

Learnability of Linear Port-Hamiltonian Systems

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Abstract

A complete structure-preserving learning scheme for single-input/single-output (SISO) linear port-Hamiltonian systems is proposed. The construction is based on the solution, when possible, of the unique identification problem for these systems, in ways that reveal fundamental relationships between classical notions in control theory and crucial properties in the machine learning context, like structure-preservation and expressive power. In the canonical case, it is shown that, up to initializations, the set of uniquely identified systems can be explicitly characterized as a smooth manifold endowed with global Euclidean coordinates, which allows concluding that the parameter complexity necessary for the replication of the dynamics is only $\mathcal{O}(n)$ and not $\mathcal{O}(n^2)$, as suggested by the standard parametrization of these systems. Furthermore, it is shown that linear port-Hamiltonian systems can be learned while remaining agnostic about the dimension of the underlying data-generating system. Numerical experiments show that this methodology can be used to efficiently estimate linear port-Hamiltonian systems out of input-output realizations, making the contributions in this paper the first example of a structure-preserving machine learning paradigm for linear port-Hamiltonian systems based on explicit representations of this model category.

Keywords: Linear port-Hamiltonian system, machine learning, structure-preserving algorithm, systems theory, physics-informed machine learning, unique identification problem, controllable representation, observable representation, canonical representation.

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1. Introduction

Machine learning has experienced substantial development in recent years due to significant advances in algorithmics and a fast growth in computational power. The universal approximation properties of neural networks (Cybenko (1989); Hornik et al. (1989)) and other similar families make it possible for them to learn any function with very few prior assumptions. A typical modus operandi in supervised machine learning is first to choose a neural network architecture, to perform forward propagation using available data, to compute some loss function, and then to carry out backward propagation, that is, gradient descent, to recursively optimize the parameters. This paradigm has proved to be very successful in the learning of numerous complicated tasks, including time-series forecasting (Hochreiter and Schmidhuber (1997)), computer vision (Krizhevsky et al. (2012)), and natural language processing (Devlin et al. (2018)).

In physics and engineering, machine learning is called to play an essential role in predicting and integrating the equations associated with physical dynamical systems. Physical systems are primarily formulated in terms of ordinary, time-delay, and partial differential equations that can be deduced mostly from variational principles. Consequently, some researchers propose to learn adequately discretized versions of their corresponding vector fields (see, for instance, Raissi and Karniadakis (2017), Qin et al. (2019), Long et al. (2018), and references therein). In addition to vector fields learning, researchers have proposed “model-free” methods like *transformers* (Shalova and Oseledets (2020); Acciaio et al. (2022)), *reservoir computing* (Jaeger and Haas (2004); Lu et al. (2018); Pathak et al. (2018a,b)), *recurrent neural networks* (Bailer-Jones et al. (1998)), *convolutional neural networks* (Mukhopadhyay and Banerjee (2020)), or *LSTMs* (Wang (2017)).

Various universal approximation properties theoretically explain the empirical success of some of these approaches (see, for instance, Grigoryeva and Ortega (2018a,b); Gonon and Ortega (2020, 2021)) of some of these learning paradigms. Nevertheless, for physics-related problems, like in mechanics or optics, it is natural to build into the learning algorithm any prior knowledge that we may have about the system based on physics’ first principles. This may include specific forms of the laws of motion, conservation laws, symmetry invariance, as well as other underlying geometric and variational structures. This observation regarding the construction of structure-preserving schemes has been profusely exploited with much success before the emergence of machine learning in the field of numerical integration (Gonzalez (2000); Marsden and West (2001); Leimkuhler and Reich (2004); McLachlan and Quispel (2006)). Many examples in that context show how the failure to maintain specific conservation laws can lead to physically inconsistent solutions.

The translation of this idea to the context of machine learning has led to the emergence of a new domain collectively known as *physics-informed machine learning* (see Raissi et al. (2017); Wu et al. (2018); Karniadakis et al. (2021) and references therein). In the specific case of Hamiltonian systems, the two main structural constraints are that the flow is symplectic and the energy, that is, the Hamiltonian, is conserved along the flow. Additionally, symmetries are frequently present, which carries the emergence of additional conserved quantities in the form of the so-called momentum maps via Noether’s Theorem (Abraham and Marsden (1978); Marsden and Ratiu (1999); Ortega and Ratiu (2004)). These are all examples of qualitative properties to be preserved by the learning algorithms. Needless

to say, the above-mentioned “model-free” approaches generically fail to preserve all these structures. With these in mind, several attempts have been made in the literature to develop tailor-made learning algorithms for Hamiltonian systems. For example, in Greydanus et al. (2019); Celledoni et al. (2023), neural methods are proposed to learn the Hamiltonian function directly. In Chen et al. (2020), a symplectic recurrent neural network is proposed that uses symplectic integration while matching the predictions and observations and leads to a structure-preserving paradigm. Other structure-preserving methods include the so-called SympNet (Jin et al. (2020)), the generating function neural networks (GFNN) in Chen and Tao (2021), and the symplectic reversible neural networks in Valperga et al. (2022). SympNet constructs a universal approximating family of symplectic maps, while GFNN applies a modified KAM theory to control long-term prediction error. Symplectic reversible neural networks are also proposed as a family of universal approximating maps that concern, in particular, reversible symplectic dynamics. In Zhong et al. (2020), a parametric framework of learning Hamiltonian state dynamics with control is proposed, assuming that the Hamiltonian is separable. Under the same assumption, Tong et al. (2021) proposes to learn with a parametrized Hamiltonian in a Taylor series form.

This paper’s focus differs from the references mentioned above in two ways. First, these methods are designed to learn the state evolution of Hamiltonian systems, whereas our approach focuses on *learning the input-output dynamics of port-Hamiltonian systems while remaining agnostic about the physical state space*. As will be introduced later, these systems have an underlying Dirac structure that describes the geometry of numerous physical systems with external inputs (van der Schaft and Jeltsema (2014)) and includes the dynamics of the observations of Hamiltonian systems as a particular case. Even though various learning schemes for these systems have already been proposed in the literature (Nagesh Rao et al. (2015); Cherifi (2020); Desai et al. (2021); Beckers et al. (2022)), most works on the learning of Hamiltonian systems deal with autonomous (separable) Hamiltonian systems on which one assumes access to the entire phase space and not only to its observations. Second, instead of a general nonlinear system for which only approximation error can be possibly estimated, we consider, as a first approach *exclusively linear systems*, in which case, we can obtain explicit representations of linear port-Hamiltonian systems in normal form and characterize the symmetries and quotient spaces associated to the invariance by system automorphisms. Thereby, we propose a structure-preserving learning paradigm with a provable minimal parameter space.

The contributions in this paper are contained in several results that we briefly introduce in the following lines. In Section 2, we define the notion of linear port-Hamiltonian systems in normal form and present some necessary introductory concepts. We start in Theorem 7 by introducing system morphisms that allow us to represent any linear port-Hamiltonian system in normal form as the image of another linear system of the same dimension in which the state equation is in controllable canonical form. An obvious observation is that since the constructed linear system and the original port-Hamiltonian system are linked by a system morphism, the input/output relations of the former are input/output relations of the latter once the initial state conditions have been properly set up. In particular, the new system can be used to learn to reproduce the input/output dynamics of the original port-Hamiltonian system (for a subspace of initial conditions) and *this learning paradigm is structure-preserving by construction*. Similarly, Theorem 7 also contains another type of

system morphisms that link any linear port-Hamiltonian system in normal form to some linear system of the same dimension in observable canonical form. Consequently, the input-output relations of the original port-Hamiltonian system with respect to any initial condition can be captured by the observable Hamiltonian representation. Both representations are derived based on classical techniques from control theory, the Cayley-Hamilton theorem, and are ultimately corollaries of the Williamson normal form (Williamson (1936, 1937); Ikramov (2018)). We show that the controllable and observable representations are closely related to each other, and both system morphisms become isomorphisms for canonical port-Hamiltonian systems. However, for the purpose of learning a general port-Hamiltonian system that may not be canonical, we reveal that there is a trade-off between the structure-preserving property and the expressive power. These results establish a strong link between classical notions in the control theory, that is, controllability and observability, and those in machine learning, namely, structure-preservation and expressive power.

Based on these explicit constructions and using the parametrizations that come with them, we aim to tackle in Section 4 the unique identifiability of input-output dynamics of linear port-Hamiltonian systems in normal form. Such a characterization is obviously needed to solve the model estimation problem since, in applications, we only have access to input/output data, and different state space systems can induce the same filter that produces that data. This fact has important implications when it comes to the learning of port-Hamiltonian systems out of finite-sample realizations of a given data-generating process because such degeneracy makes impossible its exact recovery. Said differently, it is not the space of port-Hamiltonian systems that needs to be characterized but its quotient space with respect to the equivalence relation defined by the constraint on inducing the same input/output filter. We shall see in Subsection 4.1 that the presence of non-canonical systems in PH_n and possible initialization inconsistencies make it, in general, difficult to directly characterize that quotient space by filter-equivalence and we shall settle for the closest to it that we can get, namely, the quotient space by system automorphisms that, as it will be justified, approximates the general case in a certain sense and admits an explicit characterization as a Lie groupoid orbit space (Subsection 4.3). In Subsection 4.4, we restrict our identification analysis to canonical port-Hamiltonian systems and show, first, that in that situation eliminating the system isomorphisms completely identifies the set of input/output systems up to state initializations (Sussmann (1976)), and second, that the corresponding quotient spaces can be characterized as orbit spaces with respect to a group (as opposed to a groupoid in the general unrestricted case) action, where the group is explicitly given by a semi-direct product. Moreover, (see Subsection 4.6) this orbit space can be explicitly endowed with a smooth manifold structure that has global Euclidean coordinates that can be used at the time of constructing estimation algorithms. Consequently, up to state initializations, canonical port-Hamiltonian dynamics can be identified fully and explicitly in either the controllable or the observable Hamiltonian representations and learned by estimating an initial state condition and a unique set of parameters in a smooth manifold that is obtained as a group orbit space.

Another learning-related problem that we tackle is that, in applications, one is obliged to remain agnostic as to the dimension of the underlying data-generating port-Hamiltonian system. This leads to the difficulty of choosing the dimension of the controllable/observable Hamiltonian representations. We solve this issue by proving in Theorem 34 that, for $m \geq n$,

any $2n$ -dimensional linear port-Hamiltonian system in normal form can be regarded as the restriction of a $2m$ -dimensional one to some subspace. This fact, together with some subsequent results, guarantees theoretically that we can choose a sufficiently large m in practice and parametrize the observable Hamiltonian representation in dimension $2m$ and use it for learning without assuming any knowledge about the dimension of the data generating system. The paper concludes with some numerical examples in Section 7 that illustrate the viability of the method that we propose in systems with various levels of complexity and dimensions, as well as the computational advantages associated with using the parameter space in which unique identification is guaranteed. For the reader's convenience, the Python code necessary to reproduce these numerics is public and can be found in <https://github.com/YINDAIYING/Learnability-of-Linear-Port-Hamiltonian-Systems>.

2. Preliminaries

In this section, we introduce various notions and preliminary results necessary to understand the context and the contributions of the paper.

2.1 State-space systems and morphisms

A continuous time state-space system is given by the following two equations

$$\begin{cases} \dot{\mathbf{z}} = F(\mathbf{z}, u), \\ y = h(\mathbf{z}), \end{cases} \quad (1)$$

where $u \in \mathcal{U}$ is the *input*, $\mathbf{z} \in \mathcal{Z}$ is the *internal state* and $F : \mathcal{Z} \times \mathcal{U} \rightarrow \mathcal{Z}$ is called the *state map*. The first equation is called the *state equation* while the second one is usually referred to as the *observation equation*. The solutions of (1) (when available and unique) yield an input/output map that is by construction causal and time-invariant. State-space systems will be sometimes denoted using the triplet (\mathcal{Z}, F, h) .

Definition 1 *A map $f : \mathcal{Z}_1 \rightarrow \mathcal{Z}_2$ is called a system morphism (see Grigoryeva and Ortega (2021)) between the continuous-time state-space systems $(\mathcal{Z}_1, F_1, h_1)$ and $(\mathcal{Z}_2, F_2, h_2)$ if it satisfies the following two properties:*

- (i) *System equivariance: $f(F_1(\mathbf{z}_1, u)) = F_2(f(\mathbf{z}_1), u)$, for all $\mathbf{z}_1 \in \mathcal{Z}_1$ and $u \in \mathcal{U}$.*
- (ii) *Readout invariance: $h_1(\mathbf{z}_1) = h_2(f(\mathbf{z}_1))$ for all $\mathbf{z}_1 \in \mathcal{Z}_1$.*

As a direct consequence of this definition, the composition of system morphisms is again a system morphism. In the case f is invertible and f^{-1} is also a morphism, we say that f is a system isomorphism. An elementary but very important fact is that if $f : \mathcal{Z}_1 \rightarrow \mathcal{Z}_2$ is a linear system-equivariant map between $(\mathcal{Z}_1, F_1, h_1)$ and $(\mathcal{Z}_2, F_2, h_2)$ (\mathcal{Z}_1 and \mathcal{Z}_2 are in this case vector spaces) then, for any solution $\mathbf{z}_1 \in C^1(I, \mathcal{Z}_1)$ of the state equation associated to F_1 and to the input $u \in C^1(I, \mathcal{U})$, with $I \subset \mathbb{R}$ an interval, its image $f \circ \mathbf{z}_1 \in C^1(I, \mathcal{Z}_2)$ is a solution for the state space system associated to F_2 with the same input. Indeed, for any $t \in I$ we have, by the linearity and the system equivariance of f :

$$\frac{d}{dt}[f(\mathbf{z}_1(t))] = Df(\mathbf{z}_1(t)) \cdot \dot{\mathbf{z}}_1(t) = f(\dot{\mathbf{z}}_1(t)) = f(F_1(\mathbf{z}_1(t), u(t))) = F_2(f(\mathbf{z}_1(t)), u(t)).$$

Notice that if at time $t = 0$, the output of both systems $(\mathcal{Z}_1, F_1, h_1)$ and $(\mathcal{Z}_2, F_2, h_2)$ are the same, that is, the initial conditions $\mathbf{z}_1(0)$ and $\mathbf{z}_2(0)$ at the time of integrating (1) are chosen so that $h_1(\mathbf{z}_1(0)) = h_2(f(\mathbf{z}_1(0)))$, then the two systems $(\mathcal{Z}_1, F_1, h_1)$ and $(\mathcal{Z}_2, F_2, h_2)$ have the same associated input/output relation, in the sense that we introduce later on in definition (7). This observation has an important consequence, namely that, in general, input/output systems *are not uniquely identified* since all the system-isomorphic state-space systems with appropriate initializations yield the same input/output map.

2.2 Hamiltonian and port-Hamiltonian systems

Hamiltonian systems are dynamical systems whose behavior is governed by Hamilton's variational principle. Even though these autonomous systems can be in general formulated on any symplectic manifold (Abraham and Marsden (1978)), we will restrict in this paper to the case in which the phase space is the even-dimensional vector space \mathbb{R}^{2n} endowed with the Darboux canonical symplectic form. In this case, the *Hamiltonian system* determined by the *Hamiltonian function* $H \in C^1(\mathbb{R}^{2n})$ is given by the differential equation

$$\dot{\mathbf{z}} = \mathbb{J} \frac{\partial H}{\partial \mathbf{z}}, \quad (2)$$

where $\mathbb{J} = \begin{bmatrix} 0 & \mathbb{I}_n \\ -\mathbb{I}_n & 0 \end{bmatrix}$ is the so-called the *canonical symplectic matrix*. Note that $-\mathbb{J} = \mathbb{J}^T = \mathbb{J}^{-1}$ and hence endows \mathbb{R}^{2n} also with a complex structure. In this paper, we will denote the canonical symplectic matrix as \mathbb{J} , unless the context requires to specify the dimension, in which case we denote it by \mathbb{J}_n .

A *linear* Hamiltonian system is determined by a quadratic Hamiltonian function $H(\mathbf{z}) = \frac{1}{2} \mathbf{z}^T Q \mathbf{z}$, where $\mathbf{z} \in \mathbb{R}^{2n}$ and $Q \in \mathbb{M}_{2n}$ is a square matrix that without loss of generality can be assumed to be symmetric. In this case, Hamilton's equations (2) reduce to

$$\dot{\mathbf{z}} = \mathbb{J} Q \mathbf{z}. \quad (3)$$

Port-Hamiltonian systems (see van der Schaft and Jeltsema (2014)) are state-space systems that generalize autonomous Hamiltonian systems to the case in which external signals or inputs control in a time-varying way the dynamical behavior of the Hamiltonian system. The family of input-state-output port-Hamiltonian systems are those port-Hamiltonian systems with no algebraic constraints on the state-space variables, and where the flow and effort variables of the resistive, control and interaction ports are split into conjugated pairs. In such cases, the implicit representation may be proved (see van der Schaft and Jeltsema (2014)) to be equivalent to the following explicit form:

$$\begin{cases} \dot{\mathbf{x}} = [J(\mathbf{x}) - R(\mathbf{x})] \frac{\partial H}{\partial \mathbf{x}}(\mathbf{x}) + g(\mathbf{x})u, \\ y = g^T(\mathbf{x}) \frac{\partial H}{\partial \mathbf{x}}(\mathbf{x}), \end{cases} \quad (4)$$

where (u, y) is the input-output pair (corresponding to the control and output conjugated ports), $J(\mathbf{x})$ is a skew-symmetric interconnection structure and $R(\mathbf{x})$ is a symmetric positive-definite dissipation matrix. Our work concerns *linear* port-Hamiltonian systems in the

normal form which we define now: a linear port-Hamiltonian system (4) is in normal form if the skew-symmetric matrix J is constant and equal to the canonical symplectic matrix \mathbb{J} , the Hamiltonian matrix Q is symmetric positive-definite, and the energy dissipation matrix $R = 0$, in which case (4) takes the form:

$$\begin{cases} \dot{\mathbf{z}} = \mathbb{J}Q\mathbf{z} + Bu, \\ y = B^T Q\mathbf{z}, \end{cases} \quad (5)$$

with $\mathbf{z} \in \mathbb{R}^{2n}$, $u, y \in \mathbb{R}$, and where $B \in \mathbb{R}^{2n}$ specifies the interconnection structure simultaneously at the input and output levels. By definition, such systems are fully determined by the pair (Q, B) , and hence we define by

$$\Theta_{PH_n} := \{(Q, B) | 0 < Q \in \mathbb{M}_{2n}, Q = Q^T, B \in \mathbb{R}^{2n}\} \quad (6)$$

the space of *parameters* of (5). Let $\theta_{PH_n} : \Theta_{PH_n} \rightarrow PH_n$ the map that associates to the parameter $(Q, B) \in \theta_{PH_n}$ the corresponding port-Hamiltonian state space system. For convenience, *we shall often use (Q, B) to denote elements in PH_n unless there is a risk of confusion*. Note that the condition $Q > 0$ implies that the origin is a Lyapunov stable equilibrium of (3). All these systems have the existence and uniqueness of solutions property and hence determine a family of *input/output systems*, also known as *filters*, that will be denoted by \mathcal{PH}_n . More specifically, the elements in \mathcal{PH}_n are maps $U_{(Q,B)} : C^1([0, 1]) \times \mathbb{R}^{2n} \rightarrow C^1([0, 1])$ given by

$$\begin{aligned} U_{(Q,B)} : C^1([0, 1]) \times \mathbb{R}^{2n} &\longrightarrow C^1([0, 1]) \\ (u, \mathbf{x}_0) &\longmapsto U_{(Q,B)}(u, \mathbf{x}_0)_t = B^T Q e^{\mathbb{J}Qt} \left[\int_0^t e^{-\mathbb{J}Qs} Bu(s) ds + \mathbf{x}_0 \right], \end{aligned} \quad (7)$$

$t \in [0, 1]$. Note that PH_n includes as a special case linear observations of autonomous linear Hamiltonian systems (case $B = 0$). Note that as a manifold $\Theta_{PH_n} = \mathcal{S}_{2n}^+ \times \mathbb{R}^{2n}$, where \mathcal{S}_{2n}^+ denotes the space of symmetric positive-definite matrices (SPD). We recall that \mathcal{S}_{2n}^+ has a natural differentiable manifold structure whose tangent space at any point is the vector space of symmetric matrices \mathcal{S}_{2n} (see Quang Minh and Murino (2018), and references therein).

Port-Hamiltonian systems are also closely linked to the so-called *affine Hamiltonian input-output systems* that have been considered as a natural extension of Hamiltonian systems with external forces and studied extensively in the literature (see Crouch and van der Schaft (1987) for the deterministic case and Bismut (1982); Lázaro-Camí and Ortega (2008) for stochastic extensions), which take the form

$$\begin{cases} \dot{\mathbf{x}} = X_H(\mathbf{x}) + X_g(\mathbf{x})u, \\ \tilde{y} = g(\mathbf{x}), \end{cases} \quad (8)$$

where X_H and X_g are the Hamiltonian vector fields of $H, g \in C^1(\mathbb{R}^{2n})$. In the linear case, (8) reduces to

$$\begin{cases} \dot{\mathbf{z}} = \mathbb{J}Q\mathbf{z} - \mathbb{J}Bu, \\ \tilde{y} = B^T \mathbf{z}, \end{cases} \quad (9)$$

The relation between (9) and (5) is that $\dot{y} = B^T \dot{z} = B^T \mathbb{J} Q z = (-\mathbb{J} B)^T Q z$, showing that the time derivative of the affine Hamiltonian input-output system has a port-Hamiltonian structure. Note that in the last equality, we used that $B^T \mathbb{J} B = 0$ since \mathbb{J} is antisymmetric.

Consider now a general linear single-input/single-output system that takes the form

$$\begin{cases} \dot{\mathbf{x}} = A\mathbf{x} + Bu, \\ y = C^T \mathbf{x}, \end{cases} \quad (10)$$

where $A \in \mathbb{M}_n$, $B, C \in \mathbb{R}^n$. Very often in control theory, it is the so-called transfer matrix rather than the input/output system which is studied. The transfer matrix $G(s)$ of (10) is defined as $G(s) = C^T (\mathbb{I}s - A)B$ and converts the differential equations in the time domain to an algebraic equation in the Laplace frequency domain. It can be proved that the transfer matrix of the port-Hamiltonian systems (5) satisfies $G(s) = -G(-s)$ and that of systems of the type (9) satisfies $G(s) = G(-s)$. The converse statements also hold for canonical realizations (see the definition in the next section and Brockett and Rahimi (1972), Maschke and van der Schaft (1992)). These facts are a strong indication that the systems (5) and (9) carry intrinsic symmetries that should be explicitly characterized. We shall do so in Section 4 for port-Hamiltonian systems but only using the original state-space representation.

