D. P. and Ba, J. L. Adam: A method for stochastic optimization. In Proceedings of the 3rd International Conference on Learning Representations, 2015.

Legaad, C. M., Schranz, T., Schweiger, G., Drgoňa, J., Falay, B., Gomes, C., Iosifidis, A., Abkar, M., and Larsen, P. G. Constructing Neural Network-Based Models for Simulating Dynamical Systems. ACM Computing Surveys, 1(1), 2021.

Ljung, L. System Identification: Theory for the User. Prentice Hall PTR, Englewood Cliffs, New Jersey, 1987.

Lusch, B., Kutz, J. N., and Brunton, S. L. Deep learning for universal linear embeddings of nonlinear dynamics. Nature Communications, 9, 2018.

Manek, G. and Kolter, Z. Learning stable deep dynamics models. In Advances in Neural Information Processing Systems, 2019.

Massaroli, S., Poli, M., Bin, M., Park, J., Yamashita, A., and Asama, H. Stable Neural Flows. arXiv preprint arXiv:2003.08063, 2020a.

Massaroli, S., Poli, M., Park, J., Yamashita, A., and Asama, H. Dissecting neural ODEs. In Advances in Neural Information Processing Systems 34, pp. 3952–3963, 2020b.

Mehta, V., Char, I., Neiswanger, W., Chung, Y., Schneider, J., Nelson, A. O., Boyer, M. D., and Kolemen, E. Neural Dynamical Systems. In International Conference on Learning Representations - Integration of Deep Neural Models and Differential Equations Workshop, 2020.

Nelles, O. Nonlinear System Identification. Springer, Berlin, Heidelberg, 2001.

Nguyen-Tuong, D. and Peters, J. Model learning for robot control: A survey. Cognitive Processing, 12:319–340, 2011.

Norcliffe, A., Bodnar, C., Day, B., Simidjievski, N., and Liô, P. On second order behaviour in augmented neural ODEs. In The Symbiosis of Deep Learning and Differential Equations Workshop (NeurIPS 2021), 2021.

Praly, L., Marconi, L., and Isidori, A. A new observer for an unknown harmonic oscillator. In Proceedings of the 17th International Symposium on Mathematical Theory of Networks and Systems, pp. 996–1001, 2006.

Rath, L., Geist, A. R., and Trimpe, S. Using Physics Knowledge for Learning Rigid-body Forward Dynamics with Gaussian Process Force Priors. In Proceedings of the 5th Conference on Robot Learning, pp. 101–111, 2021.

Raue, A., Schilling, M., Bachmann, J., Matteson, A., Schelke, M., Kaschek, D., Hug, S., Kreutz, C., Harms, B. D., Theis, F. J., Klingmüller, U., and Timmer, J. Lessons Learned from Quantitative Dynamical Modeling in Systems Biology. PLoS ONE, 8(9), 2013.

Ribeiro, A. H., Tiels, K., Umenberger, J., Schön, T. B., and Aguirre, L. A. On the smoothness of nonlinear system identification. Automatica, 121, 2020.

Rubanova, Y., Chen, R. T., and Duvenaud, D. Latent ODEs for irregularly-sampled time series. In Advances in Neural Information Processing Systems 33, 2019.

Schittkowski, K. Numerical Data Fitting in Dynamical Systems. Springer, Boston, MA, 2002.

Schlaginhaufen, A., Wenk, P., Krause, A., and Dörfler, F. Learning Stable Deep Dynamics Models for Partially Observed or Delayed Dynamical Systems. In Advances in Neural Information Processing Systems 35, 2021.

Schoukens, J. and Ljung, L. Nonlinear System Identification: A User-Oriented Roadmap. IEEE Control Systems Magazine, 39(6):28–99, 2019.

Shankar, V., Portwood, G. D., Mohan, A. T., Mitra, P. P., Krishnamurthy, D., Rackauckas, C., Wilson, L. A., Schmidt, D. P., and Viswanathan, V. Validation and parameterization of a novel physics-constrained neural dynamics
model applied to turbulent fluid flow. *arXiv preprint arXiv:2110.11528*, 2021.

