Unconstrained Parametrization of Dissipative and Contracting Neural Ordinary Differential Equations

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Abstract—In this work, we introduce and study a class of Deep Neural Networks (DNNs) in continuous-time. The proposed architecture stems from the combination of Neural Ordinary Differential Equations (Neural ODEs) with the model structure of recently introduced Recurrent Equilibrium Networks (RENs). We show how to endow our proposed NodeRENs with contractivity and dissipativity — crucial properties for robust learning and control. Most importantly, as for RENs, we derive parametrizations of contractive and dissipative NodeRENs which are unconstrained, hence enabling their learning for a large number of parameters. We validate the properties of NodeRENs, including the possibility of handling irregularly sampled data, in a case study in nonlinear system identification.

I. Introduction

Learning complex nonlinear mappings from data is a fundamental problem in many engineering applications, including computer vision, healthcare, internet of things, and smart cities [1]. Deep Neural Networks (DNNs) have emerged as an effective tool for dealing with this task, thanks to their flexibility and ability to generalize their predictions by using massive amounts of data. Despite their effectiveness, DNNs tend to lack robustness: a slight change in the input data may yield highly different outputs, eventually leading to poor generalization capabilities [2]-[5]. Such behavior is especially problematic when DNNs are implemented in physical systems, such as safety-critical power grids or robots that interact with humans. In these applications, sensor measurements are inevitably affected by multiple sources of noise and uncertainty, and a lack of robustness may result in significant losses.

To endow DNN models with formal stability and robustness guarantees, [4] proposes to equip DNN layers with a dynamical system interpretation. The work [6] establishes dynamical DNN models which universally approximate all nonlinear dynamical systems defined in discrete-time and proposes a set of convex constraints that enforce the stability of the DNN model during training. In [7], the authors have developed discrete-time Recurrent Equilibrium Networks (RENs) that result from the closed-loop interconnection of a discrete-time linear dynamical system

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with a static nonlinearity. A main contribution of [7] is to provide an unconstrained parametrization (also known as *direct* parametrization) of a class of RENs with properties of stability and dissipativity that are *built-in*, i.e., that hold for any choice of the parameters, and without the need to constrain them to a subset. This property enables parameter optimization for very deep models through unconstrained-gradient-descent-based algorithms, while ensuring stability and dissipativity at any iteration.

The usefulness of RENs for system identification and optimal control has been demonstrated in [7] and [8], respectively. However, the corresponding stability and dissipative guarantees are only compatible with discrete-time or sampled-data systems. Studying how the properties of nonlinear discrete-time dynamics port to their continuous-time counterpart is usually a challenging problem [9].

The recently proposed Neural Ordinary Differential Equations (Neural ODEs) [10] bridge the concepts of DNNs and continuous-time dynamics. Specifically, the authors of [10] suggest unfolding infinitely many DNN layers as specified by a parametrized ODE, and training the network by using the adjoint sensitivity method [11]. Neural ODEs enjoy several advantages over discrete DNN models such as [4], [6], [7], including memory savings, adaptive computations beyond Euler-like integration methods, and the ability to include data that arrive at arbitrary instants in the time continuum. Starting from Neural ODEs, in [12], the authors proposed a continuous-time analogous of Recurrent Neural Networks, although without guarantees of stability or dissipativity. The work [13] has proposed stable Hamiltonian Neural ODEs which further exhibit non-vanishing gradient flows. A class of Hamiltonian ODEs that further enjoy contractivity has been developed in [5]. Furthermore, while [14] derives architectures with guaranteed convergence of the flow to some stable set. However, an architecture that combines the strong stability, robustness, and expressivity properties of [6], [7] with the benefits of Neural ODEs is not available to the best of our knowledge.

A. Contributions

In this paper, we establish an alternative version of the REN architecture of [7] that is compatible with Neural ODEs in continuous-time. Consequently, we call our architectures *NodeRENs*. After showing that NodeRENs induce well-posed dynamical systems in continuous-time, we establish that our models enjoy stability and dissipativity properties by design, i.e., without any constraints on the space of the parameters that describe the DNNs — akin to their discrete-

time counterpart [7]. At the same time, NodeRENs inherit the advantages of Neural ODEs in continuous-time; they are compatible with any integration scheme that can be chosen based on a trade-off between accuracy and computational resources, and they can be evaluated at any chosen time instant, without the requirement to be uniformly sampled in time.

The paper is structured as follows. In Section II, we provide a description of the problem setting, along with the definition of contractivity and Integral Quadratic Constraints (IQCs). In Section III, the NodeREN model is introduced. We present the steps to obtain NodeRENs that are contracting and dissipative by design. Moreover, in Section IV the NodeRENs are validated on a nonlinear system identification problem. Finally, Section V summarizes the conclusions of this work and suggests future developments.

B. Notation

We denote the set of non-negative real numbers as \mathbb{R}^+_0 . For T>0, let $PC([0,T],\mathbb{R}^n)$ be the space of piecewise-continuous functions in the time interval [0,T]. We represent the Euclidean norm of $v\in\mathbb{R}^n$ with |v|. For a square matrix X, we use the notation $X\succ 0$ ($X\succeq 0$) and $X\prec 0$ ($X\preceq 0$) to denote positive (semi-) definiteness and negative (semi-) definiteness, respectively. The minimum and maximum eigenvalues of the square matrix X are denoted as $\lambda_{min}(X)$ and $\lambda_{max}(X)$, respectively. We use (*) to represent a symmetric term in a quadratic expression, e.g., $(X+Y)Q(*)^\top=(X+Y)Q(X+Y)^\top$, for some $Q\in\mathbb{R}^{n\times n}$ and $X,Y\in\mathbb{R}^{q\times n}$. With (*), we also indicate elements in symmetric matrices that can be obtained by symmetry. We use $[M]_{p\times m}$ to indicate the block matrix with the first p rows and m columns of $M\in\mathbb{R}^{n\times n}$ with $n\geq m$ and $n\geq p$.