2.3 Controllability and observability

Given a general linear system like (10), we recall that its *controllability* and *observability matrices* are defined by

$$[B \mid AB \mid \dots \mid A^{n-1}B] \quad \text{and} \quad \begin{bmatrix} C^T \\ C^T A \\ \vdots \\ C^T A^{n-1} \end{bmatrix}, \quad \text{respectively.}$$

The system is called *controllable* (respectively, *observable*) if its controllability (respectively, observability) matrix has full rank. Any linear controllable (respectively, observable) system can be transformed into the so-called controllable (respectively, observable) canonical forms by using appropriate linear system isomorphisms (see Polderman and Willems (1998)). Conversely, systems in these canonical forms are automatically controllable (respectively, observable). In the next section, we characterize the controllable/observable/canonical systems in the linear port-Hamiltonian category.

Controllability and observability are intertwined concepts in the linear port-Hamiltonian category. Indeed, it can be proved (see Medianu et al. (2013)) that if a linear port-Hamiltonian system without dissipation is controllable and $\det(Q) \neq 0$, then it is also observable. Conversely, if it is observable, then this implies that $\det(Q) \neq 0$ and it is also controllable (see Medianu et al. (2013)). As it is customary in systems theory, we say a linear port-Hamiltonian system in normal form is *canonical* if it is both controllable and observable. In view of the results that we just recalled, if $\det(Q) \neq 0$, then either controllability or observability is equivalent to the system being canonical. Furthermore, it can be shown that being canonical is a generic property, that is, the set of canonical systems forms an open and dense subset. We shall denote by $PH_n^{can} \subset PH_n$ the subset of PH_n made of

canonical linear port-Hamiltonian systems. Later on in the paper, the significance of these observations will become apparent.

2.4 The symplectic Lie group and its Lie algebra

A square matrix $S \in \mathbb{M}_{2n}$ in dimension $2n$ is called *symplectic* if it satisfies $S^T \mathbb{J} S = \mathbb{J}$. The set of all symplectic matrices forms a Lie group denoted by $Sp(2n, \mathbb{R})$. It is well-known that if $S \in Sp(2n, \mathbb{R})$ then $\det(S) = \pm 1$ and hence $Sp(2n, \mathbb{R})$ is a subgroup of the general linear group $GL(2n, \mathbb{R})$. The Lie algebra $\mathfrak{sp}(2n, \mathbb{R})$ of $Sp(2n, \mathbb{R})$ is given by the matrices $A \in \mathbb{M}_{2n}$ that satisfy the identity $A^T \mathbb{J} + \mathbb{J} A = 0$. Equivalently, $A \in \mathfrak{sp}(2n, \mathbb{R})$ if and only if $A = \mathbb{J} R$, where $R \in \mathbb{M}_{2n}$ is symmetric. We will refer to the elements in $Sp(2n, \mathbb{R})$ as *symplectic matrices* and to those in $\mathfrak{sp}(2n, \mathbb{R})$ as *infinitesimally symplectic*.

Notably, the eigenvalues of the elements in $\mathfrak{sp}(2n, \mathbb{R})$ appear in specific patterns that are spelled out in the following classical proposition (see (Abraham and Marsden, 1978, Section 3.1)).

Proposition 2 *The characteristic polynomial of any matrix in $A \in \mathfrak{sp}(2n, \mathbb{R})$ is even. Thus, if λ is an eigenvalue of A then so are $-\lambda$, $\bar{\lambda}$, and $-\bar{\lambda}$.*

The importance of this group in our developments is that the (constant) vector field associated with the Hamilton's equations (3) is an element in $\mathfrak{sp}(2n, \mathbb{R})$. Its flow determines a one-parameter subgroup of elements in $Sp(2n, \mathbb{R})$. We also introduce the unitary group $U(n, \mathbb{C})$, which consists of matrices $U \in \mathbb{M}_n(\mathbb{C})$ with $UU^* = U^*U = \mathbb{I}_n$, where U^* denotes the conjugate transpose of U . We denote by $U(n)$ (see De Gosson (2006)) the image of $U(n, \mathbb{C})$ in $Sp(2n, \mathbb{R})$ by the monomorphism

$$A + iB \rightarrow \begin{bmatrix} A & -B \\ B & A \end{bmatrix}. \quad (11)$$

The so-called *2-out-of-3 property* (Arnold (1989)) implies that $U(n) = O(2n, \mathbb{R}) \cap GL(n, \mathbb{C}) \cap Sp(2n, \mathbb{R})$, and it is indeed the intersection of any two out of the three groups.

2.5 Williamson's normal form

The following classical result can be found in Williamson (1936, 1937); Ikramov (2018); De Gosson (2006).

Theorem 3 *Let $M \in \mathbb{M}_{2n}$ be a positive-definite symmetric real matrix. Then*

(i) *There exists a symplectic matrix $S \in Sp(2n, \mathbb{R})$ such that $M = S^T \begin{bmatrix} D & 0 \\ 0 & D \end{bmatrix} S$, with $D = \text{diag}(\mathbf{d})$ an n -dimensional diagonal matrix with positive entries and $\mathbf{d} = (d_1, \dots, d_n)^T$.*

(ii) *The values d_1, \dots, d_n are independent, up to reordering, on the choice of the symplectic matrix S used to diagonalize M .*

(iii) Assume S and S' are two elements of $Sp(2n, \mathbb{R})$ such that $M = S^T \begin{bmatrix} D & 0 \\ 0 & D \end{bmatrix} S = S'^T \begin{bmatrix} D & 0 \\ 0 & D \end{bmatrix} S'$, where D is as above, then $S(S')^{-1} \in U(n)$.

Later in this paper, we always use the notation $D = \text{diag}(\mathbf{d})$ to denote that D is a diagonal matrix with diagonal entries given by the vector $\mathbf{d} = (d_1, \dots, d_n)^T$. The elements d_i in the above theorem are called the *symplectic eigenvalues* of M since they are also the eigenvalues of $\mathbb{J}M$.

Remark 4 The above theorem can be generalized to *positive-semidefinite* real symmetric matrices. Indeed, it can first be shown that if the kernel of M is a symplectic subspace of \mathbb{R}^{2n} of dimension $2m$, then the statement of Theorem 3 still holds true with the only added feature that exactly m of the diagonal entries in D are equal to 0 (see Son and Stykel (2022)). More generally, without the symplecticity assumption, all that it can be said is that there exists $S \in Sp(2n, \mathbb{R})$ such that $M = S^T \begin{bmatrix} D_1 & 0 \\ 0 & D_2 \end{bmatrix} S$ where D_1 and D_2 may contain diagonal zero entries (see Idel et al. (2017); Egusquiza and Parra-Rodriguez (2022)).

3. Controllable and observable Hamiltonian representations

In this section, we state two representation results for linear port-Hamiltonian systems in normal form, which are the main building blocks in our learnability results. More precisely, we define two subfamilies of linear systems of the type (10), that are respectively called controllable/observable Hamiltonian representations, that are by construction controllable/observable (Definition 5). We subsequently show in Theorem 7 that morphisms can be established between the elements in these families and those in the category PH_n of normal form port-Hamiltonian systems.

As it will be spelled out later on in detail, the existence of these morphisms immediately guarantees that the complexity of the family of filters \mathcal{PH}_n is actually not $\mathcal{O}(n^2)$, as it could be guessed from (5), but $\mathcal{O}(n)$. However, our proposed representations have certain limitations for non-canonical port-Hamiltonian systems. For example, the observable representation is guaranteed to capture all possible input-output dynamics of port-Hamiltonian systems (full expressive power), but it does not always produce port-Hamiltonian dynamics (fails to be structure-preserving). In the controllable case, structure preservation is guaranteed, but there is, in general, no full expressive power. Fortunately, for canonical port-Hamiltonian systems, all the morphisms that we shall introduce become isomorphisms, meaning that they are both structure-preserving and have full expressive power. Roughly speaking, the more canonical a port-Hamiltonian system is, the better the corresponding representations behave in terms of structure-preserving properties and expressive power.

The representations introduced below can be seen as a reparametrization of the elements $(Q, B) \in PH_n$ in terms of a diagonal matrix $D = \text{diag}(\mathbf{d}) \in \mathbb{M}_n$, $\mathbf{d} \in \mathbb{R}^n$, and a vector $\mathbf{v} \in \mathbb{R}^{2n}$, where D is obtained from Williamson's Theorem 3 as $Q = S^T \begin{bmatrix} D & 0 \\ 0 & D \end{bmatrix} S$ and $\mathbf{v} = S \cdot B$. This makes it obvious that the learning problem for port-Hamiltonian systems

has parameter complexity of at most $\mathcal{O}(n)$ even if the Hamiltonian matrix has complexity $\mathcal{O}(n^2)$.

We emphasize that even in the canonical situation, the availability of the controllable/observable representations does not yet provide a well-specified learning problem for this category since the invariance of these systems under system automorphisms implies the existence of symmetries (or degeneracies) in the parametrizations, which will be the focus of the next section.

The proofs of all our results are provided in the appendices.

Definition 5 Given $\mathbf{d} = (d_1, \dots, d_n)^T \in \mathbb{R}^n$, with $d_i > 0$, and $\mathbf{v} \in \mathbb{R}^{2n}$, we say that a $2n$ -dimensional linear state space system is a controllable Hamiltonian (respectively, observable Hamiltonian) representation if it takes the form

$$\begin{cases} \dot{\mathbf{s}} = g_1^{ctr}(\mathbf{d}) \cdot \mathbf{s} + (0, 0, \dots, 0, 1)^T \cdot u, \\ y = g_2^{ctr}(\mathbf{d}, \mathbf{v}) \cdot \mathbf{s}, \end{cases} \quad \left(\text{resp.}, \begin{cases} \dot{\mathbf{s}} = g_1^{obs}(\mathbf{d}) \cdot \mathbf{s} + g_2^{obs}(\mathbf{d}, \mathbf{v}) \cdot u, \\ y = (0, 0, \dots, 0, 1) \cdot \mathbf{s}, \end{cases} \right) \quad (12)$$

where $g_1^{ctr}(\mathbf{d}) \in \mathbb{M}_{2n}$ and $g_2^{ctr}(\mathbf{d}, \mathbf{v}) \in \mathbb{M}_{1,2n}$ (respectively, $g_1^{obs}(\mathbf{d}) \in \mathbb{M}_{2n}$ and $g_2^{obs}(\mathbf{d}, \mathbf{v}) \in \mathbb{R}^{2n}$) are constructed as follows:

(i) Given $\mathbf{d} \in \mathbb{R}^n$, let $\{a_0, a_1, \dots, a_{2n-1}\}$ be the real coefficients that make $\lambda^{2n} + \sum_{i=0}^{2n-1} a_i \cdot \lambda^i = (\lambda^2 + d_1^2)(\lambda^2 + d_2^2) \dots (\lambda^2 + d_n^2)$ an equality between the two polynomials in λ . Let $a_{2n} = 1$ by convention. Note that the entries a_i with an odd index i are zero. Define:

$$g_1^{ctr}(\mathbf{d}) := \begin{bmatrix} 0 & 1 & 0 & \dots & 0 \\ 0 & 0 & 1 & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \dots & 1 \\ -a_0 & -a_1 & -a_2 & \dots & -a_{2n-1} \end{bmatrix}_{2n \times 2n},$$

(respectively, $g_1^{obs}(\mathbf{d}) = g_1^{ctr}(\mathbf{d})^\top$).

(ii) Given \mathbf{d} and \mathbf{v} , then

$$g_2^{ctr}(\mathbf{d}, \mathbf{v}) := [0 \ c_{2n-1} \ 0 \ c_{2n-3} \ \dots \ 0 \ c_1], \quad (\text{resp.}, g_2^{obs}(\mathbf{d}, \mathbf{v}) = g_2^{ctr}(\mathbf{d}, \mathbf{v})^\top)$$

where

$$c_{2k+1} = \mathbf{v}^\top \begin{bmatrix} F_k & 0 \\ 0 & F_k \end{bmatrix} \mathbf{v},$$

for $k = 0, \dots, n-1$, and

$$F_k = \begin{bmatrix} f_1 & & & & \\ & f_2 & & & 0 \\ & & \ddots & & \\ & & & f_{n-1} & \\ 0 & & & & f_n \end{bmatrix}$$

with $f_l = d_l \cdot \sum_{\substack{j_1, \dots, j_k \neq l \\ 1 \leq j_1 < \dots < j_k \leq n}} (d_{j_1} d_{j_2} \dots d_{j_k})^2$, $l = 1, \dots, n$.

We denote CH_n (respectively, OH_n) the set of all systems of the form (12), and we call them controllable Hamiltonian (respectively, observable Hamiltonian) representations. The symbol \mathcal{CH}_n (respectively, \mathcal{OH}_n) denotes the set of input/output systems induced by the state space systems in CH_n (respectively, OH_n). We emphasize that the elements of both CH_n and OH_n can be parameterized with the set

$$\Theta_{CH_n} = \Theta_{OH_n} := \{(\mathbf{d}, \mathbf{v}) \mid d_i > 0, \mathbf{v} \in \mathbb{R}^{2n}\}.$$

Sometimes later on in the paper we shall write $a_i(\mathbf{d})$ and $c_j(\mathbf{d}, \mathbf{v})$ to indicate that a_i and c_j are functions of \mathbf{d} and \mathbf{v} .

Remark 6 Observe that the controllable and the observable Hamiltonian representations of port-Hamiltonian systems are closely related to each other. The controllable Hamiltonian matrix g_1^{ctr} is the transpose of the observable Hamiltonian matrix g_1^{obs} . Moreover, as can be directly observed from the construction, the input and readout matrices of the two representations, that is, g_2^{ctr} and g_2^{obs} , are transpose of each other.

Consider now the maps $\theta_{CH_n} : \Theta_{CH_n} \rightarrow CH_n$ and $\theta_{OH_n} : \Theta_{OH_n} \rightarrow OH_n$ that associate to each parameter values the corresponding state-space system. Note that the elements in CH_n (respectively, in OH_n) of the form (12) are in canonical controllable (respectively, observable) form in the sense of Sontag (1998) and they are hence controllable (respectively, observable). Our main result below establishes a relationship between port-Hamiltonian systems and controllable (respectively, observable) Hamiltonian representations as defined above, which will be used later on for considerations on the structure preservation and expressiveness in the modeling of PH_n .

Theorem 7 (i) *There exists, for each $S \in Sp(2n, \mathbb{R})$, a map*

$$\begin{aligned} \varphi_S : \quad CH_n &\longrightarrow PH_n \\ \theta_{CH_n}(\mathbf{d}, \mathbf{v}) &\longmapsto \theta_{PH_n} \left(S^T \begin{bmatrix} D & 0 \\ 0 & D \end{bmatrix} S, S^{-1}\mathbf{v} \right), \end{aligned}$$

with $D = \text{diag}(\mathbf{d})$, such that the controllable Hamiltonian system $\theta_{CH_n}(\mathbf{d}, \mathbf{v}) \in CH_n$ and the port-Hamiltonian image $\varphi_S(\theta_{CH_n}(\mathbf{d}, \mathbf{v})) \in PH_n$ are linked by a linear system morphism $f_S^{(\mathbf{d}, \mathbf{v})} : \mathbb{R}^{2n} \rightarrow \mathbb{R}^{2n}$.

(ii) *Given a port-Hamiltonian system $\theta_{PH_n}(Q, B) \in PH_n$, there exists an explicit linear system morphism $f^{(Q, B)} : \mathbb{R}^{2n} \rightarrow \mathbb{R}^{2n}$ between the state space of $\theta_{PH_n}(Q, B) \in PH_n$ and that of an observable Hamiltonian system $\theta_{OH_n}(\mathbf{d}, \mathbf{v}) \in OH_n$, where $(\mathbf{d}, \mathbf{v}) \in \Theta_{OH_n}$ is determined by the Williamson's normal form decomposition of Q determined by $S \in Sp(2n, \mathbb{R})$, that is, $Q = S^T \begin{bmatrix} D & 0 \\ 0 & D \end{bmatrix} S$, $D = \text{diag}(\mathbf{d})$ and $\mathbf{v} = S \cdot B$.*

Remark 8 We emphasize that given $(Q, B) \in \Theta_{PH_n}$, the pair $(\mathbf{d}, \mathbf{v}) \in \Theta_{CH_n}/\Theta_{OH_n}$ is not uniquely determined by Williamson's decomposition. This can be seen from Theorem 3 because the element $S \in Sp(2n, \mathbb{R})$ in its statement is not unique and the entries d_i of \mathbf{d} are independent of S up to their ordering.

Remark 9 (Controllability, observability, and invertibility)

(i) In the proof of the theorem above (available in the Appendix), we define the linear system morphism $f_S^{(\mathbf{d}, \mathbf{v})} : \mathbb{R}^{2n} \rightarrow \mathbb{R}^{2n}$ as $\mathbf{z} = f_S^{(\mathbf{d}, \mathbf{v})}(\mathbf{s}) := L\mathbf{s}$ and an explicit construction of the matrix L is provided. It turns out that, the matrix L is invertible if and only if the image port-Hamiltonian system (5) is controllable, or equivalently, observable. Indeed, using the same notation as in the proof of Theorem 7, we have

$$L = S^{-1} [L_1 \mathbf{v} \quad L_2 \mathbf{v} \quad \cdots \quad L_{2n} \mathbf{v}] = [S^{-1} L_1 \mathbf{v} \quad S^{-1} L_2 \mathbf{v} \quad \cdots \quad S^{-1} L_{2n} \mathbf{v}],$$

where

$$\begin{aligned} S^{-1} L_{2n-k} \mathbf{v} &= S^{-1} \left[\left(\mathbb{J}_n \begin{bmatrix} D & 0 \\ 0 & D \end{bmatrix} \right)^k + a_{2n-1} \cdot \left(\mathbb{J}_n \begin{bmatrix} D & 0 \\ 0 & D \end{bmatrix} \right)^{k-1} + \cdots + a_{2n-k} \cdot \mathbb{I}_{2n} \right] \cdot \mathbf{v} \\ &= S^{-1} \left((\mathbb{J}_n S^{-T} Q S^{-1})^k + a_{2n-1} \cdot (\mathbb{J}_n S^{-T} Q S^{-1})^{k-1} + \cdots + a_{2n-k} \cdot \mathbb{I}_{2n} \right) \cdot S B \\ &= S^{-1} \left((S \mathbb{J}_n Q S^{-1})^k + a_{2n-1} \cdot (S \mathbb{J}_n Q S^{-1})^{k-1} + \cdots + a_{2n-k} \cdot \mathbb{I}_{2n} \right) \cdot S B \\ &= \left((\mathbb{J}_n Q)^k + a_{2n-1} \cdot (\mathbb{J}_n Q)^{k-1} + \cdots + a_{2n-k} \cdot \mathbb{I}_{2n} \right) \cdot B. \end{aligned}$$

Therefore, L can be transformed by elementary column operations into the controllability matrix of (5) and hence L being invertible, that is, the two systems being isomorphic, is equivalent to the controllability matrix of (5) having full rank (regardless of the choice of $S \in Sp(2n, \mathbb{R})$), which is again equivalent to (5) being canonical. Additionally, the condition for $f_S^{(\mathbf{d}, \mathbf{v})}$ to be invertible can also be formulated in terms of D and \mathbf{v} directly, which we will discuss in Subsection 4.4.

(ii) Systems in CH_n are by construction in controllable canonical form, and are therefore always controllable. If the image system (5) by φ_S that we want to learn is controllable (or equivalently, observable), then by the previous point L is necessarily an invertible matrix which means that (12) and (5) are isomorphic systems by construction. As a consequence, (12) is not only controllable but also observable.

Remark 10 (Application to structure-preserving system learning)

As a corollary of the previous result, we can use controllable Hamiltonian representations to learn port-Hamiltonian systems in an efficient and structure-preserving fashion. Indeed, given a realization of a port-Hamiltonian system, a system of the type $\theta_{CH_n}(\mathbf{d}, \mathbf{v}) \in CH_n$ can be estimated using an appropriate loss (see Section 7). A representation of this type is more advantageous than the original port-Hamiltonian one for two reasons:

- (i) The *model complexity* of the controllable Hamiltonian representation is only of order $\mathcal{O}(n)$, as opposed to $\mathcal{O}(n^2)$ for the original port-Hamiltonian one.
- (ii) This learning scheme is automatically *structure-preserving*. Indeed, once a system $\theta_{CH_n}(\mathbf{d}, \mathbf{v}) \in CH_n$ has been estimated for a given realization, we have shown that there exists a family of linear morphisms, each of which is between the state space of $\theta_{CH_n}(\mathbf{d}, \mathbf{v}) \in$

CH_n and some $\theta_{PH_n}(Q, B) \in PH_n$, such that any solution of (12) is automatically a solution of some system in PH_n . Hence, even in the presence of estimation errors for $(\mathbf{d}, \mathbf{v}) \in \Theta_{CH_n}$, the solutions of $\theta_{CH_n}(\mathbf{d}, \mathbf{v})$ still correspond to a port-Hamiltonian system and hence this structure is *preserved* by the learning scheme.