Shtessel, Y., Edwards, C., Fridman, L., and Levant, A. Sliding Mode Control and Observation. In *Control Engineering*. Birkhäuser, New York, 2016.

Sjöberg, J., Zhang, Q., Ljung, L., Benveniste, A., Delyon, B., Glorennec, P. Y., Hjalmarsson, H., and Juditsky, A. Nonlinear black-box modeling in system identification: a unified overview. *Automatica*, 31(12):1691–1724, 1995.

Viberg, M. Subspace-based methods for the identification of linear time-invariant systems. *Automatica*, 31(12):1835–1851, 1995.

Vigné, M. *Estimation and Control of the Deformations of an Exoskeleton using Inertial Sensors*. PhD thesis, Mines ParisTech - Université PSL, 2021.

Villaverde, A. F., Pathirana, D., Fröhlich, F., Hasenauer, J., and Banga, J. R. A protocol for dynamic model calibration. *arXiv preprint arXiv:1902.11136*, 2021.

Wang, R. and Yu, R. Physics-Guided Deep Learning for Dynamical Systems: A survey. *arXiv preprint arXiv:2107.01272*, 2021.

Winkel, B. 2017-Gustafson, G. B. - Differential Equations Course Materials, 2017. URL https://www.simiode.org/resources/3892.

Wu, J. L., Michelén-Ströfer, C., and Xiao, H. Physics-informed covariance kernel for model-form uncertainty quantification with application to turbulent flows. *Computers and Fluids*, 193, 2019.

Xu, X., Hasan, A., Elkhalil, K., Ding, J., and Tarokh, V. Characteristic Neural Ordinary Differential Equations. *arXiv preprint arXiv:2111.13207*, 2021.

Yin, Y., Le Guen, V., Dona, J., de Bézenac, E., Ayed, I., Thome, N., and Gallinari, P. Augmenting physical models with deep networks for complex dynamics forecasting. In *Proceedings of the 9th International Conference on Learning Representations*, 2021.

Zhong, Y. D., Dey, B., and Chakraborty, A. Symplectic ODE-Net: Learning Hamiltonian Dynamics with Control. In *International Conference on Learning Representations*, 2020.
8. Supplementary Material

8.1. More detailed background on KKL observers

We recall the main existence results on KKL observers. Correctly stating these results requires more formalism than what is used in the main body of the paper. However, the assumptions and the reasoning are identical. We start with the main existence result on autonomous systems, then recall the extension to nonautonomous systems.

8.1.1. Autonomous Systems

Consider the following autonomous nonlinear dynamical system

\[ \dot{x} = f(x), \quad y = h(x) \tag{12} \]

where \( x \in \mathbb{R}^{d_x} \) is the state, \( y \in \mathbb{R}^{d_y} \) is the measured output, \( f \) is a \( C^1 \) function and \( h \) is a continuous function. The goal of observer design is to compute an estimate of the state \( x(t) \) using the past values of the output \( y(s), \ 0 \leq s \leq t \). We make the following assumptions:

**Assumption 1** There exists a compact set \( \mathcal{X} \) such that for any solution \( x \) of (18), \( x(t) \in \mathcal{X} \ \forall \ t \geq 0 \).

**Assumption 2** There exists an open bounded set \( \mathcal{O} \) containing \( \mathcal{X} \) such that (18) is backward \( \mathcal{O} \)-distinguishable on \( \mathcal{X} \), i.e., for any trajectories \( x_a \) and \( x_b \) of (18), there exists \( t > 0 \) such that for any \( t \geq \ell \) such that \( (x_a(t), x_b(t)) \in \mathcal{X} \times \mathcal{X} \) and \( x_a(t) \neq x_b(t) \), there exists \( s \in [t - \ell, t] \) such that

\[ h(x_a(s)) \neq h(x_b(s)) \]

and \( (x_a(\tau), x_b(\tau)) \in \mathcal{O} \times \mathcal{O} \) for all \( \tau \in [s, t] \). In other words, their respective outputs become different in backward finite time before leaving \( \mathcal{O} \).