II. PROBLEM FORMULATION

Consider a nonlinear system Σ_{θ} in continuous-time

$$\Sigma_{\theta} = \begin{cases} \dot{x}(t) = f_{\theta}(x(t), u(t)) \\ y(t) = g_{\theta}(x(t), u(t)) \end{cases} , \tag{1}$$

where $x(t) \in \mathbb{R}^n$, $y(t) \in \mathbb{R}^p$ and $u(t) \in \mathbb{R}^m$ denote the state, output and input of the system at any time $t \in \mathbb{R}_0^+$, respectively, and $x(0) = x_0$. In (1), $\theta \in \mathbb{R}^{n_\theta}$ denotes a vector of parameters affecting the behavior of the system. The idea behind Neural ODEs [10] is to interpret some specific DNNs (e.g., ResNets [15]) as discretized ODEs. Then, the family of Neural ODEs can be obtained when the discretization step converges to zero, effectively passing from discrete-time DNNs to continuous-time models as (1). Accordingly, in this paper we consider the following learning problem:

$$\min_{\theta} L(\theta, \mathcal{Z})
\text{subject to (1)}.$$

 1 For instance, standard ResNet models whose hidden states evolve as $h_{k+1}=h_k+\Delta t\,f(h_k,\theta_k)$ can be interpreted as the ODE $\dot{h}(t)=f(h(t),\theta(t))$ as the discretization step Δt tends to zero.

L is a scalar loss function that can depend on the trajectories x(t) and y(t) of (1), for $t \in [0,T]$ with T>0, and $\mathcal Z$ is a given training dataset. For instance, in a classification task, y(T) can play the role of the DNN output layer which is compared to the label y_{label}^j of the point $x^j(0)$ contained in a dataset $\mathcal Z = \left\{ (x^j(0), y_{label}^j) \right\}_{j=1}^N$ for $N \in \mathbb N$. Neural ODEs can exploit any chosen numerical method to perform the forward propagation and the gradient computations through (1), including those based on adaptive sampling in order to guarantee a desired level of precision (e.g., Dormand-Prince, Bogacki-Shampine [16]). Although possible, back-propagating through numerical solver's operations can be highly expensive in terms of memory and introduce numerical errors. As an alternative, to solve (2) one can use the adjoint method — we refer to [10] for full details.

Neural-ODEs in their general form are not guaranteed to yield stable or dissipative dynamical flows. Such properties are fundamental in optimal control and system identification, as well as in robust learning problems dealing with noisy features [5] and adversarial attacks [17]. Specifically, motivated by [7], in this paper, we focus on continuous-time systems that are contracting, and systems that satisfy incremental IQCs. We proceed with formally defining both.

Firstly, given a system Σ_{θ} with initial condition $a \in \mathbb{R}^n$ and an input function $u^{[1]} \in PC([0,\infty],\mathbb{R}^m)$, let $x_a^{[1]}$ and $y_a^{[1]}$ denote the corresponding state and output trajectories, respectively.

Definition 1. A system Σ_{θ} in the form (1) is said to be contracting if for any two initial conditions $a,b \in \mathbb{R}^n$ and given the same input trajectory $u^{[1]} \in PC([0,\infty],\mathbb{R}^m)$, the corresponding state trajectories $x_a^{[1]}$ and $x_b^{[1]}$ satisfy:

$$|x_a^{[1]}(t) - x_b^{[1]}(t)| \le \kappa e^{-ct} |a - b|,$$
 (3)

for all $t \in \mathbb{R}_0^+$ and for some c > 0, $\kappa > 0$.

The Definition 1 can be interpreted as follows: a contracting system 'forgets' the initial condition exponentially fast as time progresses. Hence, all trajectories converge to each other, independently of the initial state.

Next, we define dissipative systems that satisfy incremental IQCs. Dissipative systems cannot increase their internal energy despite external inputs (e.g., feedback control actions or disturbances). As such, they can be designed to possess finite input-output gains, a crucial property in nonlinear control theory [18], as well as robust learning [19]. In order to formally define these properties, let $a,b \in \mathbb{R}^n$ be two initial conditions and $u^{[1]},u^{[2]} \in PC([0,\infty],\mathbb{R}^m)$ be two input trajectories. Define the relative displacements as

$$\Delta y(t) = y_a^{[1]}(t) - y_b^{[2]}(t) , \ \Delta u(t) = u^{[1]}(t) - u^{[2]}(t) ,$$

$$\Delta x(t) = x_a^{[1]}(t) - x_b^{[2]}(t) .$$
(4)

Let

$$s_{\Delta}(\Delta u(t), \Delta y(t)) = \begin{bmatrix} \Delta y(t) \\ \Delta u(t) \end{bmatrix}^{\top} \begin{bmatrix} Q & S^{\top} \\ S & R \end{bmatrix} \begin{bmatrix} \Delta y(t) \\ \Delta u(t) \end{bmatrix}, \quad (5)$$

be a quadratic function $s_{\Delta}: \mathbb{R}^m \times \mathbb{R}^p \to \mathbb{R}$ parametrized by $Q \in \mathbb{R}^{p \times p}$, $S \in \mathbb{R}^{m \times p}$, $R \in \mathbb{R}^{m \times m}$. We recall the definition of dissipative systems that satisfy IQCs according to the supply rate (5).

Definition 2. A system Σ_{θ} in form (1) satisfies the *incremental* IQC defined by the matrices (Q, S, R), with $Q \leq 0$ and $R = R^{\top}$, if there exists a function $\mathcal{S} : \mathbb{R}^n \to \mathbb{R}_0^+$ such that, for any two initial conditions $a, b \in \mathbb{R}^n$ and any two possible input functions $u^{[1]}, u^{[2]} \in PC([0, \infty], \mathbb{R}^m)$,

$$S(\Delta x(t_1)) \le S(\Delta x(t_0)) + \int_{t_0}^{t_1} s_{\Delta}(\Delta u(t), \Delta y(t)) dt, \quad (6)$$

for every $t_1 \ge t_0$, where Δx , Δy and Δu are defined in (4) and the supply rate s_{Δ} is defined in (5).

If the function $S(\Delta x(t))$ is continuous and differentiable, (6) can be rewritten as:

$$\frac{d}{dt} \left(\mathcal{S}(\Delta x(t)) \right) \le s_{\Delta} \left(\Delta u(t), \Delta y(t) \right). \tag{7}$$

Despite being restricted to quadratic supply functions according to (5), IQCs can certify many incremental properties by appropriately selecting the values of (Q,S,R). It is worth noting that the assumptions in Definition 2

$$Q \le 0 \,, \quad R = R^{\top} \,, \tag{8}$$

are fulfilled for several incremental properties of interest, see Table I.