Remark 11 (System learning and expressive power)

Expressive power is an important property of any machine learning paradigm. As a continuation of the previous remarks, we emphasize that there is an important relation between the controllability of a system in PH_n and the expressive power of the corresponding representation in CH_n . Indeed, if (5) is controllable, by point (ii) in Remark 9, the corresponding preimage system $\theta_{CH_n}(\mathbf{d}, \mathbf{v}) \in CH_n$ can capture all possible solutions of (5), which amounts to the learning scheme based on Θ_{CH_n} having full expressive power. To see this, let \mathbf{z}_0 be an initial state of the controllable system $\theta_{PH_n}(Q, B) \in PH_n$ in (5). Since in that case we can find an invertible system isomorphism $f_S^{(\mathbf{d}, \mathbf{v})}$ that links it to some $\theta_{CH_n}(\mathbf{d}, \mathbf{v}) \in \Theta_{CH_n}$, there exists some corresponding initial state $\mathbf{s}_0 = \left(f_S^{(\mathbf{d}, \mathbf{v})}\right)^{-1}(\mathbf{z}_0)$. Then, by Theorem 7 and the uniqueness of the solutions of ODEs, the solution of (12) with initial state \mathbf{s}_0 is a representation of the solution of (5) with initial state \mathbf{z}_0 . However, if (5) fails to be controllable (that is, $f_S^{(\mathbf{d}, \mathbf{v})}$ not invertible), then such an initial condition \mathbf{s}_0 may not exist. As a rule of thumb, the more controllable a system of the type (5) is, the higher the rank of $f_S^{(\mathbf{d}, \mathbf{v})}$ is, and then the more expressive the corresponding controllable Hamiltonian representations are.

Remark 12 (Expressive power and structure-preservation)

We emphasize that systems in OH_n always have *full expressive power* guaranteed by the system morphism in Theorem 7. This implies that any input-output dynamics generated by the original port-Hamiltonian system will be captured by some of the observable Hamiltonian representations in the statement. However, unlike in the controllable case, the system morphism is between $\theta_{PH_n}(Q, B) \in PH_n$ and $\theta_{OH_n}(\mathbf{d}, \mathbf{v}) \in OH_n$. Therefore, unless (Q, B) is canonical, in which case the morphism becomes an isomorphism, we *cannot, in general, assert the structure-preserving property of this representation.*

Remark 13 (Positive semi-definite Hamiltonians)

The above results can be easily generalized to positive semi-definite (PSD) Hamiltonians with the aid of the generalized Williamson's theorem in the references Son and Stykel (2022); Idel et al. (2017); Egusquiza and Parra-Rodriguez (2022) that we briefly discussed in Section 2.5. In general, the number of unknown parameters in the vector \mathbf{d} is doubled (because of the matrices D_1 and D_2 that appear in this case), and their relation with the coefficients $\{a_0, a_1, \dots, a_{2n-1}\}$ has to be modified accordingly, that is, $\lambda^{2n} + \sum_{i=0}^{2n-1} a_i \cdot \lambda^i = (\lambda^2 + d_1 d_{n+1})(\lambda^2 + d_2 d_{n+2}) \dots (\lambda^2 + d_n d_{2n})$, where some of the d_i 's could be 0. The expression

we emphasize that a given filter can be realized by state-space systems that are not even system-isomorphic (see Example 1 later on). On the other hand, \sim_{filter} -equivalence requires that the outputs of the two systems at time $t = 0$ are consistent with exactly the same initializations, whereas this is not part of the definition of \sim_{sys} -equivalence. Motivated by this fact, we study in Subsection 4.1 how \sim_{filter} and \sim_{sys} are related in terms of PH_n and the controllable Hamiltonian representations CH_n (which by Theorem 7 automatically induce port-Hamiltonian dynamics). In Subsection 4.2, we lower our expectations and characterize PH_n / \sim_{sys} as an approximation to PH_n / \sim_{filter} . The term *approximation* in this sentence is justified because \sim_{filter} and \sim_{sys} coincide on the set of canonical Hamiltonian representations CH_n^{can} , which is system-isomorphic as a set to PH_n^{can} , which is open and dense in PH_n . In particular, unique identifiability can be achieved in CH_n^{can} by studying \sim_{sys} , that is, $\Theta_{CH_n}^{can} / \sim_{filter} \cong \Theta_{CH_n}^{can} / \sim_{sys}$.

In addition to the discussion regarding \sim_{filter} and \sim_{sys} , recall that in the previous section, we have established a link between PH_n and the representation spaces CH_n and OH_n which, as we saw in Definition 5, are both parametrized by the set

$$\Theta_{CH_n} = \Theta_{OH_n} = \{(\mathbf{d}, \mathbf{v}) \mid \mathbf{v} \in \mathbb{R}^{2n}, \mathbf{d} \in \mathbb{R}^n, d_i > 0, i \in \{1, \dots, n\}\}. \quad (13)$$

Now, it is a natural question to ask what is the equivalence relation that corresponds to \sim_{sys} on the parameter space Θ_{CH_n} , and if it is possible to explicitly characterize the quotient space PH_n / \sim_{sys} on Θ_{CH_n} in a certain sense. All these questions are addressed step-by-step in the following subsections.

In Subsection 4.1, we show that two canonical controllable Hamiltonian representations are \sim_{filter} -equivalent if and only if they are \sim_{sys} -equivalent. In Subsection 4.2, we define an equivalence relation \sim_* on Θ_{CH_n} and we show that $PH_n / \sim_{sys} \cong \Theta_{CH_n} / \sim_*$ (see Theorem 22). In Subsection 4.3, we characterize the equivalence classes PH_n / \sim_{sys} and Θ_{CH_n} / \sim_* as *Lie groupoid* orbit spaces.

In Subsection 4.4, we exclusively restrict our analysis to *canonical port-Hamiltonian systems* PH_n^{can} . We first show that the parameter subset $\Theta_{CH_n}^{can} \subset \Theta_{CH_n}$ that corresponds to PH_n^{can} is open and dense in Θ_{CH_n} as it is determined by certain generic non-resonance and nondegeneracy conditions. If we define on Θ_{CH_n} the equivalence relation \sim_{sys} of system automorphisms of the corresponding controllable/observable Hamiltonian representations (see Definition 17), then it can be proved that, restricted to the canonical subset $\Theta_{CH_n}^{can}$, the equivalence relation \sim_* coincides with \sim_{sys} , and hence

$$PH_n^{can} / \sim_{sys} \cong \Theta_{CH_n}^{can} / \sim_* \cong \Theta_{CH_n}^{can} / \sim_{sys}.$$

In Subsection 4.5, we prove that the fact that we restricted the above equivalence relations to canonical subsets allows us to characterize the corresponding quotients as orbit spaces with respect to a *group* (as opposed to groupoids in the general unrestricted case) action, where the group is given by a semi-direct product $S_n \rtimes_{\phi} \mathbb{T}^n$ that will be specified in detail later on. Finally, in Subsection 4.6, we show that the orbit space $\Theta_{CH_n}^{can} / (S_n \rtimes_{\phi} \mathbb{T}^n)$ can be explicitly identified as a smooth manifold $\mathbb{R}_{+\uparrow}^n \times \mathbb{R}_+^n$ and endowed with global Euclidean coordinates, and hence

$$PH_n^{can} / \sim_{sys} \cong \Theta_{CH_n}^{can} / \sim_* \cong \Theta_{CH_n}^{can} / \sim_{filter} \cong \Theta_{CH_n}^{can} / \sim_{sys} \cong \Theta_{CH_n}^{can} / (S_n \rtimes_{\phi} \mathbb{T}^n) \cong \mathbb{R}_{+\uparrow}^n \times \mathbb{R}_+^n.$$

Consequently, up to initializations, canonical port-Hamiltonian dynamics can be identified fully and explicitly in either the controllable or the observable Hamiltonian representations (12) and learned by estimating an initial state condition and a unique set of parameters in a smooth manifold that is obtained as a group orbit space.

4.1 The unique identification problem for filters in \mathcal{PH}_n

In the context of model estimation/machine learning, we would like to characterize and identify the filters that constitute the elements in \mathcal{PH}_n . In Section 2.1, we have seen that two systems that are system isomorphic and are initialized according to the isomorphism induce the same input-output dynamics, which indicates that these isomorphisms are redundancies/symmetries in PH_n . Our aim is to quotient out the symmetries given by system automorphisms and to investigate whether the quotient space uniquely identifies the filters in \mathcal{PH}_n .

Definition 15 (*PH_n with equivalence relations \sim_{sys} and \sim_{filter}*)

- (i) *The fact that two systems $\theta_{PH_n}(Q_1, B_1)$ and $\theta_{PH_n}(Q_2, B_2)$ in PH_n induce the same filter defines an equivalence relation in PH_n , which we denote by $(Q_1, B_1) \sim_{filter} (Q_2, B_2)$. Consequently, we have by definition $\mathcal{PH}_n = PH_n / \sim_{filter}$, which we call the unique identifiability space.*
- (ii) *We observe that $\theta_{PH_n}(Q_1, B_1)$ and $\theta_{PH_n}(Q_2, B_2)$ in PH_n are linearly system isomorphic according to Definition 1 if and only if there exists an invertible matrix L such that*

$$\begin{cases} L\mathbb{J}Q_1 = \mathbb{J}Q_2L \\ LB_1 = B_2 \\ B_1^T Q_1 = B_2^T Q_2L. \end{cases} \quad (14)$$

It is straightforward to check that system isomorphisms determine an equivalence relation on PH_n . If $\theta_{PH_n}(Q_1, B_1)$ and $\theta_{PH_n}(Q_2, B_2)$ are system isomorphic, we write $(Q_1, B_1) \sim_{sys} (Q_2, B_2)$. We denote by PH_n / \sim_{sys} the quotient space. The equivalence class in PH_n / \sim_{sys} that contains the element $\theta_{PH_n}(Q, B)$ is denoted by $[Q, B] \in PH_n / \sim_{sys}$.

It is a natural question to ask about the relation between PH_n / \sim_{sys} and PH_n / \sim_{filter} , and if they are the same. However, in general, neither of the two equivalence relations \sim_{sys} and \sim_{filter} implies the other. To see \sim_{filter} does not imply \sim_{sys} , we note that in the next Example 1, a filter in \mathcal{PH}_n could be realized by two elements in PH_n that are not \sim_{sys} -equivalent since filters identify exclusively the canonical part (that is, the minimal realization, see Kalman (1963)). To see the other direction, that is, \sim_{sys} does not imply \sim_{filter} , we can simply consider the value of the filter at time $t = 0$ induced by two systems $(Q_1, B_1) \sim_{filter} (Q_2, B_2)$ from (7), which gives $B_1^T Q_1 \mathbf{z}_0 = B_2^T Q_2 \mathbf{z}_0$ for any \mathbf{z}_0 , leading to $B_1^T Q_1 = B_2^T Q_2$. On the other hand, we have seen in (14) that $(Q_1, B_1) \sim_{sys} (Q_2, B_2)$ only guarantees $B_1^T Q_1 = B_2^T Q_2 L$, but not $B_1^T Q_1 = B_2^T Q_2$, unless L can be shown to be the identity matrix.

Example 1 Consider two systems $\theta_{PH_n}(Q_1, B_1), \theta_{PH_n}(Q_2, B_2) \in PH_n$ where

$$Q_1 = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}, Q_2 = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 2 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 3 \end{bmatrix}, B_1 = B_2 = \begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \end{bmatrix}.$$

Both systems induce the same filter $y(u, \mathbf{z}_0)_t = \int_0^t \cos(t-s)u(s)ds + (\cos t, 0, \sin t, 0)^T \cdot \mathbf{z}_0$, where \mathbf{z}_0 is the initial state. However, these two systems cannot be system isomorphic, since by (14) in that case there would exist an invertible L such that $L\mathbb{J}Q_1 = \mathbb{J}Q_2L$, and hence $\mathbb{J}Q_1$ would have the same set of eigenvalues as $\mathbb{J}Q_2$, which is not the case.

We have seen from the above that, in general, PH_n / \sim_{filter} and PH_n / \sim_{sys} are different objects, and neither one is a subset of the other. In practice, we are more interested in characterizing the former, which appears to be difficult due to issues that involve initialization consistency. Nevertheless, we can partially solve the problem by restricting to the generic subset of canonical port-Hamiltonian systems PH_n^{can} , and consider their corresponding controllable Hamiltonian representations $\theta_{CH_n}(\Theta_{CH_n}^{can})$ by system isomorphisms, then, on those representations, the two equivalence relations will coincide exactly, that is., $\Theta_{CH_n}^{can} / \sim_{filter} \cong \Theta_{CH_n}^{can} / \sim_{sys}$, which we ultimately characterize in Section 4.5. We present rigorous definitions of these equivalence relations on the parameter space before we state our main result Theorem 19.

Lemma 16 For $(\mathbf{d}_1, \mathbf{v}_1)$ and $(\mathbf{d}_2, \mathbf{v}_2) \in \Theta_{CH_n} = \Theta_{OH_n}$, $\theta_{CH_n}(\mathbf{d}_1, \mathbf{v}_1) \sim_{sys} \theta_{CH_n}(\mathbf{d}_2, \mathbf{v}_2)$ if and only if $\theta_{OH_n}(\mathbf{d}_1, \mathbf{v}_1) \sim_{sys} \theta_{OH_n}(\mathbf{d}_2, \mathbf{v}_2)$

Proof The proof is basically a restatement of the fact that $g_1^{ctr}(\mathbf{d}) = g_1^{obs}(\mathbf{d})^T$ and $g_2^{ctr}(\mathbf{d}, \mathbf{v}) = g_2^{obs}(\mathbf{d}, \mathbf{v})^T$. \blacksquare

Definition 17 (Θ_{CH_n} with equivalence relations \sim_{sys} and \sim_{filter})

- (i) We shall denote $(\mathbf{d}_1, \mathbf{v}_1) \sim_{sys} (\mathbf{d}_2, \mathbf{v}_2)$ if $\theta_{CH_n}(\mathbf{d}_1, \mathbf{v}_1)$ and $\theta_{CH_n}(\mathbf{d}_2, \mathbf{v}_2)$ are system isomorphic for $(\mathbf{d}_1, \mathbf{v}_1), (\mathbf{d}_2, \mathbf{v}_2) \in \Theta_{CH_n}$. Note that system isomorphisms for controllable/observable Hamiltonian representations are indeed equivalent as we showed in Lemma 16.
- (ii) We shall denote $(\mathbf{d}_1, \mathbf{v}_1) \sim_{filter} (\mathbf{d}_2, \mathbf{v}_2)$ if $\theta_{CH_n}(\mathbf{d}_1, \mathbf{v}_1)$ and $\theta_{CH_n}(\mathbf{d}_2, \mathbf{v}_2)$ induce the same filter for $(\mathbf{d}_1, \mathbf{v}_1), (\mathbf{d}_2, \mathbf{v}_2) \in \Theta_{CH_n}$. Note that, unlike \sim_{sys} , \sim_{filter} is defined specifically for Θ_{CH_n} , and could be different if one replace Θ_{CH_n} with Θ_{OH_n} .

Proposition 18 Given $(\mathbf{d}_1, \mathbf{v}_1)$ and $(\mathbf{d}_2, \mathbf{v}_2)$ in Θ_{CH_n} , then

- (I) $\theta_{CH_n}(\mathbf{d}_1, \mathbf{v}_1) \sim_{sys} \theta_{CH_n}(\mathbf{d}_2, \mathbf{v}_2)$ if and only if $a_i(\mathbf{d}_1) = a_i(\mathbf{d}_2)$ and $c_i(\mathbf{d}_1, \mathbf{v}_1) = c_i(\mathbf{d}_2, \mathbf{v}_2)$ for all $i = 1, \dots, n$. In other words, there exists a permutation matrix $P_\sigma \in \mathbb{M}_n$ such that, for $D = \text{diag}(\mathbf{d})$ and $P = \begin{bmatrix} P_\sigma & 0 \\ 0 & P_\sigma \end{bmatrix}$, the following conditions hold true:

$$\begin{aligned}
 \text{(i)} \quad & P \begin{bmatrix} D_1 & 0 \\ 0 & D_1 \end{bmatrix} P^T = \begin{bmatrix} D_2 & 0 \\ 0 & D_2 \end{bmatrix} \\
 \text{(ii)} \quad & \mathbf{v}_1^T \begin{bmatrix} (F_1)_k & 0 \\ 0 & (F_1)_k \end{bmatrix} \mathbf{v}_1 = \mathbf{v}_2^T \begin{bmatrix} (F_2)_k & 0 \\ 0 & (F_2)_k \end{bmatrix} \mathbf{v}_2, \quad k = 0, \dots, n-1
 \end{aligned}$$

The matrices F_i are defined in Theorem 7.

(II) $\theta_{CH_n}(\mathbf{d}_1, \mathbf{v}_1) \sim_{\text{filter}} \theta_{CH_n}(\mathbf{d}_2, \mathbf{v}_2)$ if and only if $c_i(\mathbf{d}_1, \mathbf{v}_1) = c_i(\mathbf{d}_2, \mathbf{v}_2)$ and $e_i(\mathbf{d}_1, \mathbf{v}_1) = e_i(\mathbf{d}_2, \mathbf{v}_2)$ for all $i = 1, \dots, n$, where the scalar functions e_i are defined recursively as

$$\begin{aligned}
 e_1 &= c_1 \\
 e_2 &= c_3 - a_{2n-2} \cdot e_1 \\
 e_3 &= c_5 - a_{2n-2} \cdot e_2 - a_{2n-4} \cdot e_1 \\
 &\vdots \\
 e_n &= c_{2n-1} - a_{2n-2} \cdot e_{n-1} - a_{2n-4} \cdot e_{n-2} - \dots - a_2 \cdot e_1.
 \end{aligned} \tag{15}$$

Theorem 19 Given $(\mathbf{d}_1, \mathbf{v}_1)$ and $(\mathbf{d}_2, \mathbf{v}_2)$ in $\Theta_{CH_n}^{\text{can}}$, then $\theta_{CH_n}(\mathbf{d}_1, \mathbf{v}_1) \sim_{\text{filter}} \theta_{CH_n}(\mathbf{d}_2, \mathbf{v}_2)$ if and only if $\theta_{CH_n}(\mathbf{d}_1, \mathbf{v}_1) \sim_{\text{sys}} \theta_{CH_n}(\mathbf{d}_2, \mathbf{v}_2)$, that is, $\Theta_{CH_n}^{\text{can}} / \sim_{\text{filter}} \cong \Theta_{CH_n}^{\text{can}} / \sim_{\text{sys}}$

Proof The first part of the statement immediately follows from Proposition 18 and the fact that $e_1 = c_1 \neq 0$, which is guaranteed by the fact that we are considering canonical systems, see the characterizations in Section 4.4. \blacksquare

4.2 Equivalence classes of port-Hamiltonian systems by system isomorphisms

We have seen that PH_n / \sim_{sys} is not the set of port-Hamiltonian filters due to the presence of non-canonical systems and possible initialization inconsistencies. However, it is still informative to study the quotient space PH_n / \sim_{sys} because when restricted to the canonical systems, $PH_n^{\text{can}} / \sim_{\text{sys}}$ uniquely identifies canonical port-Hamiltonian dynamics up to initializations. Furthermore, $PH_n^{\text{can}} / \sim_{\text{sys}}$ is isomorphic to $\Theta_{CH_n}^{\text{can}} / \sim_{\text{filter}}$. In other words, $PH_n^{\text{can}} / \sim_{\text{sys}}$ uniquely identifies the set of canonical controllable Hamiltonian representations CH_n^{can} . We shall make this point clearer in Sections 4.5 and 4.6.

In this section, we introduce a manageable characterization of the quotient space PH_n / \sim_{sys} by using parameter spaces. First, motivated by Williamson's theorem, we consider the space Θ_{CH_n} defined before as the set of all pairs of the form (\mathbf{d}, \mathbf{v}) , where $\mathbf{d} = (d_1, d_2, \dots, d_n)^T$ with $d_i > 0$, and $\mathbf{v} = (v_1, v_2, \dots, v_{2n})^T \in \mathbb{R}^{2n}$. Inspired by the representation results, we now define an equivalence relation \sim_\star on Θ_{CH_n} as below whose equivalence classes are denoted by $[\mathbf{d}, \mathbf{v}]$. The importance of the next definition is that, as we shall prove in Theorem 22, the relation \sim_\star on Θ_{CH_n} plays the same role as \sim_{sys} on PH_n .

Definition 20 The pairs $(\mathbf{d}_1, \mathbf{v}_1)$ and $(\mathbf{d}_2, \mathbf{v}_2)$ in Θ_{CH_n} are \sim_\star -equivalent, that is, $(\mathbf{d}_1, \mathbf{v}_1) \sim_\star (\mathbf{d}_2, \mathbf{v}_2)$, if there exists a permutation matrix $P_\sigma \in \mathbb{M}_n$ and an invertible matrix

A such that, for $D_i = \text{diag}(\mathbf{d}_i)$, $i \in \{1, 2\}$ and $P = \begin{bmatrix} P_\sigma & 0 \\ 0 & P_\sigma \end{bmatrix}$, the following conditions hold true:

- (i) $P \begin{bmatrix} D_1 & 0 \\ 0 & D_1 \end{bmatrix} P^T = \begin{bmatrix} D_2 & 0 \\ 0 & D_2 \end{bmatrix}$
- (ii) $A^T \begin{bmatrix} D_1 & 0 \\ 0 & D_1 \end{bmatrix} A \mathbf{v}_1 = \begin{bmatrix} D_1 & 0 \\ 0 & D_1 \end{bmatrix} \mathbf{v}_1$
- (iii) $A \mathbb{J} \begin{bmatrix} D_1 & 0 \\ 0 & D_1 \end{bmatrix} = \mathbb{J} \begin{bmatrix} D_1 & 0 \\ 0 & D_1 \end{bmatrix} A$
- (iv) $\mathbf{v}_2 = P A \mathbf{v}_1$.

Proposition 21 *The relation \sim_\star defined in Definition 20 is an equivalence relation on Θ_{CH_n} .*

In the next subsection, we shall give meaning to \sim_\star in terms of groupoid orbits. Now, we aim to characterize the \sim_{sys} equivalence relation on PH_n as the \sim_\star equivalence relation on the space Θ_{CH_n} of (\mathbf{d}, \mathbf{v}) -pairs, that is, we shall prove that $\Theta_{CH_n}/\sim_\star \cong PH_n/\sim_{sys}$. This will be proved in three steps. First, we show that for an arbitrary $S \in Sp(2n, \mathbb{R})$, the map φ_S defined in Theorem 7 composed with θ_{CH_n} is compatible with the equivalence relations \sim_\star and \sim_{sys} , that is, $(\mathbf{d}_1, \mathbf{v}_1) \sim_\star (\mathbf{d}_2, \mathbf{v}_2)$ if and only if $\varphi_S(\theta_{CH_n}(\mathbf{d}_1, \mathbf{v}_1)) \sim_{sys} \varphi_S(\theta_{CH_n}(\mathbf{d}_2, \mathbf{v}_2))$. Then, we show that the unique map ψ_S induced by $\varphi_S \circ \theta_{CH_n}$ on the quotient spaces does not depend on the choice of S and hence the family of maps ψ_S parameterized by $S \in Sp(2n, \mathbb{R})$ induces a unique map $\Phi : \Theta_{CH_n}/\sim_\star \rightarrow PH_n/\sim_{sys}$ which is a homeomorphism.