This is the assumption of backward distinguishability, i.e., Definition 1 but in backward time. It means that the current state is uniquely determined by the past values of the output. On the contrary, (forward) distinguishability means that the initial state is uniquely determined by the future values of the output. If the solutions of (18) are unique, e.g., if \( f \) is \( C^1 \), then these two notions are equivalent.

The following Theorem derived in (Andrieu & Praly, 2006) proves the existence of a KKL observer.

**Theorem 1** (Andrieu & Praly, 2006) Suppose Assumptions 1 and 2 hold. Define \( d_z = d_y(d_x + 1) \). Then, there exists \( \ell > 0 \) and a set \( S \) of zero measure in \( \mathbb{C}^{d_z} \), such that for any matrix \( D \in \mathbb{R}^{d_x \times d_z} \), with eigenvalues \( \lambda_1, \ldots, \lambda_{d_z} \) in \( \mathbb{C}^{d_z} \) \( \setminus \ S \), with \( \operatorname{Re} \lambda_i < -\ell \), and any \( F \in \mathbb{R}^{d_y \times d_z} \) such that \( (D, F) \) is controllable, there exists an injective mapping \( T : \mathbb{R}^{d_z} \to \mathbb{R}^{d_z} \) that satisfies the following equation on \( \mathcal{X} \)

\[ \frac{\partial T}{\partial x}(x)f(x) = DT(x) + Fh(x), \tag{13} \]

and its pseudo-inverse \( T^* : \mathbb{R}^{d_z} \to \mathbb{R}^{d_x} \) such that the trajectories of (18) remaining in \( \mathcal{X} \) and any trajectory of

\[ \dot{z} = Dz + Fy \tag{14} \]

satisfy

\[ |z(t) - T(x(t))| \leq M |z(0) - T(x(0))| e^{-\lambda_{\min} t} \tag{15} \]

for some \( M > 0 \) and with

\[ \lambda_{\min} = \min \{ |\operatorname{Re} \lambda_1|, \ldots, |\operatorname{Re} \lambda_{d_z}| \}. \tag{16} \]

This yields

\[ \lim_{t \to +\infty} |x(t) - T^*(z(t))| = 0. \tag{17} \]

8.1.2. Nonautonomous systems

These results are extended to nonautonomous systems in (Bernard & Andrieu, 2019). The system equations are then

\[ \dot{x} = f(x, u), \quad y = h(x, u) \tag{18} \]

where \( u \in \mathcal{U} \) is the input. Assumption 2 naturally extends to nonautonomous systems if it is true for any fixed input \( u \) of interest. The following Theorem proves the existence of a KKL observer in the nonautonomous case under the weak assumption of backward distinguishability.

**Theorem 2** (Bernard & Andrieu, 2019) Take some fixed input \( u \in \mathcal{U} \). Suppose Assumptions 1 and 2 hold for this \( u \) with a certain \( \ell_u \geq 0 \). Define \( d_z = d_y(d_x + 1) \). Then, there exists a set \( S \) of zero measure in \( \mathbb{C}^{d_z} \), such that for any matrix \( D \in \mathbb{R}^{d_x \times d_z} \), with eigenvalues \( \lambda_1, \ldots, \lambda_{d_z} \) in \( \mathbb{C}^{d_z} \setminus S \), with \( \operatorname{Re} \lambda_i < -\ell_u \), and any \( F \in \mathbb{R}^{d_y \times d_z} \) such that \( (D, F) \) is controllable, there exists a mapping \( T_u : \mathbb{R} \times \mathbb{R}^{d_z} \to \mathbb{R}^{d_z} \) that satisfies the following equation on \( \mathcal{X} \)

\[ \frac{\partial T_u}{\partial x}(t, x)f(x, u(t)) + \frac{\partial T_u}{\partial t}(x) = DT_u(t, x) + Fh(x, u(t)), \tag{19} \]