Incremental Property	Q	R	S	$s_{\Delta}(\Delta u, \Delta y)$
L_2 - gain bound $(\gamma \ge 0)$	$-\frac{1}{\gamma}I$	γI	0	$ \gamma \Delta u ^2 - \frac{1}{\gamma} \Delta y ^2$
Passivity	Ó	0	$\frac{1}{2}I$	$\Delta u^{\top} \Delta y$
Input Passivity $(\nu \geq 0)$	0	$-2\nu I$	\bar{I}	$\begin{array}{ c c c c } \Delta u^{\top} \Delta y - \nu \Delta u ^2 \\ \Delta u^{\top} \Delta y - \varepsilon \Delta y ^2 \end{array}$
Output Passivity $(\varepsilon \ge 0)$	$-2\varepsilon I$	0	I	$\Delta u^{\top} \Delta y - \varepsilon \Delta y ^2$

TABLE I: Choices of (Q, S, R) to verify different incremental properties.

To summarize, our goal is to learn the parameters θ of a dynamical system (1) — i.e., a Neural ODE — that optimize a given cost as per (2), with the hard constraint that either (3) or (6) (or both) hold. This new requirement (i.e., the hard constraint) must be satisfied for all the parameters θ we optimize over. In other words, we consider a form of failsafe learning, in the sense that the property of the model to be contracting or dissipative must be guaranteed during and after parameter optimization.

Remark 1. For solving problem (2), one has to select an integration scheme for (1), which allows performing forward propagation and gradient computations. The properties of the continuous-time model (1) may not coincide with those of the discretized one, in general. While in this paper our focus is on the contractivity and dissipativity properties of the continuous-time model (1), we remark that integration methods that preserve contractivity have been proposed in [20]. Tailoring these integration methods to IQC properties, or developing new ones, is an interesting direction for future work.

III. CONTRACTIVITY AND DISSIPATIVITY OF NODERENS

In this section, we present and analyze novel DNN structures that arise from appropriately combining Neural ODEs [10] with RENs [7]. The starting idea is to define the functions f_{θ} and g_{θ} in (1) through the model utilized for the layer equation in [7]. Specifically, we consider

$$\begin{bmatrix} \dot{x}(t) \\ v(t) \\ y(t) \end{bmatrix} = \underbrace{\begin{bmatrix} A & B_1 & B_2 \\ C_1 & D_{11} & D_{12} \\ C_2 & D_{21} & D_{22} \end{bmatrix}}_{\tilde{w}(t)} \begin{bmatrix} x(t) \\ w(t) \\ u(t) \end{bmatrix} + \underbrace{\begin{bmatrix} b_x \\ b_v \\ b_y \end{bmatrix}}_{\tilde{w}(t)}, \qquad (9)$$

$$w(t) = \sigma(v(t)), \qquad (10)$$

where $x(t) \in \mathbb{R}^n$, $u(t) \in \mathbb{R}^m$ and $y(t) \in \mathbb{R}^p$ are respectively the state, the input, and output at time t. The function $\sigma(\cdot)$ represents a nonlinear map and it is applied entry-wise. The input and output of $\sigma(\cdot)$ are $v(t), w(t) \in \mathbb{R}^q$, respectively. We denote system (9)-(10) as a NodeREN, and it can be interpreted as an affine time-invariant system in closed-loop with a static nonlinearity $\sigma(\cdot)$. In NodeRENs, the set of trainable parameters $\theta \in \mathbb{R}^{n_\theta}$ consists of the set \tilde{A} of matrices $(A, B_1, B_2, C_1, C_2, D_{11}, D_{12}$ and $D_{22})$ and the set \tilde{b} of vectors (b_x, b_v, b_y) in (9).

The work [7] has established conditions that ensure contractivity and IQC properties of the *discrete-time* dynamics induced by θ . However, the same conditions on θ fail to ensure these properties for the continuous-time solutions of (9)-(10), in general.

Towards establishing contractivity and IQC-based dissipativity in continuous-time for the model (9)-(10), consider two different possible trajectories of the system, starting from two initial conditions $a, b \in \mathbb{R}^n$ and two input functions $u^{[1]}$, $u^{[2]} \in PC([0,\infty],\mathbb{R}^m)$. Then, define the *incremental form* of the system (9)-(10)

$$\begin{bmatrix} \Delta \dot{x}(t) \\ \Delta v(t) \\ \Delta y(t) \end{bmatrix} = \begin{bmatrix} A & B_1 & B_2 \\ C_1 & D_{11} & D_{12} \\ C_2 & D_{21} & D_{22} \end{bmatrix} \begin{bmatrix} \Delta x(t) \\ \Delta w(t) \\ \Delta u(t) \end{bmatrix}, \quad (11)$$

$$\Delta w(t) = \sigma(v_b^{[2]}(t) + \Delta v(t)) - \sigma(v_b^{[2]}(t)), \qquad (12)$$

where Δx , Δy and Δu are defined in (4). Moreover, $\Delta v(t) = v_a^{[1]}(t) - v_b^{[2]}(t)$, where $v_a^{[1]}$ and $v_b^{[2]}$ are the inputs of $\sigma(\cdot)$ for each trajectory. Next, we introduce two technical assumptions.

Assumption 1. The function $\sigma(\cdot)$ belongs to $PC([0,\infty],\mathbb{R})$ and its slope is restricted to the interval [0,1], that is

$$0 \le \frac{\sigma(y) - \sigma(x)}{y - x} \le 1, \quad \forall x, y \in \mathbb{R}, \quad x \ne y.$$

It is important to notice that, under Assumption 1, $\Delta v(t)$ and $\Delta w(t)$ verify the following inequality

$$\Gamma(t) = \begin{bmatrix} \Delta v(t) \\ \Delta w(t) \end{bmatrix}^{\top} \begin{bmatrix} 0 & \Lambda \\ \Lambda & -2\Lambda \end{bmatrix} [*] \ge 0, \quad \forall t \in \mathbb{R}, \quad (13)$$

for any diagonal matrix $\Lambda \succ 0$. Note that most of the popular activation functions used in the literature, such as the logistic function, $ReLU(\cdot)$ and $\tanh{(\cdot)}$, satisfy Assumption 1.

Assumption 2. The matrix D_{11} in (9) is strictly lower-triangular.