Theorem 22 (Characterization of PH_n/\sim_{sys} as Θ_{CH_n}/\sim_\star) *Given any arbitrary $S \in Sp(2n, \mathbb{R})$, the map $\varphi_S \circ \theta_{CH_n}$ induces on the quotient spaces a map $\Phi : \Theta_{CH_n}/\sim_\star \rightarrow PH_n/\sim_{sys}$ which does not depend on $S \in Sp(2n, \mathbb{R})$ and is given by*

$$\Phi([\mathbf{d}, \mathbf{v}]_\star) = \left[\begin{bmatrix} D & 0 \\ 0 & D \end{bmatrix}, \mathbf{v} \right]_{sys},$$

where $D = \text{diag}(\mathbf{d})$. Moreover, Φ is a homeomorphism with respect to the quotient topologies.

4.3 The quotient spaces as groupoid orbit spaces

Recall that from a category theory point of view, a group can be seen as a category with a single object where all morphisms are invertible. Groupoids are a natural generalization of this notion and refer to categories with possibly more than one object, where again all morphisms are invertible (see Mackenzie (2005) for a comprehensive introduction). As it is customary, groupoids will be denoted with the symbol $\alpha, \beta : \mathcal{G} \rightrightarrows M$ (or simply $\mathcal{G} \rightrightarrows M$), where α and β are the *target* and the *source* maps, respectively. Given $m \in M$, the *groupoid orbit* that contains this point is given by $\mathcal{O}_m = \alpha(\beta^{-1}(m)) \subset M$. The *orbit space* associated to $\mathcal{G} \rightrightarrows M$ is denoted by M/\mathcal{G} .

In this section, we provide an alternative point of view for Theorem 22 in terms of groupoid orbits. More precisely, we show first that the set of equivalence classes PH_n / \sim_{sys} (resp. Θ_{CH_n} / \sim_*) is the orbit space $\Theta_{PH_n} / \mathcal{G}_n$ (resp. $\Theta_{CH_n} / \mathcal{H}_n$) of a groupoid $\mathcal{G}_n \rightrightarrows \Theta_{PH_n}$ (resp. $\mathcal{H}_n \rightrightarrows \Theta_{CH_n}$) which we construct in the following paragraphs. In a second step we show that the statement in Theorem 22 is equivalent to saying that the orbit spaces PH_n / \sim_{sys} and $\Theta_{CH_n} / \mathcal{H}_n$ of the two groupoids coincide.

Definition 23

1. Let $\mathcal{G}_n := \{(L, (Q, B)) \mid L \in GL(2n, \mathbb{R}), (Q, B) \in \Theta_{PH_n} \text{ such that}$
 (i) $\mathbb{J}^T L \mathbb{J} Q L^{-1}$ is symmetric positive-definite (ii) $B = \mathbb{J}^T L^T \mathbb{J} L B\}$.
2. Let the target and source maps $\alpha, \beta : \mathcal{G}_n \rightarrow \Theta_{PH_n}$ be defined as
 $\alpha(L, (Q, B)) := (\mathbb{J}^T L \mathbb{J} Q L^{-1}, LB)$ and $\beta(L, (Q, B)) := (Q, B)$.
3. Define the set of composable pairs as
 $\mathcal{G}_n^{(2)} := \{((L_1, (Q_1, B_1)), (L_2, (Q_2, B_2))) \mid \beta((L_1, (Q_1, B_1))) = \alpha((L_2, (Q_2, B_2)))\}$.
4. Let the multiplication map $m : \mathcal{G}_n^{(2)} \rightarrow \mathcal{G}_n$ be defined as
 $m((L_1, (Q_1, B_1)), (L_2, (Q_2, B_2))) = (L_1 L_2, (Q_2, B_2))$.
5. Let the identity section $\epsilon : \Theta_{PH_n} \rightarrow \mathcal{G}_n$ be defined as $\epsilon(Q, B) := (\mathbb{I}_{2n}, (Q, B))$.
6. Let the inversion map $i : \mathcal{G}_n \rightarrow \mathcal{G}_n$ be defined as $i(L, (Q, B)) := (L^{-1}, (\mathbb{J}^T L \mathbb{J} Q L^{-1}, LB))$.

Proposition 24 *The definition above determines a Lie groupoid $\mathcal{G}_n \rightrightarrows \Theta_{PH_n}$ with \mathcal{G}_n the total space, Θ_{PH_n} the base space, and structure maps $\alpha, \beta, m, \epsilon, i$. We refer to $\mathcal{G}_n \rightrightarrows \Theta_{PH_n}$ as the port-Hamiltonian groupoid. The orbit space of this groupoid $\Theta_{PH_n} / \mathcal{G}_n$ coincides with PH_n / \sim_{sys} .*

Definition 25

1. Let $\mathcal{H}_n := \{((P_\sigma, A), (\mathbf{d}, \mathbf{v})) \mid P_\sigma \in \mathbb{M}_n \text{ is a permutation matrix, } A \in GL(2n, \mathbb{R}),$
 $(\mathbf{d}, \mathbf{v}) \in \Theta_{CH_n}, \text{ such that (i) } A^T \begin{bmatrix} D & 0 \\ 0 & D \end{bmatrix} A \mathbf{v} = \begin{bmatrix} D & 0 \\ 0 & D \end{bmatrix} \mathbf{v}, \text{ and}$
 (ii) $A \mathbb{J} \begin{bmatrix} D & 0 \\ 0 & D \end{bmatrix} = \mathbb{J} \begin{bmatrix} D & 0 \\ 0 & D \end{bmatrix} A, \text{ where } D = \text{diag}(\mathbf{d})\}$.
2. Let the target and source maps $\alpha, \beta : \mathcal{H}_n \rightarrow \Theta_{CH_n}$ be defined as
 $\alpha((P_\sigma, A), (\mathbf{d}, \mathbf{v})) := (\mathbf{d}, \mathbf{v})$ and $\beta((P_\sigma, A), (\mathbf{d}, \mathbf{v})) := (P_\sigma \mathbf{d}, P A \mathbf{v})$, where $P = \begin{bmatrix} P_\sigma & 0 \\ 0 & P_\sigma \end{bmatrix}$.
3. Define the set of composable pairs as
 $\mathcal{H}_n^{(2)} := \{(((P_{\sigma,1}, A_1), (\mathbf{d}_1, \mathbf{v}_1)), ((P_{\sigma,2}, A_2), (\mathbf{d}_2, \mathbf{v}_2))) \mid$
 $\beta((P_{\sigma,2}, A_2), (\mathbf{d}_2, \mathbf{v}_2)) = \alpha((P_{\sigma,1}, A_1), (\mathbf{d}_1, \mathbf{v}_1))\}$.
4. Let the multiplication map $m : \mathcal{H}_n^{(2)} \rightarrow \mathcal{H}_n$ be defined as
 $m(((P_{\sigma,1}, A_1), (\mathbf{d}_1, \mathbf{v}_1)), ((P_{\sigma,2}, A_2), (\mathbf{d}_2, \mathbf{v}_2)))$
 $= ((P_{\sigma,2} P_{\sigma,1}, P_{\sigma,1}^T A_2 P_{\sigma,1} A_1), (\mathbf{d}_1, \mathbf{v}_1))$.

5. Let the identity section $\epsilon : \Theta_{CH_n} \rightarrow \mathcal{H}_n$ be defined as $\epsilon(\mathbf{d}, \mathbf{v}) := ((\mathbb{I}_n, \mathbb{I}_{2n}), (\mathbf{d}, \mathbf{v}))$.
6. Let the inversion map $i : \mathcal{H}_n \rightarrow \mathcal{H}_n$ be defined as $i((P_\sigma, A), (\mathbf{d}, \mathbf{v})) := ((P_\sigma^T, P_\sigma A^{-1} P_\sigma^T), (P_\sigma \mathbf{d}, P A \mathbf{v}))$.

Proposition 26 *The definition above determines a Lie groupoid $\mathcal{H}_n \rightrightarrows \Theta_{CH_n}$ with \mathcal{H}_n the total space, Θ_{CH_n} the base space, and structure maps $\alpha, \beta, m, \epsilon, i$. We refer to $\mathcal{H}_n \rightrightarrows \Theta_{CH_n}$ as the reduced port-Hamiltonian groupoid. The orbit space of this groupoid $\Theta_{CH_n}/\mathcal{H}_n$ coincides with Θ_{CH_n}/\sim_\star .*

Theorem 22 can now be restated in terms of the elements that we just introduced.

Theorem 27 *The orbit spaces of the Lie groupoids $\mathcal{G}_n \rightrightarrows \Theta_{PH_n}$ and $\mathcal{H}_n \rightrightarrows \Theta_{CH_n}$ are isomorphic.*

4.4 Characterization of canonical port-Hamiltonian systems

In Subsections 4.2 and 4.3 we have provided a characterization of PH_n/\sim_{sys} in terms of Θ_{CH_n}/\sim_\star and groupoid orbit spaces. Recall from Subsection 4.1 that the difficulty of the unique identifiability of filters in \mathcal{PH}_n comes from two parts: the possible presence of non-canonical systems, and the possible initialization inconsistency. We have shown in Subsection 4.1 that, by restricting to canonical systems, the filters induced by controllable Hamiltonian representations CH_n^{can} can be uniquely identified, even though we still cannot do the same for PH_n^{can} . Hence, it is worth studying what the quotient spaces above look like when restricted to the subset that contains only canonical port-Hamiltonian systems. In this section, we take a step in that direction.

Recall that a port-Hamiltonian system in PH_n of the form (5) is controllable (or equivalently, observable/canonical) if and only if

$$\det \left([B \mid \mathbb{J}QB \mid \dots \mid (\mathbb{J}Q)^{2n-1}B] \right) \neq 0. \quad (16)$$

Using the Williamson decomposition of Q into D and S , and $\mathbf{v} := S \cdot B$, this is equivalent to

$$\det \left(\left[\begin{array}{c|c|c} \mathbf{v} & \mathbb{J} \begin{bmatrix} D & 0 \\ 0 & D \end{bmatrix} \mathbf{v} & \dots \\ \hline \left(\mathbb{J} \begin{bmatrix} D & 0 \\ 0 & D \end{bmatrix} \right)^{2n-1} \mathbf{v} \end{array} \right] \right) \neq 0. \quad (17)$$

By definition, we have that PH_n^{can} (respectively, $\Theta_{CH_n}^{can}$) is a subset of PH_n (respectively, Θ_{CH_n}) made of systems that satisfy (16) (respectively, (17)). We now characterize the space of pairs $(\mathbf{d}, \mathbf{v}) \in \Theta_{CH_n}$ that correspond to canonical port-Hamiltonian systems in normal form. The calculation of the determinant in (17) yields $(\prod_{i=1}^n d_i) \cdot (\prod_{1 \leq j < k \leq n} (d_j + d_k)^2 (d_j - d_k)^2) \cdot (\prod_{l=1}^n (v_l^2 + v_{n+l}^2))$ up to the sign. Therefore,

$$\Theta_{CH_n}^{can} = \{ (\mathbf{d}, \mathbf{v}) \in \Theta_{CH_n} \mid \text{entries of } \mathbf{d} \text{ are distinct and } v_l^2 + v_{n+l}^2 > 0 \text{ for } l \in \{1, \dots, n\} \}.$$

We shall refer to the statement on the entries of \mathbf{d} being all different as the *non-resonance condition* and to $v_l^2 + v_{n+l}^2 > 0$ for all $l \in \{1, \dots, n\}$ as the *nondegeneracy condition*. There might be a concern about whether different choices of the matrix S lead to different vectors \mathbf{v} and hence the notion of nondegeneracy would be ill-defined. This is indeed not a

problem since, as we show in Remark 28 below, once the non-resonance condition is assumed, different vectors \mathbf{v} are obtained by rotating the planes spanned by each and every pair of l -th and $n + l$ -th entries, which preserves the value of $v_l^2 + v_{n+l}^2$. Thus, the nondegeneracy condition is actually based on the non-resonance condition.

Remark 28 (Williamson’s decomposition in the canonical case) We have mentioned in Theorem 3 (iii) that two symplectic matrices S and S' that Williamson decompose the same Q differ by a unitary matrix. We now note that for an element Q that satisfies the non-resonance condition, S and S' do not only differ by an arbitrary $U \in U(n)$, (see (11) for the definition of $U(n)$) but by a special one R that has the form

$$R = \left[\begin{array}{cc|cc} \cos \theta_1 & 0 & -\sin \theta_1 & 0 \\ & \ddots & & \\ 0 & & \cos \theta_n & 0 \\ \hline \sin \theta_1 & & 0 & -\sin \theta_n \\ & & \cos \theta_1 & 0 \\ & & & \\ 0 & & \sin \theta_n & \cos \theta_n \end{array} \right]. \quad (18)$$

This fact accounts for part of the symmetry that we shall spell out later on. The proof of this fact is purely computational: the assumption that the diagonal entries of D are all positive and distinct, the fact that U satisfies the equation $U \begin{bmatrix} D & 0 \\ 0 & D \end{bmatrix} U^T = \begin{bmatrix} D & 0 \\ 0 & D \end{bmatrix}$ and, at the same time, $U \in U(n) = SO(2n, \mathbb{R}) \cap Sp(2n, \mathbb{R})$, guarantees the claim.

Remark 29 (Being canonical is a generic property) It is well-known that the set of canonical systems, as a subset of all linear systems, corresponds to a Zariski open set, which is open and dense in the usual topology (Tcho (1983)). In particular, this also holds for linear port-Hamiltonian systems. Therefore, PH_n^{can} is open and dense in PH_n . On the other hand, using the characterization provided above, it is clear that $\Theta_{CH_n}^{can}$ is also open and dense in Θ_{CH_n} .

The isomorphism in Theorem 22 naturally restricts to canonical subsets, that is, $PH_n^{can} / \sim_{sys} \cong \Theta_{CH_n}^{can} / \sim_\star$. On the other hand, we will see below another isomorphism result involving PH_n^{can} / \sim_{sys} .

Proposition 30 (Characterization of PH_n^{can} / \sim_{sys} as $\Theta_{CH_n}^{can} / \sim_{sys}$)

The map $\Phi : \Theta_{CH_n}^{can} / \sim_{sys} \rightarrow PH_n^{can} / \sim_{sys}$ defined by $\Phi([\mathbf{d}, \mathbf{v}]_{sys}) = \left[\begin{bmatrix} D & 0 \\ 0 & D \end{bmatrix}, \mathbf{v} \right]_{sys}$, where $D = \text{diag}(\mathbf{d})$, is an isomorphism.

We just proved that both $\Theta_{CH_n}^{can} / \sim_\star$ and $\Theta_{CH_n}^{can} / \sim_{sys}$ are isomorphic to PH_n^{can} / \sim_{sys} , and even via the same isomorphism Φ . Therefore, the equivalence relations \sim_\star and \sim_{sys} coincide when restricted to $\Theta_{CH_n}^{can}$. To summarize, we have proved in this subsection that

$$PH_n^{can} / \sim_{sys} \cong \Theta_{CH_n}^{can} / \sim_\star \cong \Theta_{CH_n}^{can} / \sim_{sys}.$$

In the next subsection, we continue the investigation of the above chain of isomorphisms.

4.5 The unique identifiability space for canonical port-Hamiltonian systems as a group orbit space

In Subsection 4.3, it is proved that the quotient space PH_n / \sim_{sys} can be treated as a Lie groupoid orbit space. We now show that the restricted quotient space to canonical port-Hamiltonian systems, that is, PH_n^{can} / \sim_{sys} , is isomorphic to the orbit space of a certain group action on $\Theta_{CH_n}^{can}$, where the group is a semi-direct product of the n -permutation group and the n -torus, that is, $S_n \rtimes_{\phi} \mathbb{T}^n$. The intuition behind this fact is that restricting to the subset of canonical systems PH_n^{can} removes the degeneracies in PH_n , which allows to reduce the symmetry of the Lie groupoid $\mathcal{G}_n \rightrightarrows \Theta_{PH_n}$ to that of the Lie group $S_n \rtimes_{\phi} \mathbb{T}^n$.

We start by defining the group action. First, let the permutation group S_n act on \mathbb{R}^n by permuting the entries d_i of the vector $\mathbf{d} \in \mathbb{R}^n$. For each $i \in \{1, \dots, n\}$ the circle S^1 acts on the plane spanned by the i -th and $(n+i)$ -th entries of \mathbf{v} by rotations. More precisely, we define the action of S_n on elements \mathbf{d} and \mathbf{v} as

$$\Gamma_{\sigma}((d_1, \dots, d_n)^T) = (d_{\sigma(1)}, \dots, d_{\sigma(n)})^T = P_{\sigma} \cdot (d_1, \dots, d_n)^T$$

where P_{σ} is the corresponding permutation matrix and

$$\Gamma_{\sigma}((v_1, \dots, v_{2n})^T) = (v_{\sigma(1)}, \dots, v_{\sigma(n)}, v_{n+\sigma(1)}, \dots, v_{n+\sigma(n)})^T = \begin{bmatrix} P_{\sigma} & 0 \\ 0 & P_{\sigma} \end{bmatrix} \cdot (v_1, \dots, v_{2n})^T,$$

respectively. Then the σ -action on a pair (\mathbf{d}, \mathbf{v}) is understood as acting on \mathbf{d} and \mathbf{v} simultaneously. We also define the action of the i -th circle of the torus \mathbb{T}^n as the planar rotation of the space spanned by the i -th and $(n+i)$ -th entries of \mathbf{v} . This torus action is understood to leave \mathbf{d} invariant. More concretely, it is the action

$$\begin{aligned} \Gamma_{\theta_i}((d_1, \dots, d_n, v_1, \dots, v_{2n})^T) \\ = (d_1, \dots, d_n, v_1, \dots, v_{i-1}, \cos\theta_i v_i - \sin\theta_i v_{n+i}, v_{i+1}, \dots, v_n, \\ v_{n+1}, \dots, v_{n+i-1}, \sin\theta_i v_i + \cos\theta_i v_{n+i}, v_{n+i+1}, \dots, v_{2n})^T. \end{aligned}$$

With these actions of the groups S_n and \mathbb{T}^n on Θ_{CH_n} we define the map $\Gamma_{(\sigma, (\theta_1, \dots, \theta_n)^T)} : (\mathbb{R}_+^n \times \mathbb{R}^{2n}) \rightarrow (\mathbb{R}_+^n \times \mathbb{R}^{2n})$ as

$$\begin{aligned} \Gamma_{(\sigma, (\theta_1, \dots, \theta_n)^T)}(\mathbf{d}, \mathbf{v}) &= \Gamma_{\theta_1} \circ \dots \circ \Gamma_{\theta_n} \circ \Gamma_{\sigma}(\mathbf{d}, \mathbf{v}) \\ &= (P_{\sigma} \cdot \mathbf{d}, \Gamma_{\theta_1} \circ \dots \circ \Gamma_{\theta_n} \left(\begin{bmatrix} P_{\sigma} & 0 \\ 0 & P_{\sigma} \end{bmatrix} \cdot \mathbf{v} \right)) = (P_{\sigma} \cdot \mathbf{d}, RP \cdot \mathbf{v}), \quad (19) \end{aligned}$$

which constitutes an action of the semi-direct product group $S_n \rtimes_{\phi} \mathbb{T}^n$, where $\phi : S_n \rightarrow \text{Aut}(\mathbb{T}^n)$ is given by the permutation $\phi(\sigma)((\theta_1, \dots, \theta_n)^T) = P_{\sigma} \cdot (\theta_1, \dots, \theta_n)^T$. Note that the matrix of $\Gamma_{\theta_1} \circ \dots \circ \Gamma_{\theta_n}$ is given by R in (18), P_{σ} is the permutation matrix that corresponds to $\sigma \in S_n$, and $P = \begin{bmatrix} P_{\sigma} & 0 \\ 0 & P_{\sigma} \end{bmatrix}$.

Proposition 31 *The map $\Gamma_{(\sigma, (\theta_1, \dots, \theta_n)^T)}$ defined as (19) for $\sigma \in S_n$ and $(\theta_1, \dots, \theta_n)^T \in \mathbb{T}^n$ is a left group action of $(S_n \rtimes_{\phi} \mathbb{T}^n)$ on Θ_{CH_n} .*

Using the definition of the $(S_n \rtimes_{\phi} \mathbb{T}^n)$ -action on Θ_{CH_n} , two elements $(\mathbf{d}_1, \mathbf{v}_1), (\mathbf{d}_2, \mathbf{v}_2) \in \Theta_{CH_n}$ are in the same orbit if and only if the following conditions hold true for some $\sigma \in S_n$:

- (i) $d_{2,i} = d_{1,\sigma(i)}$,
- (ii) $v_{2,i}^2 + v_{2,n+i}^2 = v_{1,\sigma(i)}^2 + v_{1,n+\sigma(i)}^2$, $i = 1, \dots, n$.

By Proposition 18 (I) parts (i) and (ii), it can be seen that there could be a close relation between the $(S_n \rtimes_{\phi} \mathbb{T}^n)$ -action and the equivalence relation \sim_{sys} on Θ_{CH_n} . The next proposition demonstrates that the orbit spaces of the $(S_n \rtimes_{\phi} \mathbb{T}^n)$ -action coincide with the equivalence classes of the relation \sim_{sys} when we restrict our attention to the subset $\Theta_{CH_n}^{can}$.