and a mapping \( T_u^* : \mathbb{R} \times \mathbb{R}^{d_z} \to \mathbb{R}^{d_x} \) such that \( T_u(t, \cdot) \) and \( T_u^*(t, \cdot) \) only depend on the past values of \( u \) on \( [0, t] \), and \( T_u(t, \cdot) \) is injective \( \forall \ t \geq t_u \) with a left-inverse \( T_u^*(t, \cdot) \) on \( \mathcal{X} \). Then, the trajectories of (18) remaining in \( \mathcal{X} \) and any trajectory of

\[ \dot{z} = Dz + Fy, \tag{20} \]
This yields
\[ |z(t) - T_u(t, x(t))| \leq M |z(0) - T_u(0, x(0))| e^{-\lambda_{\min} t} \] (21)
for some \( M > 0 \) and with
\[ \lambda_{\min} = \min \{ |\text{Re} \lambda_1|, \ldots, |\text{Re} \lambda_{d_1}| \}. \] (22)

This yields
\[ \lim_{t \to +\infty} |x(t) - T_u^*(t, z(t))| = 0. \] (23)

### 8.2. Implementation details

We demonstrate the proposed method in several numerical experiments and one experimental dataset obtained on a robotic exoskeleton. When comparing different recognition models, we investigate the direct method \( \bar{z}(t_c) = y_0 z_c \), the KKL method \( \bar{z}(t_c) = (z(t_c), u_0, t_c) \) forward and backward in time with \( d_z = d_y (d_x + 1) \), and the functional KKL method (denoted KKLu) \( \bar{z}(t_c) = z(t_c) \) forward and backward in time with \( d_z = (d_y + d_u) (d_x + d_\omega + 1) \). When the KKL observer is used forward in time, we solve the ODE on \( z \) forward in time on \([0, t_c]\) and learn the mapping from \( \bar{z}(t_c) \) to \( x(0) \), then only use the samples \( y(t_f) \) for \( t_f > t_c \) to train the NODE model. When the KKL observer is used backward in time, we solve the ODE on \( z \) backward in time on \([t_c, 0]\) and learn the mapping from \( z(0) \) to \( x(0) \), then use all samples to train the NODE model.

In all cases, the choice of \( D \) is important for the KKL-based recognition models. We set \( F = I_{d_x \times d_u} \) and \( D \) with the following method. We compute the poles \( p_i \) of a Butterworth filter of order \( d_z \) and cut-off frequency \( 2\pi \omega_c \) and set each block of \( D \) as
\[
D_i = \begin{cases} 
  p_i & \text{if } p_i \text{ is real} \\
  \text{Re}(p_i), \text{Im}(p_i) & \text{if } p_i \text{ is complex}
\end{cases} \]
(24)
such that \( D \) is a block-diagonal matrix, and its eigenvalues are the poles of the filter. For each considered system and for each considered method, we then optimize \( D \) once jointly with all other parameters once, then re-use the obtained value of \( D \) for all corresponding experiments. This choice ensures that the pair \((D, F)\) is controllable and that \( D \) is Hurwitz and has physically meaningful eigenvalues. Other possibilities exist, such as choosing \( D \) in companion form, as a negative diagonal... However, we found that this strategy leads to the best performance for the considered use cases. We pick \( \omega_c = 1 \) for the systems of the recognition model benchmark and the harmonic oscillator with unknown frequency. For the experimental dataset, we pick \( D = \text{diag}(-1, \ldots, -d_z) \). However, this choice is somewhat arbitrary, and the previous method with \( \omega_c = 10 \) had similar performance.

### 8.2.1. Benchmark of recognition models

We demonstrate on two numerical systems that an NN-based recognition model can estimate the initial state of a dynamical system from partial measurements. For reproducibility, we generate the training data from simulation and choose systems that can be tested again with reasonable computational overhead.