Assumption 2 enforces that each scalar entry of $\Delta v(t)$ only depends on the ones above it through (11). Hence, it becomes possibly to explicitly compute $\Delta v(t)$. This simplifies the numerical calculation of the solutions to (11)-(12), while guaranteeing that the model is very expressive thanks to the recursive application of the nonlinearity σ on successive entries of $\Delta v(t)$. The case where D_{11} is not lower-triangular is left for future work. We refer the interested reader to [7] for a discussion on implicit RENs in discrete-time.

In general, an ODE model may not admit a unique solution for a given initial condition and input trajectory [21]. We now proceed to show that (9)-(10) admits a unique solution for any choice of the parameters θ .

Lemma 1. Let Assumptions 1 and 2 hold. Then, the model (9)-(10) admits a unique solution in time for any $u(t) \in PC([0,\infty],\mathbb{R}^m), \ x(0) \in \mathbb{R}^n$ and for any choice of the parameters $\theta \in \mathbb{R}^{n_\theta}$.

The proof, reported in Appendix A for completeness, is based on deriving a global Lipschitz constant by iterating through the nonlinearities defining the vector v(t).

A. Characterization of Contracting and Dissipative NodeRENs

Here, we derive sufficient conditions over the parameters θ to guarantee contractivity and dissipativity of NodeRENs (9)-(10) according to a specified supply rate (5).

Theorem 1. A NodeREN (9)-(10) is contracting according to (3), if there exists a matrix $P \succ 0$ and a diagonal matrix $\Lambda \succ 0$ such that

$$\begin{bmatrix} -A^{\top}P - PA & -C_1^{\top}\Lambda - PB_1 \\ * & W \end{bmatrix} \succ 0, \qquad (14)$$

with

$$W = 2\Lambda - \Lambda D_{11} - D_{11}^{\mathsf{T}} \Lambda. \tag{15}$$

Proof. Define

$$V_{\Delta}(t) = \Delta x(t)^{\top} P \Delta x(t), \qquad (16)$$

and let

$$\Phi = (-A^{\top}P - PA) - (C_1^{\top}\Lambda + PB_1)W^{-1}(*)^{\top} \succ 0,$$

be the Schur complement of (14). Then, using properties of matrix inequalities, it is always possible to find an $\alpha \in (0, \lambda_{min}(\Phi)^{-1}\lambda_{max}(P)]$ such that $(\Phi - \alpha P) \succ 0$. Hence,

$$\begin{bmatrix} -A^{\top}P - PA - \alpha P & -C_1^{\top}\Lambda - PB_1 \\ * & W \end{bmatrix} \succ 0. \tag{17}$$

By left- and right-multiplying the inequality (17) with $\left[\Delta x(t)^{\top} \Delta w(t)^{\top}\right]$ and $\left[\Delta x(t)^{\top} \Delta w(t)^{\top}\right]^{\top}$, respectively, and using (13), we obtain by substitution that:

$$\dot{V}_{\Delta}(t) + \alpha V_{\Delta}(t) < -\Gamma(t) \le 0$$
.

Thus, according to Lyapunov's exponential stability theorem [22], the incremental system is globally exponentially stable, that is, it satisfies (3) with $c = \alpha/2$.

For the rest of the paper, we refer to NodeRENs that comply with (14)-(15) as C-NodeRENs.

Remark 2. One may want to impose a certain convergence rate for a C-NodeREN. For this purpose, (14) can be modified as follows:

$$\begin{bmatrix} -A^\top P - PA - 2\tilde{\alpha}P & -C_1^\top \Lambda - PB_1 \\ * & W \end{bmatrix} \succ 0 \,,$$

where the term $-2\tilde{\alpha}P$ enforces that (3) holds with $c=\tilde{\alpha}$. This can be directly seen by following the proof of Theorem 1 starting from (17).

Next, we characterize NodeRENs that comply with incremental IQCs.

Theorem 2. A NodeREN (9)-(10) satisfies the incremental IQC described by the triple (Q,S,R) fulfilling (8), if there exists a matrix $P\succ 0$ and a diagonal matrix $\Lambda\succ 0$ such that

$$\begin{bmatrix} -A^{\top}P - PA & -C_{1}^{\top}\Lambda - PB_{1} & -PB_{2} + C_{2}^{\top}S^{\top} \\ * & W & -\Lambda D_{12} + D_{21}^{\top}S^{\top} \\ * & * & \mathcal{R} \end{bmatrix}$$

$$+ \begin{bmatrix} C_{2}^{\top} \\ D_{21}^{\top} \\ D_{22}^{\top} \end{bmatrix} Q \begin{bmatrix} C_{2}^{\top} \\ D_{21}^{\top} \\ D_{22}^{\top} \end{bmatrix}^{\top} \succ 0, \quad (18)$$

with W given by (15) and

$$\mathcal{R} = R + SD_{22} + D_{22}^{\mathsf{T}}S^{\mathsf{T}}. \tag{19}$$

Proof. Consider the same function V_{Δ} as in (16). By left- and right-multiplying the inequality (18) with $\left[\Delta x(t)^{\top} \ \Delta w(t)^{\top} \ \Delta u(t)^{\top}\right]^{\top}$ respectively, we obtain by substitution

$$\dot{V}_{\Delta}(t) - \begin{bmatrix} \Delta y(t) \\ \Delta u(t) \end{bmatrix}^{\top} \begin{bmatrix} Q & S^{\top} \\ S & R \end{bmatrix} [*] < -\Gamma(t) \leq 0.$$

Thus, the inequality (7) holds.

For the rest of the paper, we refer to NodeRENs that comply with (18)-(19) as IQC-NodeRENs.

Remark 3. Note that all IQC-NodeRENs are also contracting for any choice of (Q, S, R) such that (8) holds. Indeed, if there exists $P \succ 0$ and a diagonal matrix $\Lambda \succ 0$ such that (18) holds, then (14) also holds because $Q \preceq 0$ and the left-hand-side of (14) is a principal minor of that of (18).

It should be noted that solving the minimization problem (2) using the above parametrizations of C-NodeRENs or IQC-NodeRENs requires solving a semidefinite program (SDP) multiple times during the optimization process. This can be computationally intractable for DNNs with several parameters. In the following section, we propose a parametrization of a rich class of C-NodeRENs and IQC-NodeRENs that circumevents this problem and allows for unconstrained optimization. It is worth noting that this approach is similar to [7] for discrete-time RENs, but the techniques differ due to the continuous-time nature of the proposed NodeRENs.