Proposition 32 (Characterization of $\Theta_{CH_n}^{can} / \sim_{sys}$ as $\Theta_{CH_n}^{can} / (S_n \rtimes_{\phi} \mathbb{T}^n)$) *Given $(\mathbf{d}_1, \mathbf{v}_1)$ and $(\mathbf{d}_2, \mathbf{v}_2)$ in $\Theta_{CH_n}^{can}$, then $(\mathbf{d}_1, \mathbf{v}_1) \sim_{sys} (\mathbf{d}_2, \mathbf{v}_2)$ if and only if $(\mathbf{d}_1, \mathbf{v}_1)$ and $(\mathbf{d}_2, \mathbf{v}_2)$ lie in the same orbit of the $(S_n \rtimes_{\phi} \mathbb{T}^n)$ -action.*

4.6 Global Euclidean coordinates for the unique identifiability space of canonical port-Hamiltonian systems

Recall from Section 4.4 that $\Theta_{CH_n}^{can}$ contains pairs (\mathbf{d}, \mathbf{v}) where $\mathbf{d} \in \mathbb{R}_+^n$ and $\mathbf{v} \in \mathbb{R}^{2n}$ are such that the entries d_l 's are all distinct and $v_l^2 + v_{n+l}^2 > 0$ for all $l = 1, \dots, n$. We define for convenience a function $\mathcal{R} : \mathbb{R}^{2n} \rightarrow \mathbb{R}_{\geq 0}^n$ as $\mathcal{R}((v_1, \dots, v_{2n})^T) = (v_1^2 + v_{n+1}^2, \dots, v_n^2 + v_{2n}^2)^T$.

Now observe that the quotient space $\Theta_{CH_n}^{can} / (S_n \rtimes_{\phi} \mathbb{T}^n)$ naturally has a smooth manifold structure. We briefly prove this in the following lines. Note that the torus \mathbb{T}^n is a connected abelian compact Lie group. The symmetry group S_n is a finite group, and hence compact as well. Thus, it is easy to see that the semi-direct product $S_n \rtimes_{\phi} \mathbb{T}^n$ is also a compact Lie group, and hence its action on $\Theta_{CH_n}^{can}$ is automatically proper. On the other hand, since $\Theta_{CH_n}^{can}$ is the space of (\mathbf{d}, \mathbf{v}) pairs satisfying that \mathbf{d} contains distinct entries and $\mathcal{R}(\mathbf{v})^{(l)} > 0$ for $l = 1, \dots, n$, it necessarily holds that the only element in $S_n \rtimes_{\phi} \mathbb{T}^n$ that possibly keep any element in $\Theta_{CH_n}^{can}$ invariant is the identity, which implies the $(S_n \rtimes_{\phi} \mathbb{T}^n)$ -action on $\Theta_{CH_n}^{can}$ is free. Classical results in Lie theory (Ortega and Ratiu, 2004, Proposition 2.3.8) guarantee that $\Theta_{CH_n}^{can} / (S_n \rtimes_{\phi} \mathbb{T}^n)$ admits a unique smooth structure such that the quotient map $\pi : \Theta_{CH_n}^{can} \rightarrow \Theta_{CH_n}^{can} / (S_n \rtimes_{\phi} \mathbb{T}^n)$ is a submersion. With this as a motivation, we try to find the quotient space explicitly in the following.

For a fixed \mathbf{d} , we denote by \mathbf{d}_{\uparrow} the reordered vector constructed out of \mathbf{d} by placing the entries in increasing order. Denote by $\mathbb{R}_{+\uparrow}^n$ the set of $\mathbf{d} \in \mathbb{R}_+^n$ with distinct positive entries in increasing order. We have then the following proposition that explicitly characterizes the quotient space $\Theta_{CH_n}^{can} / (S_n \rtimes_{\phi} \mathbb{T}^n)$.

Proposition 33 (Global Euclidean coordinates for orbit space $\Theta_{CH_n}^{can} / (S_n \rtimes_{\phi} \mathbb{T}^n)$) *The map $f : \Theta_{CH_n}^{can} / (S_n \rtimes_{\phi} \mathbb{T}^n) \rightarrow \mathbb{R}_{+\uparrow}^n \times \mathbb{R}_+^n$ defined by $f([\mathbf{d}, \mathbf{v}]) = (\mathbf{d}_{\uparrow}, \mathcal{R}(\Gamma_{\sigma}(\mathbf{v})))$, where $\sigma \in S_n$ is the unique permutation such that $\Gamma_{\sigma}(\mathbf{d}) = \mathbf{d}_{\uparrow}$, is an isomorphism.*

5. Linear port-Hamiltonian systems in normal form are restrictions of higher dimensional ones

In this section, we prove a theorem (Theorem 34), inspired by the classical Kalman Decomposition (Jacob and Zwart (2012)), which says the filter induced by any $(Q, B) \in PH_n$ can

be regarded as that induced by some $(Q', B') \in PH_m$, where m can be any integer that is at least n . The motivation for these considerations is given by the fact that in many practical situations in which an input/output system has to be learned, the dimension of the underlying state-space system is not known. In that situation, we may want to have the flexibility of considering the actual system that needs to be learned as a lower-dimensional restriction of a much larger-dimensional one that we have picked for the learning task.

We shall carry this out by producing an explicit injective system morphism between the state space of (Q, B) and that of (Q', B') in our next Theorem 34. In Proposition 35, we show that the quotient space PH_n / \sim_{sys} can be characterized as $PH_{m,n} / \sim_{sys}$, where $PH_{m,n} \subset PH_m$ is the space containing all the systems of the form (Q', B') . Motivated by the developments in Section 4, we then characterize the pair $(\mathbf{d}', \mathbf{v}')$ that corresponds to (Q', B') in Proposition 36. Eventually, in Proposition 37, we show that the isomorphism $PH_n / \sim_{sys} \cong \Theta_{CH_n} / \sim_*$ can be lifted to high dimension as well. We shall comment further at the end of this section on the significance of the above-mentioned results in the context of machine learning.

The following theorem states that the filter induced by $(Q, B) \in PH_n$ can be reproduced using systems in an arbitrarily higher dimension.

Theorem 34 *Given any system $(Q, B) \in PH_n$, then*

- (i) *For any $m \geq n$, there exists an orthogonal matrix $O \in O(2m, \mathbb{R})$ such that the filter induced by $(Q', B') = \left(O \begin{bmatrix} Q & 0 \\ 0 & \mathbb{I}_{2m-2n} \end{bmatrix} O^T, O \begin{bmatrix} B \\ 0 \end{bmatrix} \right) \in PH_m$ coincides with that induced by (Q, B) .*
- (ii) *The map $f : \mathbb{R}^{2n} \rightarrow \mathbb{R}^{2m}$ defined by $f(\mathbf{z}) = O \begin{bmatrix} \mathbb{I}_{2n} \\ 0 \end{bmatrix} \cdot \mathbf{z}$ is an injective system morphism between the state spaces of (Q, B) and (Q', B') .*

As it can be seen in the proof (included in Appendix 9.10), the matrix $O \in O(2m, \mathbb{R})$ above is constructed so that

$$O \begin{bmatrix} \mathbb{J}_n & 0 \\ 0 & \mathbb{J}_{m-n} \end{bmatrix} O^T = \mathbb{J}_m. \quad (20)$$

From now on, we denote by $PH_{m,n} \subset PH_m$ the space of linear port-Hamiltonian systems parametrized by pairs (Q', B') of the form $\left(O \begin{bmatrix} Q & 0 \\ 0 & \mathbb{I}_{2m-2n} \end{bmatrix} O^T, O \begin{bmatrix} B \\ 0 \end{bmatrix} \right)$, where $O \in O(2m, \mathbb{R})$ satisfies (20), and equip it with the system automorphism relation \sim_{sys} defined on PH_m . The following proposition states that, up to system isomorphism, PH_n is indeed the same as $PH_{m,n}$. This means that, with appropriate initialization, we can exactly reproduce the input/output dynamics of $2n$ -dimensional port-Hamiltonian systems in higher dimension by simply considering the elements (Q', B') in $PH_{m,n}$.

Proposition 35 *The function $f : PH_n / \sim_{sys} \rightarrow PH_{m,n} / \sim_{sys}$ defined by*

$$f([Q, B]_{sys}) = \left[O \begin{bmatrix} Q & 0 \\ 0 & \mathbb{I}_{2m-2n} \end{bmatrix} O^T, O \begin{bmatrix} B \\ 0 \end{bmatrix} \right]_{sys}$$

is an isomorphism, where $O \in O(2m, \mathbb{R})$ is as in Theorem 34 and hence satisfies (20).

Recall that for a system $(Q, B) \in PH_n$, we derive the corresponding object $(\mathbf{d}, \mathbf{v}) \in \Theta_{CH_n}$ from Williamson's decomposition $Q = S^T \begin{bmatrix} D & 0 \\ 0 & D \end{bmatrix} S$ and $\mathbf{v} = S \cdot B$. We have seen that $(Q', B') \in PH_{m,n} \subset PH_m$ is also a linear port-Hamiltonian system in normal form. Therefore, it makes sense to investigate the relation between (\mathbf{d}, \mathbf{v}) and the element $(\mathbf{d}', \mathbf{v}')$ which corresponds to (Q', B') . The following proposition asserts that \mathbf{d}' can be obtained from \mathbf{d} by padding it with ones and, similarly, \mathbf{v}' can be obtained by splitting \mathbf{v} and padding each segment with zeros.

Proposition 36 (Symplectic eigenvalues of the higher dimensional system) *Let (Q, B) and (Q', B') be as in Theorem 34, and let \mathbf{d} and \mathbf{d}' be their corresponding symplectic eigenvalues. Then, up to reordering, $\mathbf{d}' = (d_1, \dots, d_n, 1, 1, \dots, 1)^T$. Even though \mathbf{v} and \mathbf{v}' are not uniquely determined (See Remark 8), there exists a choice of \mathbf{v}' that is related to $\mathbf{v} = (v_1, \dots, v_n, v_{n+1}, \dots, v_{2n})^T$ via*

$$\mathbf{v}' = (v_1, \dots, v_n, \underbrace{0, \dots, 0}_{m-n}, v_{n+1}, \dots, v_{2n}, \underbrace{0 \dots 0}_{m-n})^T.$$

From the above proposition, we call \mathbf{d}' the extended symplectic eigenvalues and \mathbf{v}' the extended vector. Now we define the space $\Theta_{CH_{m,n}}$ as the set of all pairs of the form $(\mathbf{d}', \mathbf{v}')$ and equip $\Theta_{CH_{m,n}}$ with the equivalence relation \sim_\star as in Definition 20 but in dimension m instead of n . Recall that we proved $\Theta_{CH_n} / \sim_\star \cong PH_n / \sim_{sys}$. Now we proceed to show that the above isomorphism in dimension $2n$ can be lifted to dimension $2m$ by considering only the restricted parameter spaces with vectors of the form $(\mathbf{d}', \mathbf{v}')$ and (Q', B') .

Proposition 37 *The function $f : \Theta_{CH_{m,n}} / \sim_\star \rightarrow PH_{m,n} / \sim_{sys}$ defined by*

$$f([\mathbf{d}', \mathbf{v}']_{\sim_\star}) = \left[\begin{bmatrix} D' & 0 \\ 0 & D' \end{bmatrix}, \mathbf{v}' \right]_{sys},$$

where $D' = \text{diag}(\mathbf{d}')$, is an isomorphism.

Note that in general \mathbf{d}' contains repeated symplectic eigenvalues because of all the ones used in the extension and that $v_l'^2 + v_{m+l}'^2 = 0$ for $l > n$. Therefore, it is impossible that $\Theta_{CH_{m,n}}$ contains canonical systems for $m > n$. In other words, lifting PH_n to $PH_{m,n}$ introduces degeneracies that exclude the possibility of the systems being canonical.

We emphasize that the above-mentioned series of results are crucial in machine learning applications. Very often in practice, the dimension $2n$ of the underlying data-generating process, that is, the latent port-Hamiltonian system (5), is not known, causing a problem when choosing the dimension of the controllable/observable Hamiltonian representation for learning. This issue can be solved by composing the morphism in Theorem 34 (ii) (which is injective) and the one in Theorem 7 (not necessarily injective). The composition of system morphisms is still a system morphism, this time between the underlying system $\theta_{PH_n}(Q, B)$ and the observable Hamiltonian representation in an arbitrarily higher dimension $2m \geq 2n$. In this way, the observable Hamiltonian representations in dimension $2m$ still have full expressive power to represent any $2n$ -dimensional system in PH_n , and hence can be used for learning. Practically, one can choose a sufficiently large m , and parameterize the observable Hamiltonian representation using (\mathbf{d}, \mathbf{v}) (we use the notation (\mathbf{d}, \mathbf{v}) instead of $(\mathbf{d}', \mathbf{v}')$)

because practically we do not know what n is) and then estimate them. We emphasize that the higher-dimensional port-Hamiltonian systems are in general not canonical, hence the (\mathbf{d}, \mathbf{v}) -pair that corresponds to the data-generating process is not guaranteed to be unique. Still, we always know there is at least one choice of (\mathbf{d}, \mathbf{v}) that works no matter how large an m we choose, and which is constructed using the recipe in Proposition 36.

6. Practical implementation of the results

We start with a diagram that summarizes the results that we have proved.

Theorem 38 *The following diagram holds true using the isomorphisms explicitly constructed in all the preceding results. We denote the inclusion between one set and the other by a one-directional arrow.*

$$\begin{array}{ccccccc}
 & & \Theta_{CH_{m,n}} / \sim_{\star} & \xleftarrow{\cong} & PH_{m,n} / \sim_{sys} & & \\
 & & \updownarrow \cong & & \updownarrow \cong & & \\
 \Theta_{CH_n} / \mathcal{H}_n & \xleftarrow{\cong} & \Theta_{CH_n} / \sim_{\star} & \xleftarrow{\cong} & PH_n / \sim_{sys} & \xleftarrow{\cong} & \Theta_{PH_n} / \mathcal{G}_n \\
 & & \uparrow & & \uparrow & & \\
 & & \Theta_{CH_n}^{can} / \sim_{\star} & \xleftarrow{\cong} & PH_n^{can} / \sim_{sys} & & \\
 & & \updownarrow \cong & & \updownarrow \cong & & \\
 \Theta_{CH_n}^{can} / (S_n \times_{\phi} \mathbb{T}^n) & \xleftarrow{\cong} & \Theta_{CH_n}^{can} / \sim_{sys} & \xleftarrow{\cong} & \Theta_{CH_n}^{can} / \sim_{filter} & & \\
 & & \updownarrow \cong & & & & \\
 & & \mathbb{R}_{+\uparrow}^n \times \mathbb{R}_+^n & & & &
 \end{array}$$

We now comment on how to use the results contained in the diagram above depending on the different learning situations that we may encounter. Indeed, we can use our statements to tackle three different learning scenarios:

- Case 1: The target port-Hamiltonian system (the data generating process that we want to learn) is canonical and its state-space dimension is known, that is, $\theta_{PH_n}(Q, B) \in PH_n^{can}$ with n known. This is the most favorable situation in the sense that we can exactly represent the system $\theta_{PH_n}(Q, B)$ by either the controllable or the observable Hamiltonian representations, which are both isomorphic to the original system. Furthermore, since, in this case, the input/output map can be uniquely identified by properly setting up the initialization, it can be learned by estimating an initial state condition of the representation used and the unique parameters in $\mathbb{R}_{+\uparrow}^n \times \mathbb{R}_+^n$.
- Case 2: The target port-Hamiltonian system is not guaranteed to be canonical but its dimension is known, that is, $\theta_{PH_n}(Q, B) \in PH_n$ with n known. In this case, there is a trade-off between the controllable Hamiltonian representation and the observable one.

As mentioned before, the controllable one will be structure-preserving but its expressive power depends on the controllability of the target system $\theta_{PH_n}(Q, B)$. On the other hand, the observable one always possesses full expressive power but does not always guarantee the port-Hamiltonian structure of the induced filter.

- **Case 3:** We are agnostic about the dimension of the target port-Hamiltonian system, that is, given $\theta_{PH_n}(Q, B) \in PH_n$ with n unknown. In this case, we need to choose a sufficiently large m so that $m \geq n$, then based on composition of system morphisms, it suffices to learn some $(\mathbf{d}, \mathbf{v}) \in \Theta_{CH_m}$ and use the $2m$ -dimensional observable Hamiltonian representation to reproduce the input-output dynamics of (Q, B) . Due to the loss of the canonical property, such a (\mathbf{d}, \mathbf{v}) pair may not be unique. Additionally, we do not know the dimension $2n$ of the data generating process, and hence we are ignorant of how many ones should be padded into \mathbf{d} (and similarly, how many zeros are padded into the vector \mathbf{v}). However, we do know that an element (\mathbf{d}, \mathbf{v}) exists in some $\Theta_{CH_{m,n}} \subset \Theta_{CH_m}$ that captures the input/output dynamics, given by Proposition 36.

An important special case is when there is no input to the port-Hamiltonian system, that is, $u(t) = 0$. In this case, the port-Hamiltonian system reduces to a linear Hamiltonian system with an arbitrary linear readout matrix. We emphasize that the observable Hamiltonian representation in a higher dimension is totally independent of B since it is simply given by

$$\begin{cases} \dot{\mathbf{s}} = g_1^{obs}(\mathbf{d}) \cdot \mathbf{s}, \\ y = (0, 0, \dots, 0, 1) \cdot \mathbf{s}, \end{cases} \quad (21)$$

In other words, Hamiltonian systems with linear readout can be learned by adjusting the initial state \mathbf{s}_0 and symplectic eigenvalues d_i , without even knowing the linear readout function that yields the observations.

7. Numerical illustrations

In this section, we present two numerical examples to demonstrate the effectiveness of our representation results from a learning point of view.

7.1 Non-dissipative circuit

Similar to an example in Medianu and Lefevre (2021), we consider a circuit consisting of a power source with voltage $V = u(t)$, together with five parallelizations, each of them containing a capacitor C_i with charge Q_i and an inductor L_i with magnetic flux linkage ϕ_i for $i = 1, \dots, 5$ (see Figure 1). Using Kirchhoff laws, we obtain the following port-Hamiltonian system in normal form (22) and (23), where the Hamiltonian of the system is

$$H(Q_1, \dots, Q_5, \phi_1, \dots, \phi_5) = \frac{Q_1^2}{2C_1} + \dots + \frac{Q_5^2}{2C_5} + \frac{\phi_1^2}{2L_1} + \dots + \frac{\phi_5^2}{2L_5}.$$

$$\begin{bmatrix} \dot{Q}_1 \\ \vdots \\ \dot{Q}_5 \\ \dot{\phi}_1 \\ \vdots \\ \dot{\phi}_5 \end{bmatrix} = \begin{bmatrix} 0 & \mathbb{I}_5 \\ -\mathbb{I}_5 & 0 \end{bmatrix} \cdot \begin{bmatrix} \frac{\partial H}{\partial Q_1} \\ \vdots \\ \frac{\partial H}{\partial Q_5} \\ \frac{\partial H}{\partial \phi_1} \\ \vdots \\ \frac{\partial H}{\partial \phi_5} \end{bmatrix} + \begin{bmatrix} 0 \\ \vdots \\ 0 \\ 1 \\ \vdots \\ 1 \end{bmatrix} \cdot u \quad (22)$$

$$y = \frac{\partial H}{\partial \phi_1} + \frac{\partial H}{\partial \phi_2} + \cdots + \frac{\partial H}{\partial \phi_5}, \quad (23)$$

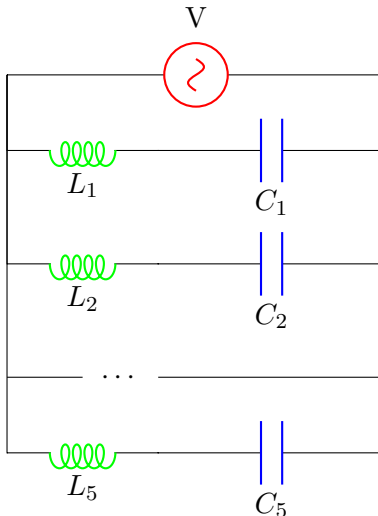


Figure 1: Lossless circuit port-Hamiltonian system

This port-Hamiltonian system treats the power supply $V = u$ as input and the current through the power supply, that is y , as output. One verifies that such a system is *non-canonical*. Our purpose is to learn the input-output behavior of this system without any access to the internal physical state and train only with input-output observations.

In our implementation, we choose for simplicity $C_i = 1$ and $L_i = 1$ for $i = 1, \dots, 5$. We choose to learn with a 10-dimensional observable Hamiltonian representation to show that the dynamics can be captured even in the non-canonical case. (Indeed, with our choice of C_i 's and L_i 's, the system is readily checked to be noncanonical). We randomly generate an initial condition for the ground-truth system and integrate it using Euler's method (see Appendix 9.14 for more sophisticated structure-preserving integration methods) with a discretization step of 0.01 for 1000 time steps. The input is chosen as $u(t) = \sin(t)$. The 1000 pairs of input and output data will be used as training data. During the training phase, we estimate the initial state $\mathbf{x} \in \mathbb{R}^{10}$ as well as the parameters $\mathbf{d} \in \mathbb{R}_+^5$ and $\mathbf{v} \in \mathbb{R}^{10}$. This is carried out via gradient descent using a learning rate of $\lambda = 0.1$ for 500 epochs. At each gradient descent iteration we integrate the state-space equations corresponding to the

current parameter values over 1000 times steps with Euler’s method and then we compute the squared error with respect to the training set.

We set a testing period of 4000 time steps and demonstrate the robustness of our approach by not only testing our trained model on the original input $u(t) = \sin(t)$ but evaluating on other three commonly used input signals (see Figure 2, 3, 4 and 5). The numerical experiments provide a strong indication that the underlying system is learned independently of the input signal and is robust with respect to various forms of inputs.

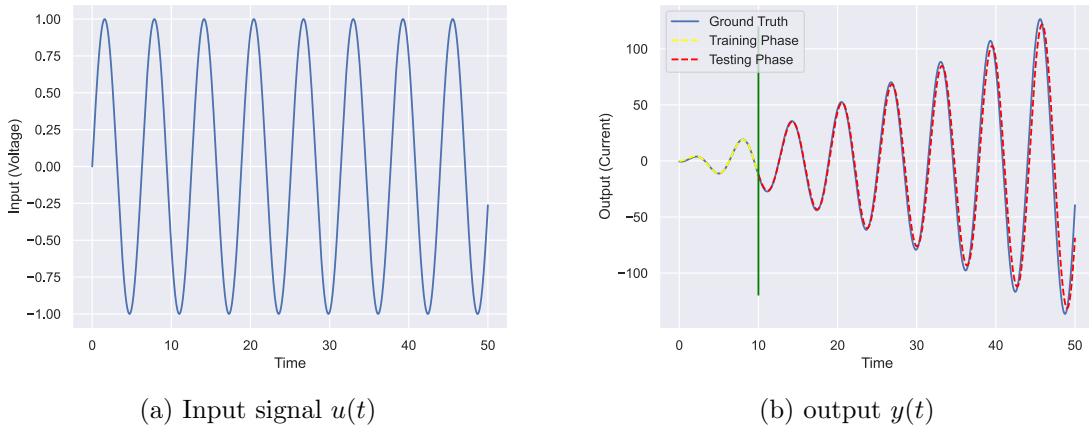


Figure 2: Training and testing on a sinusoidal signal.