**Earthquake model** A simplified model of the effects of an earthquake on a two-story building is presented in (Winkel, 2017), and an NODE is trained for it in (Karlsson & Svanström, 2019). This linear model can be written as

\[
\dot{x}_1 = x_2 \\
\dot{x}_2 = \frac{k}{m} (x_3 - 2x_1) - F_0 \omega^2 \cos(\omega t) \\
\dot{x}_3 = x_4 \\
\dot{x}_4 = \frac{k}{m} (x_1 - x_3) - F_0 \omega^2 \cos(\omega t) \\
y = x_1 + \epsilon,
\]
(25)

where \( x_1 \) and \( x_3 \) are the positions of the first and second floor respectively, \( x_2 \) and \( x_4 \) their velocities, \( F_0 \omega^2 \cos(\omega t) \) is the perturbation caused by the earthquake and only \( x_1 \) is observed with Gaussian noise of variance \( \sigma^2 = 10^{-4} \). We consider the oscillation caused by the earthquake as a disturbance, which is known when computing trajectories (because the dynamics model is assumed to be entirely known), but unknown to the recognition model: we estimate \( x(0) \) from \( y_0; t_c \) only.

We aim to learn a recognition model that estimates \( x(0) \) using only \( y_0; t_c \) with the methods described above. We set \( t_c = 40 \times \Delta t = 40 \times 0.03 = 1.2 \) s which seems to be enough to reconstitute the initial condition (after trial and error), \( N = 50 \) (each sample corresponds to a random initial condition, random \( F_0 \) and random \( \omega \)), \( n = 100 \), and design \( \psi \) as a fully connected feed-forward network, i.e., a multi-layer perceptron, with two hidden layers containing 50 neurons each, and two fully connected input and output layers with bias terms. We notice that \( t_c \) large enough and enough parameters in \( \psi \), i.e., enough flexibility of the model, are needed for good generalization performance. Also, we pick the sampling time \( \Delta t = 0.03 \) s low enough such that the obtained trajectories are reasonably smooth, otherwise analyzing the results quantitatively becomes hard due to interpolation errors getting too large.

We train the recognition model with each proposed method and evaluate the results on 100 test trajectories of random initial conditions and random input oscillation. The results on one such test trajectory are illustrated in Figure 6. We evaluate the different recognition models by computing the RMSE on the estimation of the initial condition and of the
We conduct the same tests while also optimizing $k/m$, the main parameter of the dynamics model. In our example, we have $k/m = 10$, but we initialize this variable to a random value in $[8, 12]$ and optimize it jointly with the recognition model. As usual, this problem is not well-posed and there are many local optima. Therefore, we can only hope to converge to a good estimate by starting from a reasonable guess of the main parameter. We keep everything else fixed, including the optimization routine, which might not be the best choice as it has been shown that for parametric optimization, trust region optimization routines with multiple starts often lead to better results (Raue et al., 2013). The results are shown in Figure 7 (bottom row) and in the main body of the paper. We observe that the KKL-based models achieve higher performance, which seems to indicate that the optimization problem based on $z(t)$ is better conditioned than that based on $y(t)$. 

**FitzHugh-Nagumo model** This model represents a relaxation oscillation in an excitable system. It is a simplified representation of the behavior of a spiking neuron: an external stimulus is received, leading to a short, nonlinear increase of membrane voltage then a slower, linear recovery.

$$\ddot{y} = \frac{1}{\epsilon} (v - v^3 - u) + I_{ext}$$

$$\dot{u} = \gamma v - u + \beta$$

$$y = v + \epsilon,$$

where $v$ is the membrane potential, $u$ is the value of the recovery channel, $I_{ext}$ is the value of the external stimulus (here a constant), $\epsilon = 0.1$ is a time scale parameter, and $\gamma = 1.5$, $\beta = 0.8$ are kinetic parameters. Only $v$ is measured, corrupted by Gaussian measurement noise $\epsilon$ of variance $\sigma^2 = 5 \times 10^{-4}$.