B. Direct Parametrization of NodeRENs

Our goal is to define new free parameters $\theta_C \in \mathbb{R}^{n_C}$ and $\theta_{IQC} \in \mathbb{R}^{n_{IQC}}$ that can be mapped onto the parameters θ of the NodeREN model, given by equations (9)-(10), and such that either (14) or (18) are verified. First, we focus on constructing C-NodeRENs from the parameters $\theta_C \in \mathbb{R}^{n_C}$ given by

$$\theta_C = \{X, B_2, C_2, D_{12}, D_{21}, D_{22}, \tilde{b}, U, Y_1, X_P\}, \quad (20)$$

where $X \in \mathbb{R}^{(n+q)\times(n+q)}$, $B_2 \in \mathbb{R}^{n\times m}$, $C_2 \in \mathbb{R}^{p\times n}$, $D_{12} \in \mathbb{R}^{q\times m}$, $D_{21} \in \mathbb{R}^{p\times q}$, $D_{22} \in \mathbb{R}^{p\times m}$, $\tilde{b} \in \mathbb{R}^{(n+q+p)}$ $U \in \mathbb{R}^{n\times q}$, $Y_1 \in \mathbb{R}^{n\times n}$ and $X_P \in \mathbb{R}^{n\times n}$.

Theorem 3. For any $\theta_C \in \mathbb{R}^{n_C}$ defined in (20), and $\epsilon, \epsilon_P > 0$ the two following statements hold.

There are matrices (Y, W, Z, P) of appropriate dimensions such that

$$\begin{bmatrix} -Y^{\top} - Y & -U - Z \\ * & W \end{bmatrix} = X^{\top}X + \epsilon I, \qquad (21)$$

$$P = X_P^{\dagger} X_P + \epsilon_P I \,. \tag{22}$$

2) There are matrices $\{\tilde{A}, \tilde{b}\}$ defined in terms of θ_C and the matrices (Y, W, Z, P) defined in point 1, such that the corresponding NodeREN (9)-(10) is contracting.

Moreover, matrices (Y, W, Z, P) and $\{\tilde{A}, \tilde{b}\}$ can be computed as described in the proof of the Theorem.

Proof. Part 1): Define

$$H = \begin{bmatrix} H_{11} & H_{12} \\ H_{21} & H_{22} \end{bmatrix} = X^{\top} X + \epsilon I, \qquad (23)$$

where $H_{11} \in \mathbb{R}^{n \times n}$, $H_{12} \in \mathbb{R}^{n \times q}$, $H_{21} \in \mathbb{R}^{q \times n}$ and $H_{22} \in \mathbb{R}^{q \times q}$. Then, one can set

$$Y = -\frac{1}{2}(H_{11} + Y_1 - Y_1^{\top}), \qquad (24)$$

and

$$W = H_{22}, \quad Z = -H_{12} - U.$$
 (25)

Thus, starting from H as in (23), (Y, W, Z) can be built using (24)-(25) and P using (22).

Part 2): First, note that $H \succ 0$ and $P \succ 0$ are guaranteed by construction because $X^\top X + \epsilon I$ and $X_P^\top X_P + \epsilon_P I$ are positive definite for any X and X_P . From Assumption 2, D_{11} is strictly lower triangular. Thus, using (15) and being $W = W^\top$ by construction, it is possible to split W as: $W = W_{diag} + W_{low} + W_{low}^\top$, where W_{diag} is a diagonal matrix, and W_{low} is a strictly lower triangular matrix. By setting

$$\Lambda = \frac{1}{2} W_{diag} \,, \quad D_{11} = -\Lambda^{-1} W_{low} \,,$$
 (26)

and the matrices A, B_1, C_1 can be retrieved as

$$C_1 = \Lambda^{-1} U^{\top}$$
, $A = P^{-1} Y$, $B_1 = P^{-1} Z$, (27)

where P^{-1} and Λ^{-1} exist since $P \succ 0$ and $\Lambda \succ 0$. Finally, we can show that (14) holds by substituting A, B_1 , C_1 , D_{11} , Λ , and P with their definitions in (23)-(27). Thus, the corresponding NodeREN (9)-(10) specified by $\{\tilde{A}, \tilde{b}\}$ is contracting.

In conclusion, an unconstrained parametrization of a class of C-NodeRENs is obtained by first freely choosing θ_C defined in (20), and then recovering the matrix \tilde{A} using (24)-(27).

Next, we focus on NodeRENs that satisfy IQC constraints by design, i.e. for any choice of parameters $\theta_{IQC} \in \mathbb{R}^{n_{IQC}}$ given by

$$\theta_{IQC} = \{X_R, B_2, C_2, D_{21}, \tilde{b}, X_3, T, U, Y_1, X_P\}, \quad (28)$$

where $X_R \in \mathbb{R}^{(n+q)\times(n+q)}$, $B_2 \in \mathbb{R}^{n\times m}$, $C_2 \in \mathbb{R}^{p\times n}$, $D_{21} \in \mathbb{R}^{p\times q}$, $\tilde{b} \in \mathbb{R}^{(n+p+q)}$, $X_3 \in \mathbb{R}^{s\times s}$, $T \in \mathbb{R}^{q\times m}$, $U \in \mathbb{R}^{n\times q}$, $Y_1 \in \mathbb{R}^{n\times n}$ and $X_P \in \mathbb{R}^{n\times n}$. In the next theorem, we provide a procedure to construct an IQC-NodeREN for any choice of θ_{IQC} .

Theorem 4. Let (Q,S,R) be such that (8) holds. Assume also that there exists $\delta>0$ satisfying $R-S(Q-\delta I)^{-1}S^{\top}\succ 0$. For any $\theta_{IQC}\in\mathbb{R}^{n_{IQC}}$ defined in (28), and $\epsilon,\epsilon_P>0$ the two following statements hold.