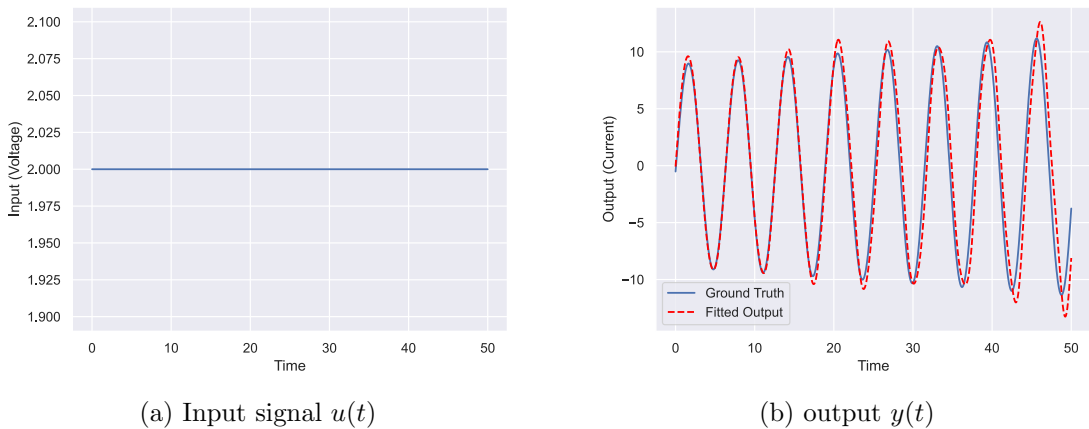


Figure 3: Testing on a constant signal. The training had been carried out using a sinusoidal signal. See Figure 2.

7.2 Positive definite Frenkel-Kontorova model

As a second example, we consider a modification of the well-known Frenkel-Kontorova model such that it becomes a linear port-Hamiltonian system with a positive-definite Hamiltonian function. Recall that the general form of Frenkel-Kontorova model describes the motion of classical particles with nearest neighbor interactions using periodic potentials. The Hamil-

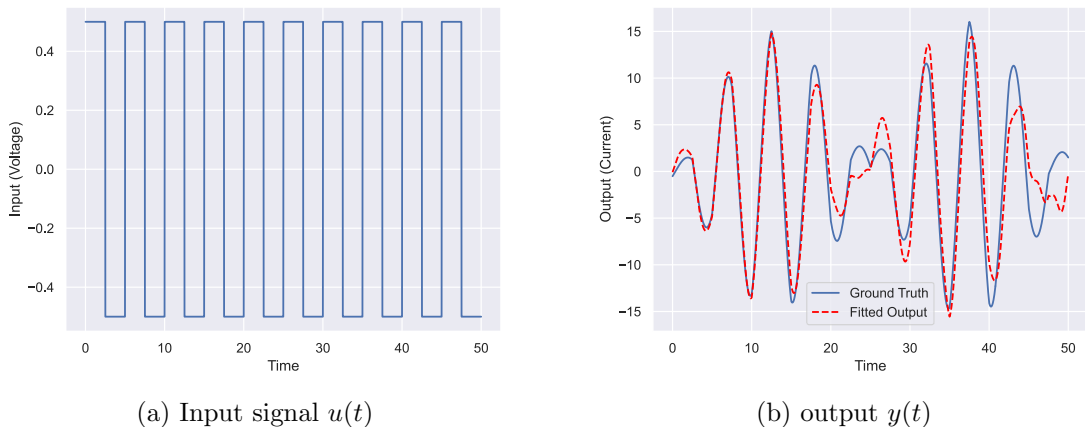


Figure 4: Testing on a square signal. The training had been carried out using a sinusoidal signal. See Figure 2.

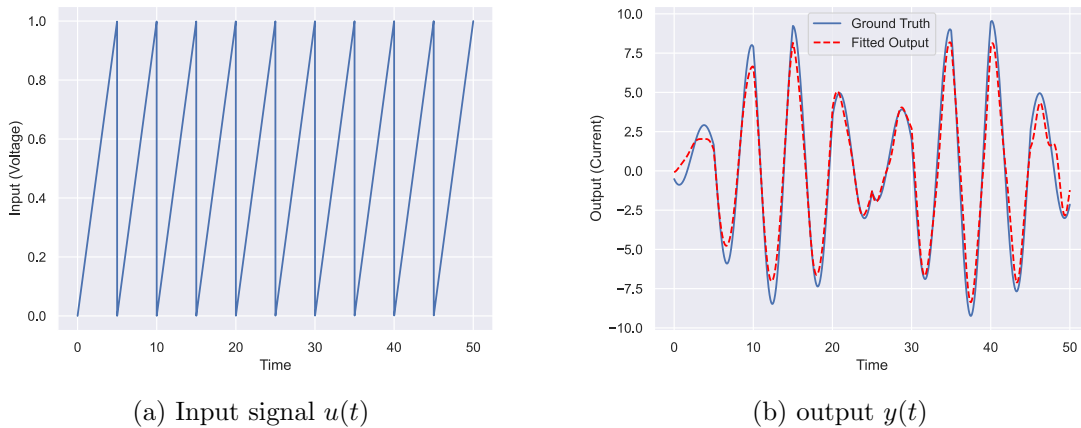


Figure 5: Testing on a ramp signal. The training had been carried out using a sinusoidal signal. See Figure 2.

tonian function can be written as

$$H = \sum_{n=1}^N \left[\frac{1}{2} \cdot \dot{q}_n^2 + \left(1 - \cos q_n + \frac{1}{2} g \cdot (q_{n+1} - q_n - a_0)^2 \right) \right].$$

Since we are dealing with linear systems, we remove the periodic potential and rescale the potential coefficient. By fixing $a_0 = 0$, we obtain the Hamiltonian

$$H = \frac{1}{2} \cdot \sum_{n=1}^N [\dot{q}_n^2 + (q_{n+1} - q_n)^2].$$

In order to consider a Hamiltonian that is strictly positive definite, we add a term $\frac{1}{2} q_1^2$ to the Hamiltonian, which carries the physical meaning that the particle q_1 interacts with

the origin via a spring. In summary, our model of interest now has the positive-definite Hamiltonian

$$H = \frac{1}{2} \cdot \sum_{n=1}^N [\dot{q}_n^2 + (q_{n+1} - q_n)^2] + \frac{1}{2} \cdot q_1^2 = \frac{1}{2} \cdot \sum_{n=1}^N [p_n^2 + (q_{n+1} - q_n)^2] + \frac{1}{2} \cdot q_1^2.$$

For the sake of simplicity, we consider in the above, a Hamiltonian system with $N = 2$ unit mass particles (so that $p_i = \dot{q}_i$) and an external force $F = u$ that is imposed on the first particle. This gives a linear port-Hamiltonian system in normal form as below with the output being the velocity of the first particle.

$$\begin{bmatrix} \dot{q}_1 \\ \dot{q}_2 \\ \dot{p}_1 \\ \dot{p}_2 \end{bmatrix} = \begin{bmatrix} 0 & \mathbb{I}_2 \\ -\mathbb{I}_2 & 0 \end{bmatrix} \cdot \begin{bmatrix} \frac{\partial H}{\partial q_1} \\ \frac{\partial H}{\partial q_2} \\ \frac{\partial H}{\partial p_1} \\ \frac{\partial H}{\partial p_2} \end{bmatrix} + \begin{bmatrix} 0 \\ 0 \\ 1 \\ 0 \end{bmatrix} \cdot u \quad (24)$$

$$y = \frac{\partial H}{\partial p_1}. \quad (25)$$

In contrast to the first example, this system is *canonical*. Therefore, based on our theoretical results, any input-output dynamics can be captured by either a controllable or an observable Hamiltonian representation, and furthermore, it is possible to uniquely identify the system by learning an initial condition, and the parameters in the quotient space $\mathbb{R}_{+\uparrow}^2 \times \mathbb{R}_+^2$.

For the sake of numerical illustration, we choose the initial state condition $\mathbf{x} = (2, 1, -3, -3)^T$ for the ground-truth system and integrate it 1000 time steps times using Euler's method with step of 0.01 (see Appendix 9.14 for more sophisticated structure-preserving integration methods), where the input is chosen as $u(t) = \sin(t)$. The 1000 pairs of input and output data are then used as training data.

As motivated above, we apply two different training mechanisms in which we learn the initial state condition and the parameter values of the model using both the natural parameters from Θ_{OH_n} of the observable Hamiltonian representation and those in the unique identifiability space $\mathbb{R}_{+\uparrow}^2 \times \mathbb{R}_+^2$. As in the previous example, we carry out the training using gradient descent with a learning rate of $\lambda = 0.02$ over 1500 epochs out of randomly chosen initial values for the initial state condition and the model parameters in Θ_{CH_n} and $\mathbb{R}_{+\uparrow}^2 \times \mathbb{R}_+^2$.

We record the validation error during the 1500 gradient descent iterations of both training mechanisms to compare their convergence rates. Heuristically, it should be expected that the rate of convergence is faster when the models are trained using the coordinates that provide unique identifiability. This is empirically confirmed in Figure 6 (indeed, unique identifiability provides exponentially faster convergence). After 1500 iterations, the prediction accuracy when training was carried out using the unique identifiability space significantly outperforms the other setting, as can be seen in Figure 7. Moreover, we found that the learned parameters $\mathbf{d} \in \mathbb{R}_{+\uparrow}^2$ are exactly the same as the eigenvalues of the Hamiltonian matrix, which is theoretically guaranteed by the unique identifiability. It is worth emphasizing that, despite the difference in the convergence rates, both mechanisms eventually lead to perfect path continuations of the input-output dynamics after enough training iterations.

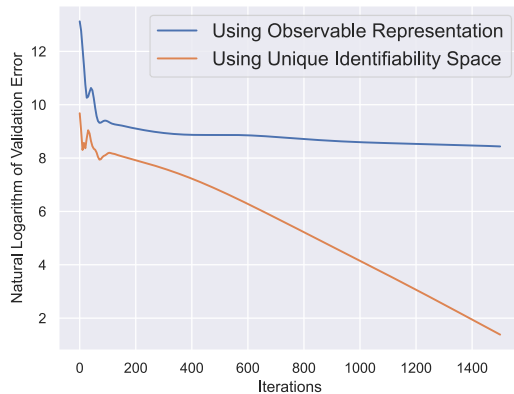
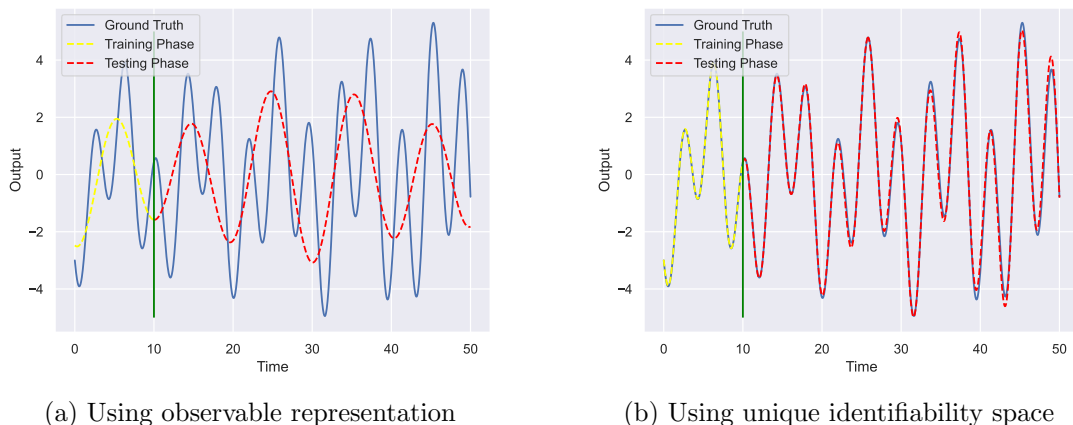


Figure 6: Logarithm of validation errors of the two training mechanisms based on using the natural parameters of the observable representation and the unique identifiability space



(a) Using observable representation

(b) Using unique identifiability space

Figure 7: Training and testing performance of the two training mechanisms after 1500 gradient descent iterations based on using the natural parameters of the observable representation (pane (a)) and the unique identifiability space (pane (b))

8. Conclusions

In this paper, we have introduced a complete structure-preserving learning scheme for single-input/single-output (SISO) linear port-Hamiltonian systems. The construction is based on the solution, when possible, of the unique identification problem for these systems, in ways that reveal fundamental relationships between classical notions in control theory and crucial properties in the machine learning context, like structure-preservation and expressive power.

The main building block in our construction is a representation result that we introduced for linear port-Hamiltonian systems in normal form that provides two subfamilies of linear systems that are by construction controllable and observable (Definition 5). We showed that morphisms can be established between the elements in these families and those in the category of normal form port-Hamiltonian systems. The existence of these morphisms immediately guarantees that the complexity of a generic subset of the family of

port-Hamiltonian filters is actually not $\mathcal{O}(n^2)$, as it could be guessed from the standard parametrization of this family, but $\mathcal{O}(n)$. We showed that the expressive power of our proposed representations is limited for non-canonical port-Hamiltonian systems. Indeed, we saw that the observable representation is guaranteed to capture all possible input-output dynamics of port-Hamiltonian systems (full expressive power), but it does not always produce port-Hamiltonian dynamics (fails to be structure-preserving). In the controllable case, structure preservation is guaranteed, but there is, in general, no full expressive power. For canonical port-Hamiltonian systems, these representations are both structure-preserving and have full expressive power.

We saw that even in the canonical situation, the availability of the controllable/observable representations did not yet provide a well-specified learning problem for this category since the invariance of these systems under system automorphisms implies the existence of symmetries (or degeneracies) in those parametrizations. We tackled this problem by solving the unique identifiability of input-output dynamics of linear port-Hamiltonian systems in normal form up to initializations by characterizing the quotient space by system automorphisms as a Lie groupoid orbit space. Moreover, we showed that in the canonical case the corresponding quotient spaces can be characterized as orbit spaces with respect to an explicit group action and can be explicitly endowed with a smooth manifold structure that has global Euclidean coordinates that can be used at the time of constructing estimation algorithms. Consequently, we showed that canonical port-Hamiltonian dynamics can be identified fully and explicitly in either the controllable or the observable Hamiltonian representations and learned by estimating an initial state condition and a unique set of parameters in a smooth manifold obtained as a group orbit space. Additionally, we complemented this learning scheme with results that allow us to extend it to situations where we remain agnostic regarding the dimension of the underlying data-generating port-Hamiltonian system.

We concluded the paper with some numerical examples that illustrate the viability of the method we propose in systems with various levels of complexity and dimensions and the computational advantages associated with using the parameter space in which unique identification is guaranteed.

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Glossary of Symbols

$\Theta_{CH_{m,n}}$	The space of parameters $(\mathbf{d}', \mathbf{v}')$ for $PH_{m,n}$
\mathbb{R}_{\uparrow}^n	The set of n -tuples of distinct positive real numbers in increasing order
\mathbb{T}^n	The n -torus
$\mathcal{CH}_n/\mathcal{OH}_n$	The space of filters induced by CH_n/OH_n
$\mathcal{G}_n \rightrightarrows \Theta_{PH_n}$	Port-Hamiltonian groupoid, see Proposition 24

$\mathcal{H}_n \rightrightarrows \Theta_{CH_n}$	Reduced port-Hamiltonian groupoid, see Proposition 26
\mathcal{PH}_n	The space of input-output dynamics/filters induced by systems in PH_n
\mathcal{PH}_n^{can}	The space of input-output dynamics/filters induced by systems in PH_n^{can}
$\mathfrak{sp}(2n, \mathbb{R})$	Lie algebra of the symplectic group
\sim_*	An equivalence relation defined on Θ_{CH_n}
\sim_{filter}	The equivalence relation of inducing the same filter
\sim_{sys}	The equivalence relation of system automorphism
$\Theta_{CH_n}/\Theta_{OH_n}$	The space of parameters (\mathbf{d}, \mathbf{v}) for CH_n and/or OH_n , which are the same
$\theta_{CH_n}/\theta_{OH_n}$	The map that send parameters in for $\Theta_{CH_n}/\Theta_{OH_n}$ to the corresponding state space system in CH_n/OH_n
$\Theta_{CH_n}^{can}$	The subset of Θ_{CH_n} that corresponds to canonical systems
Θ_{PH_n}	The space of parameters (Q, B) for PH_n
θ_{PH_n}	The map that sends parameters in for Θ_{PH_n} to the corresponding state space system in PH_n
B	Input matrix of a port-Hamiltonian system in normal form
CH_n/OH_n	The space of $2n$ -dimensional controllable/observable Hamiltonian representations
$F : \mathcal{Z} \times \mathcal{U} \rightarrow \mathcal{Z}$	State equation
$H : \mathbb{R}^{2n} \rightarrow \mathbb{R}$	Hamiltonian function
PH_n	The space of $2n$ -dimensional linear normal form port-Hamiltonian systems (5)
PH_n^{can}	The subspace of PH_n consisting of canonical linear normal form port-Hamiltonian systems
$PH_{m,n}$	The subspace of PH_m containing all $(Q', B') = \left(O \begin{bmatrix} Q & 0 \\ 0 & \mathbb{I}_{2m-2n} \end{bmatrix} O^T, O \begin{bmatrix} B \\ 0 \end{bmatrix} \right)$, $(Q, B) \in PH_n$, $O \in O(2m, \mathbb{R})$
Q	Quadratic form that determines a linear Hamiltonian system
S_n	Permutation group of n -elements
$Sp(2n, \mathbb{R})$	Symplectic group
$\mathbb{J}_n = \begin{bmatrix} 0 & \mathbb{I}_n \\ -\mathbb{I}_n & 0 \end{bmatrix}$	Canonical symplectic matrix

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9. Appendices

9.1 Proof of Theorem 7 (i)

Let $(\mathbf{d}, \mathbf{v}) \in \Theta_{CH_n}$ and let

$$\begin{cases} \dot{\mathbf{s}} = g_1^{ctr}(\mathbf{d}) \cdot \mathbf{s} + (0, 0, \dots, 0, 1)^T \cdot u, \\ y = g_2^{ctr}(\mathbf{d}, \mathbf{v}) \cdot \mathbf{s}, \end{cases} \quad (26)$$

be the corresponding linear controllable state-space system. In the following paragraphs, we construct for every $S \in Sp(2n, \mathbb{R})$, a linear system morphism $f_S^{(\mathbf{d}, \mathbf{v})} : \mathbb{R}^{2n} \rightarrow \mathbb{R}^{2n}$ between (26) and the port-Hamiltonian system $(Q, B) = \varphi_S(\theta_{CH_n}(\mathbf{d}, \mathbf{v})) \in PH_n$ in the statement. Notice, first of all that Q is by construction symmetric and positive-definite. Let now $L \in \mathbb{M}_{2n}$ be the matrix implementing the linear map $f_S^{(\mathbf{d}, \mathbf{v})}$, that is, $f_S^{(\mathbf{d}, \mathbf{v})}(\mathbf{s}) = L\mathbf{s}$, $\mathbf{s} \in \mathbb{R}^{2n}$. We now explicitly construct L and prove that it provides a system morphism.

We start by denoting $A := \mathbb{J}_n \begin{bmatrix} D & 0 \\ 0 & D \end{bmatrix}$, and define for each $k = 1, \dots, 2n$, a matrix $L_k \in \mathbb{M}^{2n}$ as

$$L_{2n-k} := A^k + a_{2n-1} \cdot A^{k-1} + \dots + a_{2n-k} \cdot \mathbb{I}_{2n}.$$

In particular, $L_{2n} = \mathbb{I}_{2n}$. Then, L is constructed as $L' := [L_1 \mathbf{v} \quad L_2 \mathbf{v} \quad \dots \quad L_{2n} \mathbf{v}]$, and $L := S^{-1} L'$.

We now check that $f_S^{(\mathbf{d}, \mathbf{v})}(\mathbf{s}) = L\mathbf{s}$ is indeed a system morphism between (26) and the port-Hamiltonian system (5) with $Q = S^T \begin{bmatrix} D & 0 \\ 0 & D \end{bmatrix} S$ and $B = S^{-1} \mathbf{v}$. This amounts to checking that

- (i) $L \cdot g_1^{ctr}(\mathbf{d}) = \mathbb{J}_n Q L$
- (ii) $L \cdot (0, 0, \dots, 0, 1)^T = B$

(iii) $g_2^{ctr}(\mathbf{d}, \mathbf{v}) = B^T Q L$.