Our aim is to learn a recognition model that estimates $(v(0), u(0))$ using $y(t)$, and $I_{ext}$ with the methods described above. We set $t_c = 40 \times \Delta t = 40 \times 0.03 = 1.2$ s, $N = 50$ for 50 random initial conditions and external stimulus, $n = 100$, and design $\psi$ as a fully connected feedforward network, i.e., a multi-layer perceptron, with two hidden layers containing 50 neurons each, and two fully connected input and output layers with bias terms.

We train the recognition model with each proposed method and evaluate the results on 100 test trajectories with random initial conditions and random stimulus. The results on one such test trajectory are illustrated in Figure 8. We evaluate...
the different recognition models as above; we show the corresponding box plots in Figure 9 (top row). This time, we observe that the forward KKL method leads to slightly better results than the direct method, but the backward KKL method to slightly worse results. However, the obtained performances are very close, and these differences might not be significant.

We also combine the previous experiments with the estimation of the main dynamic parameters $\epsilon, \beta, \gamma$ which are initialized randomly in $[0.05, 0.15]$, $[0.75, 2.25]$ and $[0.4, 1.2]$ respectively. The results are illustrated in Figure 9 (bottom row) and in the main body of the paper. We observe once again that the KKL-based methods lead to lower error when jointly optimizing $\psi$ and the dynamical parameters.

### 8.2.2. Synthetic Dataset: Harmonic Oscillator with Unknown Frequency

We demonstrate the performance of structured NODEs to learn the dynamics of a harmonic oscillator with unknown frequency from partial observations with varying degrees of structure. We train on $N = 20$ trajectories from 20 random initial states in $[-1, 1]^2$ and frequency $\omega^2 = 1$ Hz (i.e., period 6.3 s), of $n = 50$ time steps each for an overall length of 3 s, corrupted by Gaussian measurement noise of variance $\sigma^2 = 10^{-4}$. We use $t_c = 20 \times \Delta t = 1.2$ s for the recognition model. We optimize the parameters using Adam (Kingma & Ba, 2015) and a learning rate of 0.005.

The obtained results are depicted in Figure 10 with the backward KKL recognition model. We show the prediction of a random test trajectory with random initial state: $y_0 x t_c$ is measured for this trajectory, used by the recognition model to estimate $x(0)$. Then, the learned NODE is simulated to predict the whole state trajectory for 500 time steps, i.e., ten times longer than the training time.

### No Structure

We start without imposing any structure, i.e., learning a general latent NODE model of the system as in (4). The NODE fits the observations $y = x_1$, but not $x_2$ as it has learned the dynamics in another coordinate system, which is expected for general latent NODEs. It also does not conserve energy, which is not surprising when no structure is imposed, as discussed e.g., in (Greydanus et al., 2019).

### Hamiltonian State-Space Model

We now assume the user has some physical insight about the system at hand: it derives from a Hamiltonian function, i.e., there exists $H$ such that

$$
\begin{align*}
\dot{x}_1 &= \frac{\partial H}{\partial x_2}(x), \\
\dot{x}_2 &= -\frac{\partial H}{\partial x_1}(x).
\end{align*}
$$

(27)

We approximate $H$ directly with a NN $H_\theta$ of weights $\theta$, such that the NODE has form (27), and inject this into the optimization problem as in (10). This formulation enforces the constraint that the dynamics derive from a Hamiltonian function, whose choice is free. In that case, we do not necessarily find the "physical" state-space realization, as several Hamiltonian functions can fit the data. However, the obtained state-space model conserves energy due to the Hamiltonian structure.
We optimize the weights $\theta$ where $\omega > 0$ is the unknown frequency. We approximate $\omega$ with a parameter $\theta$, which is initialized randomly in $[0.5, 2]$. We optimize the weights $\theta_v$ and $\theta$ jointly. We obtain excellent results with this method, as $\theta$ is estimated correctly up to $10^{-2}$ and the trained recognition model gives satisfying results. This demonstrates that our framework can recover both the dynamics and the recognition model in the physical coordinates imposed by the parametric model from partial and noisy measurements in this simple use case.