1) There are matrices (Y, W, Z, P, D_{22}) of appropriate dimensions such that

$$\tilde{\mathcal{R}} = R + SD_{22} + D_{22}^{\top}S^{\top} + D_{22}^{\top}QD_{22} \succ 0, \quad (29)$$

$$\begin{bmatrix} -Y^{\top} - Y & -U - Z \\ * & W \end{bmatrix} - \Psi = X_R^{\top} X_R + \epsilon I , \quad (30)$$

where P is constructed as in (22), and

$$\Psi = \begin{bmatrix} V \\ \tilde{T} \end{bmatrix} \tilde{\mathcal{R}}^{-1} \begin{bmatrix} * \end{bmatrix}^{\top} - \begin{bmatrix} C_2^{\top} \\ D_{21}^{\top} \end{bmatrix} Q \begin{bmatrix} * \end{bmatrix}^{\top}, \quad (31)$$

$$\tilde{T} = -T + D_{21}^{\mathsf{T}} S^{\mathsf{T}} + D_{21}^{\mathsf{T}} Q D_{22} , \qquad (32)$$

$$V = -PB_2 + C_2^{\top} S^{\top} + C_2^{\top} Q D_{22}.$$
 (33)

2) There are matrices $\{\tilde{A}, \tilde{b}\}$ defined in terms of θ_{IQC} and the matrices (Y, Z, W, P, D_{22}) defined in point 1, such that the corresponding NodeREN (9)-(10) satisfies the incremental IQCs parametrized by (Q, S, R).

Moreover, matrices (Y, W, Z, P) and $\{A, b\}$ can be computed as described in the proof of the Theorem.

The proof of Theorem 4 shares similarities with the one of Proposition 2 in [7] and it is reported in Appendix B. Note that the assumption that there exists a δ such that $R-S(Q-\delta I)^{-1}S^{\top}\succ 0$ is not restrictive. Indeed, for all the most relevant cases, reported in Table I, finding an appropriate value of δ is straightforward. In conclusion, an unconstrained parametrization of IQC-NodeRENs is obtained by first freely choosing the parameters $\theta_{IQC}\in\mathbb{R}^{n_{IQC}}$, then constructing D_{22} as per (42) in Appendix B, and last recovering the matrices of \tilde{A} using (24)-(27), (42) and (43).

IV. SIMULATIONS & RESULTS

In this section, we demonstrate the use of NodeRENs for the identification of a stable nonlinear system. First, we evaluate the performance of NodeRENs through different integration methods during the training phase — not possible in discrete-time systems. Second, we illustrate the benefits of contractivity-by-design by training a general noncontractive NodeREN (11)-(12), which fails to learn a stable behavior for the same task. Last, we show the ability of NodeRENs to learn from data that are not sampled regularly in time, while maintaining the guarantees by design. The code used in this work is available at https://github.com/DecodEPFL/NodeREN.

We remark that the trajectories of NodeRENs are reversible in time due to Lemma 1, and hence they cannot intersect for different initial conditions. To increase the expressivity of the model, in the simulations we use augmented state vectors and initialize to zero the additional scalar states. This technique, also known as feature augmentation, has been proposed in [23] for general Neural ODEs.

A. Continuous-Time System Identification

Here, we consider the system identification of a black-box system. For this experiment, we assume that the unknown system dynamics are those of a nonlinear pendulum

$$\ell\ddot{\alpha}(t) + \beta\dot{\alpha}(t) + g\sin\alpha(t) = 0, \qquad (34)$$

where $\alpha(t)$ is the angle position of the pendulum at time t with respect to the vertical axis, $\beta>0$ is the viscous damping coefficient, g is the gravitational acceleration and $\ell>0$ is the length of the pendulum. For our experiments, we have chosen $\ell=0.5\,\mathrm{m}$ and $\beta=1.5\,\mathrm{m\,s^{-1}}$.

We consider the scenario where the system dynamics (34) to identify are completely unknown and the only prior knowledge we have is that the system is stable around the origin. Hence, we choose to train a C-NodeREN, which is guaranteed to be contracting (and so, stable around the origin if \tilde{b} is null) for any choice of the trainable parameters θ_C — i.e. even if we stop the optimization prematurely.

The training data are given by noisy measurements of $\alpha(t)$ and $\dot{\alpha}(t)$ across $N \in \mathbb{N}$ different experiments performed in the time interval $[0,T_{end}] \subset \mathbb{R}$ with T_{end} . For each experiment $i=1,\ldots,N$, the system (34) starts from a different and known initial condition $\alpha_i(0)$ and $\dot{\alpha}_i(0)$. Due to the possibility of random time delays during data acquisition, we assume that trajectory measurements are taken at various time instants across the real number line for each experiment. It is worth noting that inconsistent measurement times are a common occurrence in control applications; however, incorporating this feature into discrete-time systems would pose a significant modeling challenge.

Precisely, the training data consist of $\mathcal{Z} = \{\mathcal{Z}_i\}_{i=1}^N$, where

$$\mathcal{Z}_i = \{(t_i, z_i), \text{ for all } t_i \in \mathcal{T}_i \subset [0, T_{end}] \subset \mathbb{R} \},$$
 (35)

where $T_{end} = 3 \,\mathrm{s}$, \mathcal{T}_i contains $n_i \in \mathbb{N}$ time instants, and for each experiment $i = 1, \ldots, N$, the vector $z_j \in$

 \mathbb{R}^2 is measured as $z_j = \begin{bmatrix} \alpha(t_j) & \dot{\alpha}(t_j) \end{bmatrix}^\top + w(t_j)$ with $w(t_j) \sim \mathcal{N}(0, 0.01I_2)$ being drawn according to a Gaussian distribution. We minimize over θ_C the mean squared error function

$$L(\theta_C, \mathcal{Z}) = \frac{1}{N} \sum_{i=1}^{N} \frac{1}{n_i} \sum_{(t_j, z_j) \in \mathcal{Z}_i} |y(t_j) - z_j|^2,$$

where, with a slight abuse of notation, $y(t_j) \in \mathbb{R}^2$ denotes the output at time t_j of the C-NodeREN with parameters θ_C .

The chosen C-NodeREN architecture has n=4 and q=5. It comes with $\theta_C \in \mathbb{R}^{\sim 150}$, and it is trained using one of the following integration methods: forward Euler (euler), Runge-Kutta of order 4 (rk4), and Dormand-Prince-Shampine of order 5 (dopri5). The training is performed with N=200 experiments and using Adam [24].

In order to test the prediction performance of our trained models, we construct a test dataset \mathcal{Z}_{test} in the same way as (35), using a longer time window $[0,T_{end}^{test}]$ with $T_{end}^{test}=8\,\mathrm{s}$ and new sets of time instants \mathcal{T}_i^{test} . We then compute the test loss $L(\theta_C^\star,\mathcal{Z}_{test})$, where θ_C^\star are the parameters where the training converged to.