We note that (ii) trivially holds. Now, (i) is equivalent to

$$\begin{aligned} S^{-1} L' g_1^{ctr}(\mathbf{d}) &= \mathbb{J}_n S^T \begin{bmatrix} D & 0 \\ 0 & D \end{bmatrix} S S^{-1} L' = S^{-1} \mathbb{J}_n \begin{bmatrix} D & 0 \\ 0 & D \end{bmatrix} S S^{-1} L' \\ \iff L' g_1^{ctr}(\mathbf{d}) &= \mathbb{J}_n \begin{bmatrix} D & 0 \\ 0 & D \end{bmatrix} L' \\ \iff [L_1 \mathbf{v} \quad L_2 \mathbf{v} \quad \cdots \quad L_{2n} \mathbf{v}] &\begin{bmatrix} 0 & 1 & 0 & \cdots & 0 \\ 0 & 0 & 1 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & 1 \\ -a_0 & -a_1 & -a_2 & \cdots & -a_{2n-1} \end{bmatrix} = A [L_1 \mathbf{v} \quad L_2 \mathbf{v} \quad \cdots \quad L_{2n} \mathbf{v}] \end{aligned}$$

We compare the k -th columns of the left and the right-hand sides in this equality. When $k = 1$, the difference between the first columns in the left and the right-hand side is

$$\begin{aligned} A L_1 \mathbf{v} + a_0 \mathbf{v} &= A(A^{2n-1} + a_{2n-1} \cdot A^{2n-2} + \cdots + a_1 \cdot \mathbb{I}) \mathbf{v} + a_0 \mathbf{v} \\ &= (A^{2n} + a_{2n-1} A^{2n-1} + \cdots + a_1 A + a_0) \mathbf{v} = 0. \end{aligned} \quad (27)$$

The last equality holds as a consequence of the Cayley-Hamilton theorem. Indeed, by the definition of the entries $\{a_0, a_1, \dots, a_{2n-1}\}$ we have that the characteristic polynomial of A is

$$\begin{aligned} \det(\lambda \mathbb{I}_{2n} - A) &= \det\left(\lambda \mathbb{I}_{2n} - \begin{bmatrix} 0 & D \\ -D & 0 \end{bmatrix}\right) = \det\left(\begin{bmatrix} \lambda \mathbb{I}_n & -D \\ D & \lambda \mathbb{I}_n \end{bmatrix}\right) \\ &= \det(\lambda \mathbb{I}_{2n}) \cdot \det\left(\lambda \mathbb{I}_{2n} - (-D) \left(\frac{1}{\lambda} \mathbb{I}_n\right) D\right) \\ &= (\lambda^2 + d_1^2)(\lambda^2 + d_2^2) \cdots (\lambda^2 + d_n^2) = \lambda^{2n} + \sum_{i=0}^{2n-1} a_i \cdot \lambda^i. \end{aligned}$$

Consequently, since by the Cayley-Hamilton theorem, A solves its characteristic polynomial, we can conclude that $A^{2n} + a_{2n-1} A^{2n-1} + \cdots + a_1 A + a_0 = 0$ and hence (27) follows. When $1 < k \leq 2n$, the difference between the k -th columns in the left and the right-hand side is

$$(L_{k-1} \mathbf{v} - a_{k-1} \mathbf{v}) - A L_k \mathbf{v} = (L_{k-1} - a_{k-1} \mathbb{I}_{2n} - A L_k) \mathbf{v} = 0,$$

since

$$\begin{aligned} L_{k-1} - a_{k-1} \mathbb{I}_{2n} - A L_k &= (A^{2n-k+1} + a_{2n-1} \cdot A^{2n-k} + \cdots + a_{k-1} \cdot \mathbb{I}_{2n}) - a_{k-1} \cdot \mathbb{I}_{2n} \\ &\quad - A(A^{2n-k} + a_{2n-1} \cdot A^{2n-k-1} + \cdots + a_k \cdot \mathbb{I}_{2n}) = 0. \end{aligned}$$

We have hence proved that (i) holds. We now proceed to check (iii). This amounts to computing

$$\begin{aligned} B^T Q L &= (S^{-1} \mathbf{v})^T S^T \begin{bmatrix} D & 0 \\ 0 & D \end{bmatrix} S S^{-1} L' = \mathbf{v}^T \begin{bmatrix} D & 0 \\ 0 & D \end{bmatrix} L' \\ &= \mathbf{v}^T \begin{bmatrix} D & 0 \\ 0 & D \end{bmatrix} [L_1 \mathbf{v} \quad L_2 \mathbf{v} \quad \cdots \quad L_{2n} \mathbf{v}]. \end{aligned} \quad (28)$$

Let us denote

$$B^T Q L = [c_{2n} \quad c_{2n-1} \quad c_{2n-2} \quad \cdots \quad c_2 \quad c_1]. \quad (29)$$

Then we observe that for $k = 1, \dots, n$,

$$\begin{aligned}
 c_{2k} &= \mathbf{v}^T \begin{bmatrix} D & 0 \\ 0 & D \end{bmatrix} L_{2n-2k+1} \mathbf{v} \\
 &= \mathbf{v}^T \begin{bmatrix} D & 0 \\ 0 & D \end{bmatrix} \left[\left(\mathbb{J}_n \begin{bmatrix} D & 0 \\ 0 & D \end{bmatrix} \right)^{2k-1} + a_{2n-1} \left(\mathbb{J}_n \begin{bmatrix} D & 0 \\ 0 & D \end{bmatrix} \right)^{2k-2} + \dots + a_{2n-2k+1} \cdot \mathbb{I}_{2n} \right] \mathbf{v} \\
 &= \mathbf{v}^T \begin{bmatrix} D & 0 \\ 0 & D \end{bmatrix} \left[\left(\mathbb{J}_n \begin{bmatrix} D & 0 \\ 0 & D \end{bmatrix} \right)^{2k-1} + a_{2n-2} \left(\mathbb{J}_n \begin{bmatrix} D & 0 \\ 0 & D \end{bmatrix} \right)^{2k-3} + \dots + a_{2n-2k+2} \left(\mathbb{J}_n \begin{bmatrix} D & 0 \\ 0 & D \end{bmatrix} \right) \right] \mathbf{v} \\
 &= \mathbf{v}^T \left[\mathbb{J}_n^{2k-1} \cdot \begin{bmatrix} D & 0 \\ 0 & D \end{bmatrix}^{2k} + a_{2n-2} \cdot \mathbb{J}_n^{2k-3} \cdot \begin{bmatrix} D & 0 \\ 0 & D \end{bmatrix}^{2k-2} + \dots + a_{2n-2k+2} \cdot \mathbb{J}_n \cdot \begin{bmatrix} D & 0 \\ 0 & D \end{bmatrix}^2 \right] \mathbf{v} = 0,
 \end{aligned}$$

The last equation follows from the fact that each summand is a skew-symmetric matrix. On the other hand, for $k = 0, \dots, n-1$,

$$\begin{aligned}
 c_{2k+1} &= \mathbf{v}^T \begin{bmatrix} D & 0 \\ 0 & D \end{bmatrix} L_{2n-2k} \mathbf{v} \\
 &= \mathbf{v}^T \begin{bmatrix} D & 0 \\ 0 & D \end{bmatrix} \left[\left(\mathbb{J}_n \begin{bmatrix} D & 0 \\ 0 & D \end{bmatrix} \right)^{2k} + a_{2n-1} \left(\mathbb{J}_n \begin{bmatrix} D & 0 \\ 0 & D \end{bmatrix} \right)^{2k-1} + \dots + a_{2n-2k} \cdot \mathbb{I}_{2n} \right] \mathbf{v} \\
 &= \mathbf{v}^T \begin{bmatrix} D & 0 \\ 0 & D \end{bmatrix} \left[\left(\mathbb{J}_n \begin{bmatrix} D & 0 \\ 0 & D \end{bmatrix} \right)^{2k} + a_{2n-2} \left(\mathbb{J}_n \begin{bmatrix} D & 0 \\ 0 & D \end{bmatrix} \right)^{2k-2} + \dots + a_{2n-2k} \cdot \mathbb{I}_{2n} \right] \mathbf{v} \\
 &= \mathbf{v}^T \left[(-1)^k \cdot \begin{bmatrix} D & 0 \\ 0 & D \end{bmatrix}^{2k+1} + a_{2n-2} \cdot (-1)^{k-1} \cdot \begin{bmatrix} D & 0 \\ 0 & D \end{bmatrix}^{2k-1} + \dots + a_{2n-2k} \cdot \begin{bmatrix} D & 0 \\ 0 & D \end{bmatrix} \right] \mathbf{v}.
 \end{aligned}$$

Substitute the values of coefficients a_{2k} as expressions in terms of d_i 's, we obtain that

$$c_{2k+1} = \mathbf{v}^T \begin{bmatrix} F_k & 0 \\ 0 & F_k \end{bmatrix} \mathbf{v},$$

for $k = 0, \dots, n-1$, and

$$F_k = \begin{bmatrix} f_1 & & & & \\ & f_2 & & & \\ & & \ddots & & \\ & & & \ddots & \\ 0 & & & & f_{n-1} \\ & & & & & f_n \end{bmatrix}$$

with $f_l = d_l \cdot \sum_{\substack{j_1, \dots, j_k \neq l \\ 1 \leq j_1 < \dots < j_k \leq n}} (d_{j_1} d_{j_2} \cdots d_{j_k})^2$, $l = 1, \dots, n$. This is exactly how we define $g_2^{ctr}(\mathbf{d}, \mathbf{v})$. Hence, (iii) is also verified.

9.2 Proof of Theorem 7 (ii)

Let $(Q, B) \in PH_n$. Obtain \mathbf{d} and \mathbf{v} from (Q, B) as in the statement of the theorem. We aim to construct a linear system morphism $f_S^{(Q, B)} : \mathbb{R}^{2n} \rightarrow \mathbb{R}^{2n}$ between the port-Hamiltonian system $(Q, B) \in PH_n$ and the observable Hamiltonian representation associated to $(\mathbf{d}, \mathbf{v}) \in \Theta_{OH_n}$, that is,

$$\begin{cases} \dot{\mathbf{s}} = g_1^{obs}(\mathbf{d}) \cdot \mathbf{s} + g_2^{obs}(\mathbf{d}, \mathbf{v}) \cdot u, \\ y = (0, 0, \dots, 0, 1) \cdot \mathbf{s}. \end{cases} \quad (30)$$

Denote by $L \in \mathbb{M}_{2n}$ the matrix implementing the linear map $f_S^{(Q, B)}$, that is, $f_S^{(Q, B)}(\mathbf{s}) = L\mathbf{s}$, $\mathbf{s} \in \mathbb{R}^{2n}$. We now construct a L which yields a system morphism. We start by writing $A := \mathbb{J}_n \begin{bmatrix} D & 0 \\ 0 & D \end{bmatrix}$ and define,

for each $k = 1, \dots, 2n$, a matrix $L_k \in \mathbb{M}^{2n}$ as

$$\begin{aligned} L_{2n-k} &:= (\mathbb{J}_n Q)^k + a_{2n-1} \cdot (\mathbb{J}_n Q)^{k-1} + \dots + a_{2n-k} \cdot \mathbb{I}_{2n} \\ &= (S^{-1}AS)^k + a_{2n-1} \cdot (S^{-1}AS)^{k-1} + \dots + a_{2n-k} \cdot \mathbb{I}_{2n} \\ &= S^{-1}(A^k + a_{2n-1} \cdot A^{k-1} + \dots + a_{2n-k} \cdot \mathbb{I}_{2n}) \cdot S. \end{aligned}$$

In particular, $L_{2n} = \mathbb{I}_{2n}$. Then, define L is as $L := \begin{bmatrix} B^T Q L_1 \\ B^T Q L_2 \\ \vdots \\ B^T Q L_{2n} \end{bmatrix}_{2n \times 2n}$.

We now check that $f_S^{(Q,B)}(\mathbf{s}) = L\mathbf{s}$ is indeed a system morphism between the port-Hamiltonian system (5) and the observable Hamiltonian representation (30) with $Q = S^T \begin{bmatrix} D & 0 \\ 0 & D \end{bmatrix} S$ and $B = S^{-1}\mathbf{v}$. This amounts to checking that

- (i) $g_1^{obs}(\mathbf{d}) \cdot L = L\mathbb{J}_n Q$
- (ii) $LB = g_2^{obs}(\mathbf{d}, \mathbf{v})$
- (iii) $B^T Q = (0, 0, \dots, 0, 1) \cdot L$.

We note that (iii) is straightforward. Now, (i) is equivalent to

$$\begin{bmatrix} 0 & 0 & \dots & 0 & -a_0 \\ 1 & 0 & \dots & 0 & -a_1 \\ 0 & 1 & \dots & 0 & -a_2 \\ \vdots & \vdots & \dots & \vdots & \vdots \\ 0 & 0 & \dots & 1 & -a_{2n-1} \end{bmatrix} \begin{bmatrix} B^T Q L_1 \\ B^T Q L_2 \\ \vdots \\ B^T Q L_{2n} \end{bmatrix} = \begin{bmatrix} B^T Q L_1 \\ B^T Q L_2 \\ \vdots \\ B^T Q L_{2n} \end{bmatrix} \cdot S^{-1}AS.$$

Compare now the k -th rows of the left and the right-hand sides of this equality. When $k = 1$, the difference between the first rows in the left and the right-hand sides are

$$\begin{aligned} B^T Q L_1 S^{-1}AS + a_0 B^T Q L_{2n} &= B^T Q (L_1 S^{-1}AS + a_0 \mathbb{I}_{2n}) \\ &= B^T Q S^{-1}(A^{2n} + a_{2n-1}A^{2n-1} + \dots + a_1 A + a_0 \cdot \mathbb{I}_{2n})S = B^T Q \cdot 0 = 0. \end{aligned}$$

The last equality follows, as in the proof of Theorem 7, from the Cayley-Hamilton theorem.

When $1 < k \leq 2n$, the difference between the k -th rows in the left and the right-hand sides are:

$$\begin{aligned} B^T Q L_{k-1} - a_{k-1} B^T Q L_{2n} - B^T Q L_k S^{-1}AS &= B^T Q (L_{k-1} - a_{k-1} \cdot \mathbb{I}_{2n} - L_k S^{-1}AS) \\ &= B^T Q S^{-1} \left[(A^{2n-k+1} + a_{2n-1} \cdot A^{2n-k} + \dots + a_{k-1} \cdot \mathbb{I}_{2n}) - a_{k-1} \cdot \mathbb{I}_{2n} \right. \\ &\quad \left. - (A^{2n-k} + a_{2n-1} \cdot A^{2n-k-1} + \dots + a_k \cdot \mathbb{I}_{2n})A \right] S = 0, \end{aligned}$$

which shows that (i) holds. We now proceed to check (ii). This is equivalent to computing

$$LB = \begin{bmatrix} B^T Q L_1 \\ B^T Q L_2 \\ \vdots \\ B^T Q L_{2n} \end{bmatrix} B.$$

Let us denote $LB = [c_{2n} \ c_{2n-1} \ c_{2n-2} \ \dots \ c_2 \ c_1]^T$. Then we have, for $k = 1, \dots, 2n$,

$$\begin{aligned} c_{2n-k+1} &= B^T Q L_k B = (S^{-1}\mathbf{v})^T S^T \begin{bmatrix} D & 0 \\ 0 & D \end{bmatrix} S S^{-1}(A^{2n-k} + a_{2n-1} \cdot A^{2n-k-1} + \dots + a_k \cdot \mathbb{I}_{2n}) S S^{-1}\mathbf{v} \\ &= \mathbf{v}^T \begin{bmatrix} D & 0 \\ 0 & D \end{bmatrix} (A^{2n-k} + a_{2n-1} \cdot A^{2n-k-1} + \dots + a_k \cdot \mathbb{I}_{2n})\mathbf{v}, \end{aligned}$$

which coincides exactly with the expression of c_{2n-k+1} in the equations (28) and (29) that we provided in the controllable Hamiltonian case. Thus, for (iii) to hold, we simply need to require that $g_2^{obs}(\mathbf{d}, \mathbf{v}) = (g_2^{ctr}(\mathbf{d}, \mathbf{v}))^T$.

9.3 Proof of Proposition 18

Proof of part (i). We have that $(\mathbf{d}_1, \mathbf{v}_1) \sim_{sys} (\mathbf{d}_2, \mathbf{v}_2)$ implies the existence of an invertible matrix L such that

$$\begin{cases} L \cdot g_1^{ctr}(\mathbf{d}_1) = g_1^{ctr}(\mathbf{d}_2) \cdot L \\ L \cdot (0, 0, \dots, 0, 1)^T = (0, 0, \dots, 0, 1)^T \\ g_2^{ctr}(\mathbf{d}_1, \mathbf{v}_1) = g_2^{ctr}(\mathbf{d}_2, \mathbf{v}_2) \cdot L \end{cases}$$

The first condition implies that $\det(\lambda \mathbb{I} - g_1^{ctr}(\mathbf{d}_1)) = \det(\lambda \mathbb{I} - g_1^{ctr}(\mathbf{d}_2))$, meaning that

$$(\lambda^2 + d_{1,1}^2) \dots (\lambda^2 + d_{1,n}^2) = (\lambda^2 + d_{2,1}^2) \dots (\lambda^2 + d_{2,n}^2).$$

Therefore, (i) is clear. With the symmetry in (i), it is clear that $g_1^{ctr}(\mathbf{d}_1) = g_1^{ctr}(\mathbf{d}_2)$. Note that the second condition says the last column of L is $(0, 0, \dots, 0, 1)^T$. Bring both facts into the first condition $L \cdot g_1^{ctr}(\mathbf{d}_1) = g_1^{ctr}(\mathbf{d}_2) \cdot L$ and compare both sides. This will deduce L can only be the identity. Thus the third condition becomes $g_2^{ctr}(\mathbf{d}_1, \mathbf{v}_1) = g_2^{ctr}(\mathbf{d}_2, \mathbf{v}_2)$, which is exactly (ii).

Conversely, with (i) and (ii) hold, we can check L being identity works. Thus, $(\mathbf{d}_1, \mathbf{v}_1) \sim_{sys} (\mathbf{d}_2, \mathbf{v}_2)$.

Proof of part (ii). Since $\theta_{CH_n}(\mathbf{d}_i, \mathbf{v}_i)$ ($i = 1, 2$) are linear systems, we can explicitly write down the filters as

$$(y_i(u), \mathbf{z}_0)_t = g_2^{ctr}(\mathbf{d}_i, \mathbf{v}_i) \int_0^t e^{g_1^{ctr}(\mathbf{d}_i)(t-s)} \cdot (0, 0, \dots, 0, 1)^T u(s) ds + g_2^{ctr}(\mathbf{d}_i, \mathbf{v}_i) e^{g_1^{ctr}(\mathbf{d}_i)t} \cdot \mathbf{z}_0.$$

We consider two special cases. In the first case, we take time $t = 0$, then $(y_i(u), \mathbf{z}_0)_0 = g_2^{ctr}(\mathbf{d}_i, \mathbf{v}_i) \cdot \mathbf{z}_0$. Since \mathbf{z}_0 can be arbitrary, the two filters coincide if and only if $c_j(\mathbf{d}_1, \mathbf{v}_1) = c_j(\mathbf{d}_2, \mathbf{v}_2)$ for all $j = 1, \dots, n$. In the second case, we take $\mathbf{z}_0 = \mathbf{0}$, then

$$(y_i(u), \mathbf{0})_t = g_2^{ctr}(\mathbf{d}_i, \mathbf{v}_i) \int_0^t \left[\mathbb{I} + g_1^{ctr}(\mathbf{d}_i)(t-s) + (g_1^{ctr}(\mathbf{d}_i))^2 \frac{(t-s)^2}{2!} + \dots \right] \cdot (0, 0, \dots, 0, 1)^T u(s) ds.$$

By differentiating the above with respect to t , and using the fact that the input $u(t)$ is arbitrary (and hence can choose $u(0)$ arbitrarily), we see that y_1 and y_2 coincide as filters if and only if $g_2^{ctr}(\mathbf{d}_1, \mathbf{v}_1)(g_1^{ctr}(\mathbf{d}_1))^k \cdot (0, 0, \dots, 0, 1)^T = g_2^{ctr}(\mathbf{d}_2, \mathbf{v}_2)(g_1^{ctr}(\mathbf{d}_2))^k \cdot (0, 0, \dots, 0, 1)^T$ for all $k \in \mathbb{N}$. Moreover, one verifies that $g_2^{ctr}(\mathbf{d}, \mathbf{v})(g_1^{ctr}(\mathbf{d}))^k \cdot (0, 0, \dots, 0, 1)^T = 0$ for odd k . Thus, if we define $e_i(\mathbf{d}, \mathbf{v}) = g_2^{ctr}(\mathbf{d}, \mathbf{v})(g_1^{ctr}(\mathbf{d}))^{2i} \cdot (0, 0, \dots, 0, 1)^T$, then $y_1 = y_2$ is equivalent to $e_i(\mathbf{d}_1, \mathbf{v}_1) = e_i(\mathbf{d}_2, \mathbf{v}_2)$ for all $i \in \mathbb{N}$. Now, one finds a recursion in the values of e_i 's, that is,, for all $m \leq n$

$$e_m(\mathbf{d}, \mathbf{v}) = -a_{2n-2} \cdot e_{m-1}(\mathbf{d}, \mathbf{v}) - a_{2n-4} \cdot e_{m-2}(\mathbf{d}, \mathbf{v}) - \dots - a_2 \cdot e_1(\mathbf{d}, \mathbf{v}) - a_0 \cdot e_{m-n}(\mathbf{d}, \mathbf{v}).$$

More precisely, it can be checked that the following recursion holds true

$$\begin{aligned} e_1 &= c_1 \\ e_2 &= c_3 - a_{2n-2} \cdot e_1 \\ e_3 &= c_5 - a_{2n-2} \cdot e_2 - a_{2n-4} \cdot e_1 \\ &\vdots \\ e_n &= c_{2n-1} - a_{2n-2} \cdot e_{n-1} - a_{2n-4} \cdot e_{n-2} - \dots - a_2 \cdot e_1. \end{aligned}$$

On the other hand, $(a_{2n-2}, \dots, a_2, a_0)$ happens to be the coefficients of the characteristic polynomial of $g_1^{ctr}(\mathbf{d}, \mathbf{v})$, therefore, by Cayley-Hamilton Theorem, $e_m(\mathbf{d}, \mathbf{v}) = 0$ for all $m > n$.

In conclusion, by combining the two special cases, we see that $\theta_{CH_n}(\mathbf{d}_1, \mathbf{v}_1)$ and $\theta_{CH_n}(\mathbf{d}_2, \mathbf{v}_2)$ induce the same filter if and only if $c_i(\mathbf{d}_1, \mathbf{v}_1) = c_i(\mathbf{d}_2, \mathbf{v}_2)$ and $e_i(\mathbf{d}_1, \mathbf{v}_1) = e_i(\mathbf{d}_2, \mathbf{v}_2)$ for all $0 \leq i \leq n-1$,

9.4 Proof of Theorem 22

$\varphi_S \circ \theta_{CH_n}$ is compatible with \sim_* and \sim_{sys} . Fix a choice of $S \in Sp(2n, \mathbb{R})$. We need to show that $(\mathbf{d}_1, \mathbf{v}_1) \sim_*(\mathbf{d}_2, \mathbf{v}_2)$ if and only if

$$\left(S^T \begin{bmatrix} D_1 & 0 \\ 0 & D_1 \end{bmatrix} S, S^{-1} \mathbf{v}_1 \right) := (Q_1, B_1) \sim_{sys} (Q_2, B_2) := \left(S^T \begin{bmatrix} D_2 & 0 \\ 0 & D_2 \end{bmatrix} S, S^{-1} \mathbf{v}_2 \right).$$

This means there exists an invertible L such that (14) holds. We claim that $L = S^{-1}PAS$ does the job, where P and A are given by Definition 20.