Extended state-space model We now consider the extended state-space model
\begin{equation}
\begin{aligned}
\dot{x}_1 &= x_2, \\
\dot{x}_2 &= -\omega^2 x_1,
\end{aligned}
\end{equation}
where $x_3 = \omega^2$ is a constant state representing the unknown frequency. In this case, the dynamics are completely known and only the recognition is left to train, in order to estimate the initial condition $x(0) \in \mathbb{R}^3$, where $x_3(0)$ is the unknown frequency. This is the same degree of structure as the parametric model: the dynamics are known up to the frequency. However, it also is a more open problem: since we are learning a recognition model for $x(0) \in \mathbb{R}^3$, at each new trajectory, we estimate a new value of the frequency $x_3(0)$, which was considered the same across all trajectories for the previous methods. Therefore, with this setting, we also obtain models that can predict energy-preserving trajectories in the physical parameters, but with lower accuracy due to this extra degree of freedom.

For a more quantitative comparison, we compute the RMSE on the prediction of $y = x_1$ over hundred random test trajectories. We obtain for the considered settings, in mean over ten training rounds: 0.28 for (a), 0.15 for (b), 0.07 for (c), 0.09 for (d), 0.28 for (e) as in Fig. 10. These results are coherent with the intuition that adding structure into the NODE framework leads to better prediction capabilities: with strong priors, the obtained model is not only physically interpretable but also has higher output prediction accuracy. The error is of the same order of magnitude for settings (c) and (d), even though the priors are stronger in (d): this is due to the fact that our method is not directly tailored for parametric model estimation (see (Raue et al., 2013; Villaverde et al., 2021) for settings that are more adapted to parameter estimation). Only the extended state-space model exhibits higher output prediction error. This can be explained by the fact that we do not impose that $\omega$ be constant across all training and test trajectories, as discussed above.

Figure 10: Random test trajectory of the trained NODE for the harmonic oscillator: without imposing any structure (a), imposing Hamiltonian dynamics (b), imposing $\dot{x}_1 = x_2$ (c), directly identifying a parametric model (d) and learning a recognition model of an extended state-space representation where $x_3 = \omega^2$ (e). We show the true and predicted trajectories of $x_1$ (top) and $x_2$ (bottom).
8.2.3. Experimental Case Study on a Robotic Exoskeleton

We use a set of measurements collected at Wandercraft on one of their exoskeletons and presented in (Vigne, 2021). More details on the robot, the dataset and the methods applied at Wandercraft are provided in Section 4.1.2.1 of (Vigne, 2021).

For this experiment, the robot basin is fixed to the wall and low amplitude sinusoidal inputs are sent to the front hip motor with different frequencies between 2 Hz and 16 Hz. A linear model has been identified in (Vigne, 2021) by modeling the deformation as a linear spring in the hip motor, yielding a system with $x \in \mathbb{R}^4$. The angle of the hip ($x_1$) is measured by the encoder on this motor, while a gyrometer measures the angular velocity of the thigh ($x_4$). The measurements are sampled with $\Delta t = 1 ms$. The aim is to identify the nonlinear deformations in the hip motor, which can be seen in motion capture and cause significant errors in gait planning, but are not captured by the known models of the exoskeleton.

We start by preprocessing the signal: for each input frequency and corresponding trajectory, we compute the FFT of $y$, apply a Gaussian window at $f_c = 50$ Hz on the spectrum, then apply an inverse FFT and slice out the beginning and the end (100 time steps) of each signal to get rid of the border effects. For $u$, which is not very noisy, we rather apply a Butterworth filter of order 2 and cut-off frequency 200 Hz. We cut the long trajectories for each input frequency in slices of 200 samples, and stack these training trajectories of length 0.2 s together to form our set of training trajectories. Hence, all trajectories have the same sampling times and can be simulated in parallel easily, as presented in Remark 1. We choose the length of 0.2 s because it seems long enough to capture some of the dynamics even in the low-frequency regime, but also short enough to remain acceptable in the high-frequency regime, as discussed in Remark 1.