In Figure 1, we report the resulting test losses for different methods, along with their Number of Function Evaluations (NFE) used for the prediction in the time window $[0,T_{end}^{test}]$. Both euler and rk4 have been applied using $\{100, 200\}$ and $\{50, 200\}$ integration steps, respectively, in $[0,T_{end}^{test}]$. One of the advantages of variable-steps methods such as dopri5 is the possibility to choose a tolerance value tol to fix the computational error during the ODE simulation. Indeed, it is possible to obtain a trade-off between accuracy and the required number of function evaluations just by properly setting this parameter. It is important to emphasize how for fixed-step methods (e.g., euler, rk4) the chosen number of steps may not be enough to properly capture the dynamics of the trained model. This can lead to numerical instability. Instead, adaptive methods (e.g., dopri5) can adapt the integration step on the fly, keeping the integration error bounded. As anticipated in Remark 1, it is of future work to endow C-NodeRENs with specific integration methods that preserve contractivity, e.g. [20].

Then, for the same identification task, we have trained a general NodeREN (11)-(12) (that we denote as G-NodeREN), with trainable parameters $\theta=\{\tilde{A},\tilde{b}\}$. Given the higher flexibility of G-NodeRENs with respect to C-NodeRENs, one could expect a better performance in the time window $[0,T_{end}]$ considered for the training. However, a trained G-NodeREN can exhibit unstable dynamics when simulating for longer horizons; this phenomenon is illustrated in Figure 2. Instead, C-NodeRENs limit the search to stable models only, resulting in better identification performance for the considered example. In Figure 2 we additionally plot the tubes of trajectories resulting from perturbed initial conditions. Note that the diameter of the tube associated with the C-NodeREN decreases over time, thus showcasing the contractivity property.

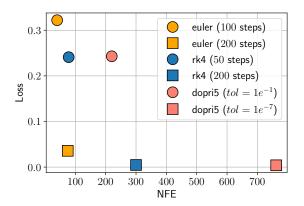


Fig. 1: Comparison between the number of function evaluations (NFE) and loss on testing dataset for different integration methods.

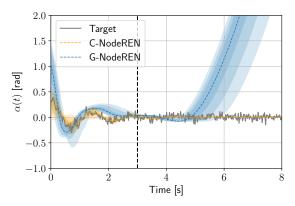


Fig. 2: Noisy test trajectory of the angular position $\alpha(t)$ of the real system (in gray). Predicted trajectories of the trained C-NodeREN (in orange) and G-NodeREN (in blue). The shaded areas represent tubes of additional trajectories resulting from perturbations on the initial state of the systems. The black dashed line indicates the end of the training horizon $T_{end}=3\,\mathrm{s}$.

B. Irregularly sampled-data

To show the robustness of C-NodeRENs with respect to the irregularly sample data, we compare the test losses of 10 C-NodeRENs trained on 10 different training datasets having the same initial conditions, but different sampling times. We observe that, despite using differently sampled data, all the models have similar test losses: they all lay in the interval $[3.7\times10^{-4};9.1\times10^{-3}]$, depending on how well the samples were distributed.

V. CONCLUSIONS

In this work, we have established a class of Neural ODEs that generalize RENs for continuous-time scenarios. Specifically, the proposed models guarantee relevant continuous-time system-theoretic properties such as contractivity and dissipativity by design. The resulting DNNs can be trained using unconstrained optimization — which enables the use of large networks — and the resulting architectures are

flexible in the choice of an ODE integration scheme that is suitable for the learning problem at hand. We have showcased performance of our NodeRENs through the identification of a nonlinear pendulum, where the data are measured at irregularly spaced time instants.

An important direction for future research is to develop integration schemes that provably preserve contractivity and IQC properties for NodeRENs. It is also relevant to study distributed NodeREN architectures and to characterize their generalization properties.

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APPENDIX

A. Proof of Lemma 1

Given $u(t) \in PC([0,\infty], \mathbb{R}^m)$, we can rewrite (9) as:

$$\dot{x}(t) = p(x(t), t) = Ax(t) + B_1 w(t) + B_2 u(t) + b_x,$$
 (36)

where we define p(x(t),t)=f(x(t),u(t),t). It is well-known that a solution exists and is unique if $p(\cdot,\cdot)$ is globally Lipschitz in its first argument and piece-wise continuous in its second (e.g., [21, Theorem 3.6]). Therefore, we prove that these properties hold for the model in (9) under Assumptions 1 and 2. First, $p(\cdot,\cdot)$ is piece-wise continuous in its second argument because it is the composition of piece-wise continuous functions under Assumption 1. Then, we prove that $p(\cdot,\cdot)$ is globally Lipschitz in its first variable, that is

$$\exists \kappa > 0 : |p(x_1, t) - p(x_2, t)| < \kappa |x_1 - x_2|,$$

for every $x_1, x_2 \in \mathbb{R}^n$ and $t \in \mathbb{R}$. For $j \in \{1, 2\}$, denote $w_j \in \mathbb{R}^q$ as $w_j = \left[w_j^1, \dots, w_j^q\right]^\top = \sigma(v_j) = \left[\sigma\left(v_j^1\right), \dots, \sigma\left(v_j^q\right)\right]^\top$, where $v_j = C_1x_j + D_{11}w_j + D_{12}\hat{u}$ for any possible value \hat{u} of the function u(t) in time. By using the triangular inequality, we obtain

$$|p(x_1,t) - p(x_2,t)| = |A(x_1 - x_2) + B_1(w_1 - w_2)|$$

$$\leq |A| |x_1 - x_2| + |B_1| |w_1 - w_2|. \quad (37)$$

Using Assumption 1 and Assumption 2 we verify that $|w_1^1-w_2^1| \leq |C_1^{1:}||x_1-x_2|$, where $C_1^{i:}$ denotes the i^{th} row of C_1 , and we define $\kappa_1 = |C_1^{1:}|$. Proceeding similarly for each entry of w_1-w_2 we derive that, for every $r=2,3,\ldots,q$, it holds that $|w_1^r-w_2^r| \leq \kappa_r |x_1-x_2|$, with Lipschitz constants $\kappa_r = |C_1^{r:}| + \sum_{\ell=1}^{r-1} |D_{11}^{r,\ell}| \kappa_\ell$, where $D_{11}^{i,j}$ denotes the element in the i^{th} row and j^{th} column of D_{11} . Finally, from (37) we conclude $|p(x_1,t)-p(x_2,t)| \leq \kappa_{tot}|x_1-x_2|$, where $\kappa_{tot} = |A| + \sum_{i=1}^q |B_1^{i:}|\kappa_i$. Thus, the differential equation $\dot{x}(t) = f(x(t),u(t),t) = p(x(t),t)$ is globally Lipschitz in x with constant $\kappa_{tot} \in \mathbb{R}_0^+$ and its solution exists and it is unique.