We then run the structured NODE framework on this data. We directly train the NODE on a random subset of training trajectories, use a subset of validation trajectories for early stopping, and a subset of test trajectories to evaluate the generalization of the learned model. In all experiments, we use a recognition model of type backward KKL with $d_z = 10$, $F = \mathbb{1}_{d_z \times d_u}$ and $D = \text{diag}(-1, \ldots, -10)$. Both recognition and dynamics models are feed-forward networks with five hidden layers of 50 respectively 100 neurons and SiLU activation.

We notice that for this complex and nonautonomous use case, the direct recognition method seems easier to train. However, it also takes longer due to the higher dimension of $\tilde{z}(t_c)$, and tends to overfit more. This is probably due to the choice of $D$, which can be hard to tune, and to the fact that the KKL observer approximates a time-dependent transformation for nonautonomous systems.

Normalization is also an important aspect in the implementation: all losses and evaluation metrics are scaled to the same range, so that all loss terms play a similar role and remain within a similar range. This ensures that the values on which the optimization is based are always numerically tractable for the chosen solver. Different scaling possibilities are discussed in Sect. 5.2.3 of (Schittkowski, 2002). In our case, since we do not know in advance the values that $x(t)$ will take, we compute the mean and standard deviation of the samples in $y(t)$ and $u(t)$ and scale all outputs $y(t)$ respectively inputs $u(t)$ according to these. We also scale all states $x(t)$ or derivatives $\dot{x}(t)$ using the scaler on $y(t)$ for the dimensions that are measured ($x_1$ and $x_4$), and a mean of the scaler on $y(t)$ for the other dimensions. This is not quite correct, but it is the best we can do without knowing the range of values that $x(t)$ will take, and it is enough to ensure that all scaled values of $x(t)$ stay within a reasonable range.

We investigate three settings: no structure, imposing $\dot{x}_1 = x_2$ and $\dot{x}_3 = x_4$ (“hard” prior), and learning the residuals from the prior linear model on $\dot{x}_2$ and $\dot{x}_4$ (“soft” prior) with $\lambda = 5 \times 10^{-7}$; we already have $\dot{x}_1 = x_2$ and $\dot{x}_3 = x_4$ in the prior model). In each setting, we learn from $N = 265$ trajectories of a subset of input frequencies: $\{2.5, 3.5, 4.5, 5.5, 6.5, 7.5, 8.5, 9.5, 11, 13, 15\}$ Hz. We then evaluate on 163 test trajectories of 0.2 s from these input frequencies, to evaluate data fitting in the trained regime, and obtain the RMSE: 9.0 (a), 0.15 (b), 0.17 (c), 0.28 (d). We also evaluate on 52 longer (2 s) test trajectories from other input frequencies, to evaluate the interpolation capabilities of the learned model: $\{2, 3, 4, 5, 6, 7, 8, 9, 10, 12, 15, 17\}$ Hz. We obtain: 113 (a), 0.64 (b), 0.61 (c), 1.1 (d). We use the Adam (Kingma & Ba, 2015) optimizer with decaying learning rate starting at $8 \times 10^{-3}$ for the first two settings, $5 \times 10^{-3}$ for the third setting.

Overall, we find that structured NODEs are able to fit this complex nonlinear dynamical system using real-world data and realistic settings. The predictions of the obtained models are not perfect, but they are much better than those of the prior model, such that they could probably be used in a closed-loop control task like the linear model currently is at Wandercraft. Adding structure leads to similar performance, but to a model that can be physically interpreted in terms of position and velocity. In the third setting (hard constraints and residual model), the accuracy is lower. This is due to the fact that the prior model leads to rather inaccurate open-loop predictions.
Learning dynamics from partial observations with structured neural ODEs

Figure 11: Structured NODEs on the experimental dataset. The dynamics and recognition models are learned from 0.2 s of partial observations. We use the backward KKL recognition model and impose varying degrees of structure in the dynamics. We show a longer test trajectory of 2 s with an input frequency that was not seen during training ($x_1$ above, $x_4$ below).