B. Proof of Theorem 4

We first need a technical lemma.

Lemma 2. Let $p, m \in \mathbb{N}$, and $s = \max(p, m)$. Let $M \in \mathbb{R}^{s \times s}$, and $M = M^{\top} \succ 0$. Define

$$F = (I - M)(I + M)^{-1}, (38)$$

and $\tilde{F} = [F]_{p \times m}$. Then it follows that $I - \tilde{F}^{\top} \tilde{F} \succ 0$.

Proof. Notice that F as defined in (38) is the Cayley transformation of M. First, we list several properties of the Cayley transformation.

P1
$$M = M^{\top} \Rightarrow F = F^{\top}$$
,

P2
$$I + F = 2(I + M)^{-1}$$
,

P3
$$I - F = 2(I + M)^{-1}M$$
.

Moreover, note that the following properties hold for any symmetric matrices M, N:

P4 If
$$M\succ 0,\ N\succ 0$$
 and $MN=NM,$ then $MN\succ 0,$ P5 $(I+M)^{-1}M=M(I+M)^{-1}.$

We are now ready to prove the lemma based on these properties.

Let M be such that $M = M^{\top} \succ 0$. First, we prove that

$$I - F^{\top} F \succ 0. \tag{39}$$

This is equivalent to proving

$$(I+F)^{\top}(I-F) \succ 0, \tag{40}$$

since $F = F^{\top}$. Using P4, we prove (40) in three steps.

- 1) From property P2, (I+F) > 0 since $2(I+M)^{-1} > 0$ thanks to M > 0.
- 2) From property P3, (I-F) > 0 since $2(I+M)^{-1}M > 0$ from properties P4 and P5.
- 3) We prove that $(I+F)^{\top}$ and (I-F) are commutative:

$$(I+F)^{\top}(I-F) = I - F + F^{\top} + F^{\top}F$$
$$= I + F^{\top} - F + FF^{\top}$$
$$= (I-F)(I+F)^{\top}$$

where the second equality is valid from P1.

Then, (40) holds and this proves that $I - F^{\top}F \succ 0$.

Last, we prove that (39) implies $I - \tilde{F}^{\top} \tilde{F} \succ 0$. Note that if p = m then $\tilde{F} = F$ and this fact is trivial. We consider the two remaining cases p > m and m > p separately.

Assume that p>m. Then, $F=\begin{bmatrix} \tilde{F} \\ F_b \end{bmatrix}$. Hence, $I-F^\top F=I-\tilde{F}$. Hence, $I-\tilde{F}^\top F=I-\tilde{F}$.

Assume that m > p. Then, $F = \begin{bmatrix} \tilde{F} & F_r \end{bmatrix}$. Hence,

$$I - F^{\top} F = \begin{bmatrix} I - \tilde{F}^{\top} \tilde{F} & -\tilde{F}^{\top} F_r \\ -F_r^{\top} \tilde{F} & I - F_r^{\top} F_r \end{bmatrix} \succ 0,$$

and by applying the Schur complement, the above equation implies $I - \tilde{F}^{\top} \tilde{F} \succ 0$.

Note that the property (38) has also been used in [7]. In this work, we have derived a full proof for completeness. We are now ready to present the proof of Theorem 4.

Proof. Part 1): Define $Q = Q - \delta I$. Since $Q \prec 0$ and $R - S(Q - \delta I)^{-1}S^{\top} \succ 0$, there exist $L_Q \succ 0$ and $L_R \succ 0$ with

$$L_Q^\top L_Q = -\mathcal{Q} \,, \quad L_R^\top L_R = R - S\mathcal{Q}^{-1} S^\top \,. \tag{41}$$

Next, define $M=X_3^{\top}X_3+\epsilon I$ and $\tilde{F}=\left[(I-M)(I+M)^{-1}\right]_{p\times m}.$ Construct D_{22} as

$$D_{22} = -Q^{-1}S^{\top} + L_Q^{-1}\tilde{F}L_R. \tag{42}$$

We now show that this choice of D_{22} leads to $\tilde{\mathcal{R}} \succ 0$. Let $\Xi = R + SD_{22} + D_{22}^{\top}S^{\top} + D_{22}^{\top}\mathcal{Q}D_{22}$. Since $\tilde{\mathcal{R}} = \Xi + \delta D_{22}^{\top}D_{22}$, it suffices to prove that $\Xi \succ 0$. After plugging (42) in the definition of Ξ , we obtain $\Xi = L_{T}^{\top}(I - \tilde{F}^{\top}\tilde{F})L_{R}$

by cancellation of addends and by using (41). By Lemma 2 and since $L_R \succ 0$, we conclude that $\Xi \succ 0$.

Finally, we indicate how to construct (Y, W, Z) so that (30) holds. Compute Ψ from (31) and define

$$H = \begin{bmatrix} H_{11} & H_{12} \\ H_{21} & H_{22} \end{bmatrix} = X_R^\top X_R + \epsilon I + \Psi \,.$$

Then, using H, it is possible to use the same steps of Theorem 3 to compute (Y, W, Z) from (24)-(25), and P from (22). This choice satisfies the equality (30) by construction.

Part 2): We show how to parametrize the matrices in \tilde{A} . First, note that $P \succ 0$ is valid due to (22). Construct Λ and D_{11} using (26), and define the matrices (A, B_1, C_1, D_{11}) according to (27). Set

$$D_{12} = \Lambda^{-1} T \,. \tag{43}$$

Then, when choosing the parameters according to part 1 of this Theorem and plugging in the matrices just defined, Ψ satisfies $\Psi=\Psi^\top\succeq 0$ since $\tilde{\mathcal{R}}\succ 0$ and $Q\preceq 0$. Moreover, $H-\Psi=X_R^\top X_R+\epsilon I\succ 0$. Thus, $H=H^\top\succ 0$, and we have $W=W^\top\succ 0$ and $\Lambda\succ 0$. Thus, the NodeREN defined by $\{\tilde{A},\tilde{b}\}$ complies with (18), and thus it satisfies the incremental IQCs parametrized by (Q,S,R). \Box