The first condition is

$$\begin{aligned} L\mathbb{J}Q_1 &= \mathbb{J}Q_2L \\ \iff L\mathbb{J}Q_1L^{-1} &= \mathbb{J}Q_2 \\ \iff S^{-1}PAS\mathbb{J}S^T \begin{bmatrix} D_1 & 0 \\ 0 & D_1 \end{bmatrix} SS^{-1}A^{-1}P^{-1}S &= \mathbb{J}S^T \begin{bmatrix} D_2 & 0 \\ 0 & D_2 \end{bmatrix} S \\ \iff S^{-1}PAS\mathbb{J}S^T \begin{bmatrix} D_1 & 0 \\ 0 & D_1 \end{bmatrix} A^{-1}P^{-1}S &= S^{-1}\mathbb{J} \begin{bmatrix} D_2 & 0 \\ 0 & D_2 \end{bmatrix} S \\ \iff PA\mathbb{J} \begin{bmatrix} D_1 & 0 \\ 0 & D_1 \end{bmatrix} A^{-1}P^{-1} &= \mathbb{J} \begin{bmatrix} D_2 & 0 \\ 0 & D_2 \end{bmatrix} \\ \iff A\mathbb{J} \begin{bmatrix} D_1 & 0 \\ 0 & D_1 \end{bmatrix} A^{-1} = P^T\mathbb{J} \begin{bmatrix} D_2 & 0 \\ 0 & D_2 \end{bmatrix} P \\ \iff A\mathbb{J} \begin{bmatrix} D_1 & 0 \\ 0 & D_1 \end{bmatrix} = \mathbb{J} \begin{bmatrix} D_1 & 0 \\ 0 & D_1 \end{bmatrix} A. \end{aligned}$$

The second condition is true by construction, namely

$$LB_1 = B_2 \iff S^{-1}PASS^{-1}\mathbf{v}_1 = S^{-1}\mathbf{v}_2 \iff \mathbf{v}_2 = PA\mathbf{v}_1.$$

The third condition is

$$\begin{aligned} B_1^T Q_1 &= B_2^T Q_2 L \\ \iff \mathbf{v}_1^T S^{-T} S^T \begin{bmatrix} D_1 & 0 \\ 0 & D_1 \end{bmatrix} S &= \mathbf{v}_2^T S^{-T} S^T \begin{bmatrix} D_2 & 0 \\ 0 & D_2 \end{bmatrix} SS^{-1}PAS \\ \iff \mathbf{v}_1^T \begin{bmatrix} D_1 & 0 \\ 0 & D_1 \end{bmatrix} = \mathbf{v}_2^T \begin{bmatrix} D_2 & 0 \\ 0 & D_2 \end{bmatrix} PA & \\ \iff \mathbf{v}_1^T \begin{bmatrix} D_1 & 0 \\ 0 & D_1 \end{bmatrix} = \mathbf{v}_1^T A^T P^T \begin{bmatrix} D_2 & 0 \\ 0 & D_2 \end{bmatrix} PA & \\ \iff \mathbf{v}_1^T \begin{bmatrix} D_1 & 0 \\ 0 & D_1 \end{bmatrix} = \mathbf{v}_1^T A^T \begin{bmatrix} D_1 & 0 \\ 0 & D_1 \end{bmatrix} A. & \end{aligned}$$

Based on the compatibility result above, we know that $\varphi_S \circ \theta_{CH_n}$ induces a unique map $\Phi_S : \Theta_{CH_n} / \sim_* \rightarrow PH_n / \sim_{sys}$ defined as $\Phi_S([\mathbf{d}, \mathbf{v}]_*) = \left[S^T \begin{bmatrix} D & 0 \\ 0 & D \end{bmatrix} S, S^{-1} \mathbf{v} \right]_{sys}$. We now verify that Φ_S does not depend on the choice of $S \in Sp(2n, \mathbb{R})$.

Φ_S is independent of S . It suffices to check that, for $S_1 \neq S_2$, we have $\left(S_1^T \begin{bmatrix} D & 0 \\ 0 & D \end{bmatrix} S_1, S_1^{-1} \mathbf{v} \right) := (Q'_1, B'_1) \sim_{sys} (Q'_2, B'_2) := \left(S_2^T \begin{bmatrix} D & 0 \\ 0 & D \end{bmatrix} S_2, S_2^{-1} \mathbf{v} \right)$, which again goes back to checking (14) holds for some

invertible L . We claim that $L = S_2^{-1}S_1$ does the job. The first condition is

$$\begin{aligned}
 L\mathbb{J}Q'_1 &= \mathbb{J}Q'_2L \\
 \iff L\mathbb{J}Q'_1L^{-1} &= \mathbb{J}Q'_2 \\
 \iff S_2^{-1}S_1\mathbb{J}S_1^T \begin{bmatrix} D & 0 \\ 0 & D \end{bmatrix} S_1S_1^{-1}S_2 &= \mathbb{J}S_2^T \begin{bmatrix} D & 0 \\ 0 & D \end{bmatrix} S_2 \\
 \iff \begin{bmatrix} D & 0 \\ 0 & D \end{bmatrix} &= \begin{bmatrix} D & 0 \\ 0 & D \end{bmatrix}.
 \end{aligned}$$

The second condition is

$$LB'_1 = B'_2 \iff S_2^{-1}S_1S_1^{-1}\mathbf{v} = S_2^{-1}\mathbf{v} \iff \mathbf{v} = \mathbf{v}.$$

The third condition is

$$\begin{aligned}
 B_1'^T Q'_1 &= B_2'^T Q'_2 L \\
 \iff \mathbf{v}^T S_1^{-T} S_1^T \begin{bmatrix} D & 0 \\ 0 & D \end{bmatrix} S_1 & \\
 &= \mathbf{v}^T S_2^{-T} S_2^T \begin{bmatrix} D & 0 \\ 0 & D \end{bmatrix} S_2 S_2^{-1} S_1 \\
 \iff \mathbf{v}^T \begin{bmatrix} D & 0 \\ 0 & D \end{bmatrix} &= \mathbf{v}^T \begin{bmatrix} D & 0 \\ 0 & D \end{bmatrix}.
 \end{aligned}$$

Since Φ_S does not depend on $S \in Sp(2n, \mathbb{R})$, we may as well choose $S = \mathbb{J}_n$ and call it Φ . Then Φ has the expression $\Phi([\mathbf{d}, \mathbf{v}]_\star) = \left[\begin{bmatrix} D & 0 \\ 0 & D \end{bmatrix}, \mathbf{v} \right]_{sys}$. We now verify that Φ is injective and surjective, and hence an isomorphism.

Φ is surjective. For an arbitrary choice $[Q, B]_{sys}$ of equivalence class, we take a representative Q and B . Since Q is symmetric positive-definite, by Williamson's theorem, $Q = S^T \begin{bmatrix} D & 0 \\ 0 & D \end{bmatrix} S$ for some $S \in Sp(2n, \mathbb{R})$ and the diagonal entries of D are nonnegative and can be identified with \mathbf{d} . Let $\mathbf{v} = S \cdot B$. Then we have $\Phi_S([\mathbf{d}, \mathbf{v}]_\star) = [Q, B]_{sys}$. Given that $\Phi_S = \Phi$ for any S , it holds that $\Phi([\mathbf{d}, \mathbf{v}]_\star) = [Q, B]_{sys}$. This concludes Φ being surjective.

Φ is injective. For $\left(\begin{bmatrix} D_1 & 0 \\ 0 & D_1 \end{bmatrix}, \mathbf{v}_1 \right) \sim_{sys} \left(\begin{bmatrix} D_2 & 0 \\ 0 & D_2 \end{bmatrix}, \mathbf{v}_2 \right)$, it means there exists some invertible L such that the conditions in (14) are all satisfied. We aim to show that $(\mathbf{d}_1, \mathbf{v}_1) \sim_\star (\mathbf{d}_2, \mathbf{v}_2)$. The first condition gives

$$\begin{aligned}
 L\mathbb{J} \begin{bmatrix} D_1 & 0 \\ 0 & D_1 \end{bmatrix} &= \mathbb{J} \begin{bmatrix} D_2 & 0 \\ 0 & D_2 \end{bmatrix} L \Rightarrow L\mathbb{J} \begin{bmatrix} D_1 & 0 \\ 0 & D_1 \end{bmatrix} L^{-1} = \mathbb{J} \begin{bmatrix} D_2 & 0 \\ 0 & D_2 \end{bmatrix} \\
 \Rightarrow \det \left(\lambda \mathbb{I} - \mathbb{J} \begin{bmatrix} D_1 & 0 \\ 0 & D_1 \end{bmatrix} \right) &= \det \left(\lambda \mathbb{I} - \mathbb{J} \begin{bmatrix} D_2 & 0 \\ 0 & D_2 \end{bmatrix} \right) \\
 \Rightarrow (\lambda^2 + d_{1,1}^2) \dots (\lambda^2 + d_{1,n}^2) &= (\lambda^2 + d_{2,1}^2) \dots (\lambda^2 + d_{2,n}^2).
 \end{aligned}$$

Therefore, $\{d_{1,i} | i = 1, \dots, n\}$ is the same as $\{d_{2,i} | i = 1, \dots, n\}$ as a set, and this implies the existence of some $\sigma \in S_n$ such that $d_{2,i} = d_{1,\sigma(i)}$ for $i = 1, \dots, n$. In other words, there exists some permutation matrix

P_σ such that $P \begin{bmatrix} D_1 & 0 \\ 0 & D_1 \end{bmatrix} P^T = \begin{bmatrix} D_2 & 0 \\ 0 & D_2 \end{bmatrix}$. Thus, (i) of Definition 20 holds. Further, we have

$$\begin{aligned} L\mathbb{J} \begin{bmatrix} D_1 & 0 \\ 0 & D_1 \end{bmatrix} &= \mathbb{J} \begin{bmatrix} D_2 & 0 \\ 0 & D_2 \end{bmatrix} L \\ \iff L\mathbb{J} \begin{bmatrix} D_1 & 0 \\ 0 & D_1 \end{bmatrix} &= \mathbb{J} P \begin{bmatrix} D_1 & 0 \\ 0 & D_1 \end{bmatrix} P^T L \\ \iff L\mathbb{J} \begin{bmatrix} D_1 & 0 \\ 0 & D_1 \end{bmatrix} &= P \mathbb{J} \begin{bmatrix} D_1 & 0 \\ 0 & D_1 \end{bmatrix} P^T L \\ \iff P^T L \mathbb{J} \begin{bmatrix} D_1 & 0 \\ 0 & D_1 \end{bmatrix} &= \mathbb{J} \begin{bmatrix} D_1 & 0 \\ 0 & D_1 \end{bmatrix} P^T L \\ \iff A \mathbb{J} \begin{bmatrix} D_1 & 0 \\ 0 & D_1 \end{bmatrix} &= \mathbb{J} \begin{bmatrix} D_1 & 0 \\ 0 & D_1 \end{bmatrix} A, \end{aligned}$$

if we denote $A := P^T L$. Thus, (iii) of Definition 20 holds true. The second condition of (14) says $\mathbf{v}_2 = L\mathbf{v}_1 = P A \mathbf{v}_1$. Thus, (iv) of Definition 20 holds true. Lastly, the third condition implies

$$\begin{aligned} \mathbf{v}_1^T \begin{bmatrix} D_1 & 0 \\ 0 & D_1 \end{bmatrix} &= \mathbf{v}_2^T \begin{bmatrix} D_2 & 0 \\ 0 & D_2 \end{bmatrix} L \\ \iff \mathbf{v}_1^T \begin{bmatrix} D_1 & 0 \\ 0 & D_1 \end{bmatrix} &= (P A \mathbf{v}_1)^T \left(P \begin{bmatrix} D_1 & 0 \\ 0 & D_1 \end{bmatrix} P^T \right) (P A) \\ \iff \mathbf{v}_1^T \begin{bmatrix} D_1 & 0 \\ 0 & D_1 \end{bmatrix} &= \mathbf{v}_1^T A^T \begin{bmatrix} D_1 & 0 \\ 0 & D_1 \end{bmatrix} A, \end{aligned}$$

Thus, (ii) in Definition 20 holds. We conclude that Φ is injective.

Φ is a homeomorphism with respect to the quotient topology. Before we prove this statement, we first quote a lemma (see, for instance, Abraham et al. (1988)).

Lemma 39 *Let X and Y be sets equipped with equivalence relations \sim_X and \sim_Y respectively. If $\phi : X \rightarrow Y$ is a map such that, for any $x_1, x_2 \in X$, $x_1 \sim_X x_2$ if and only if $\phi(x_1) \sim_Y \phi(x_2)$, then ϕ projects to a unique map $\tilde{\phi} : X/\sim_X \rightarrow Y/\sim_Y$ between the quotient spaces given by $\tilde{\phi}([x]_{\sim_X}) = [\phi(x)]_{\sim_Y}$ and such that the following diagram commutes. In particular, if ϕ is a homeomorphism between two topological spaces X and Y , then $\tilde{\phi}$ is also a homeomorphism.*

$$\begin{array}{ccc} X & \xrightarrow{\phi} & Y \\ \downarrow \pi_X & & \downarrow \pi_Y \\ X/\sim_X & \xrightarrow{\tilde{\phi}} & Y/\sim_Y \end{array}$$

We now proceed with the proof.

(i) If (Q_1, B_1) and $(Q_2, B_2) \in PH_n$ are linked by some linear symplectic map $S \in Sp(2n, \mathbb{R})$ by $(Q_2, B_2) = (S^{-T} Q_1 S^{-1}, S B_1)$, then $(Q_1, B_1) \sim_{sys} (Q_2, B_2)$. Therefore, as an immediate consequence of Williamson's normal form, we have $PH_n/\sim_{sys} = PH_n^{diag}/\sim_{sys}$, where

$$PH_n^{diag} := \left\{ \left(\begin{bmatrix} D & 0 \\ 0 & D \end{bmatrix}, \mathbf{v} \right) \mid D = \text{diag}(\mathbf{d}), d_i > 0, \mathbf{v} \in \mathbb{R}^{2n} \right\}.$$

(ii) There is an obvious homeomorphism $\varphi : \Theta_{CH_n} \rightarrow PH_n^{diag}$ given by $\varphi(\mathbf{d}, \mathbf{v}) = \left(\begin{bmatrix} D & 0 \\ 0 & D \end{bmatrix}, \mathbf{v} \right)$. Therefore, by identifying PH_n/\sim_{sys} with PH_n^{diag}/\sim_{sys} , the induced map of φ on the quotients is exactly Φ . By Lemma 39, Φ is also a homeomorphism.

To summarize, we have that the following diagram commutes.

$$\begin{array}{ccc} \Theta_{CH_n} & \xrightarrow{\varphi_S \circ \theta_{CH_n}} & PH_n \\ \downarrow \pi_* & & \downarrow \pi_{sys} \\ \Theta_{CH_n}/\sim_* & \xrightarrow[\Phi_S = \Phi]{\cong} & PH_n/\sim_{sys} \end{array}$$

9.5 Proof of Proposition 24

The axioms of being a groupoid mostly follow from the definition. Here, we only check the closure of the multiplication operation m , that is, $(L_1 L_2, (Q_2, B_2)) \in \mathcal{G}_n$. Note that

$$\mathbb{J}^T(L_1 L_2) \mathbb{J} Q_2 (L_1 L_2)^{-1} = \mathbb{J}^T L_1 \mathbb{J} (\mathbb{J}^T L_2 \mathbb{J} Q_2 L_2^{-1}) L_1^{-1} = \mathbb{J}^T L_1 \mathbb{J} Q_1 L_1^{-1}$$

is symmetric positive-definite. On the other hand, we have

$$\begin{aligned} \mathbb{J}^T(L_1 L_2)^T \mathbb{J}(L_1 L_2) B_2 &= \mathbb{J}^T L_2^T L_1^T \mathbb{J} L_1 L_2 B_2 = \mathbb{J}^T L_2^T L_1^T \mathbb{J} L_1 B_1 \\ &= \mathbb{J}^T L_2^T \mathbb{J} (\mathbb{J}^T L_1^T \mathbb{J} L_1 B_1) = \mathbb{J}^T L_2^T \mathbb{J} B_1 = \mathbb{J}^T L_2^T \mathbb{J} L_2 B_2 = B_2. \end{aligned}$$

Thus, closure of multiplication is proved. We also need to show that α and β are submersions. Indeed, for $(L, (Q, B)) \in \mathcal{G}_n$ and $(N, (P, C)) \in T_{(L, (Q, B))} \mathcal{G}_n$, it holds that

$$\begin{aligned} T_{(L, (Q, B))} \alpha(N, (P, C)) &= \left. \frac{d}{dt} \right|_{t=0} \left(\mathbb{J}^T(L + tN) \mathbb{J}(Q + tP)(L + tN)^{-1}, (L + tN)(B + tC) \right) \\ &= (\mathbb{J}^T N \mathbb{J} Q L^{-1} + \mathbb{J}^T L \mathbb{J} P L^{-1} - \mathbb{J}^T L \mathbb{J} Q L^{-1} N L^{-1}, LC + NB). \end{aligned}$$

Obviously, $LC + NB$ can traverse \mathbb{R}^{2n} with varying $N \in GL(2n, \mathbb{R})$ and $C \in \mathbb{R}^{2n}$. For the first component, we can take $N = L$ such that it becomes $\mathbb{J}^T L \mathbb{J} P L^{-1}$. Since the tangent space of an open submanifold can be identified with the tangent space of the whole manifold, plus the fact that the tangent space of a vector space can be identified with itself, we naturally conclude that $T_{(L, (Q, B))} \alpha$ is surjective and hence α is a submersion. Similarly, one check that β is a submersion.

Then, the orbit of the groupoid containing (Q, B) is given by

$$\begin{aligned} \alpha(\beta^{-1}(Q, B)) &= \alpha(\{(L, (Q, B)) | L \text{ satisfies 1.(i) and 1.(ii) in Definition 23}\}) \\ &= \left\{ (\mathbb{J}^T L \mathbb{J} Q L^{-1}, LB) | L \text{ satisfies 1.(i) and 1.(ii) in Definition 23} \right\} \\ &= \{(Q', B') | (Q', B') \sim_{sys} (Q, B)\} \end{aligned}$$

9.6 Proof of Proposition 30

f is well-defined. If $(\mathbf{d}_1, \mathbf{v}_1) \sim_{sys} (\mathbf{d}_2, \mathbf{v}_2)$, then there exists an invertible matrix L_0 such that

$$\begin{cases} L_0 \cdot g_1^{ctr}(\mathbf{d}_1) = g_1^{ctr}(\mathbf{d}_2) \cdot L_0 \\ L_0 \cdot (0, 0, \dots, 0, 1)^T = (0, 0, \dots, 0, 1)^T \\ g_2^{ctr}(\mathbf{d}_1, \mathbf{v}_1) = g_2^{ctr}(\mathbf{d}_2, \mathbf{v}_2) \cdot L_0 \end{cases}$$

Since we are restricting on canonical systems, we apply the representation theorem to deduce the existence of some invertible matrices L_i , $i = 1, 2$ such that

$$\begin{cases} L_i \cdot g_1^{ctr}(\mathbf{d}_i) = \mathbb{J} Q_i \cdot L_i \\ L_i \cdot (0, 0, \dots, 0, 1)^T = B_i \\ g_2^{ctr}(\mathbf{d}_i, \mathbf{v}_i) = B_i^T Q_i \cdot L_i \end{cases}$$

Now, check $L = L_2 L_0 L_1^{-1}$ is invertible and satisfies

$$\begin{cases} L \mathbb{J} Q_1 = \mathbb{J} Q_2 L \\ LB_1 = B_2 \\ B_1^T Q_1 = B_2^T Q_2 L. \end{cases}$$

Therefore, $(Q_1, B_1) \sim_{sys} (Q_2, B_2)$.

f is surjective. This is obvious, see the proof above.

f is injective. Given all the matrices are invertible, this can be shown by essentially reversing the proof of f being well-defined.

9.7 Proof of Proposition 31

We directly verify that

$$\begin{aligned}
 & \Gamma_{(\sigma, (\theta_1, \dots, \theta_n)^T) \circ (\bar{\sigma}, (\bar{\theta}_1, \dots, \bar{\theta}_n)^T)}(\mathbf{d}, \mathbf{v}) \\
 &= \Gamma_{(\sigma \bar{\sigma}, (\theta_1, \dots, \theta_n)^T + P_\sigma \cdot (\bar{\theta}_1, \dots, \bar{\theta}_n)^T)}(\mathbf{d}, \mathbf{v}) \\
 &= (P_\sigma \bar{\sigma} \cdot \mathbf{d}, \Gamma_{(\theta_1, \dots, \theta_n)^T} \circ \Gamma_{P_\sigma \cdot (\bar{\theta}_1, \dots, \bar{\theta}_n)^T} \left(\begin{bmatrix} P_\sigma \bar{\sigma} & 0 \\ 0 & P_\sigma \bar{\sigma} \end{bmatrix} \mathbf{v} \right)) \\
 &= (P_\sigma P_\sigma \cdot \mathbf{d}, \\
 & \quad \Gamma_{(\theta_1, \dots, \theta_n)^T} \circ \left[\begin{array}{cc|cc} \cos \bar{\theta}_{\sigma(1)} & 0 & -\sin \bar{\theta}_{\sigma(1)} & 0 \\ & \ddots & & \\ 0 & \cos \bar{\theta}_{\sigma(n)} & 0 & -\sin \bar{\theta}_{\sigma(n)} \\ \hline \sin \bar{\theta}_{\sigma(1)} & 0 & \cos \bar{\theta}_{\sigma(1)} & 0 \\ & \ddots & & \\ 0 & \sin \bar{\theta}_{\sigma(n)} & 0 & \cos \bar{\theta}_{\sigma(n)} \end{array} \right] \begin{bmatrix} P_\sigma & 0 \\ 0 & P_\sigma \end{bmatrix} \begin{bmatrix} P_\sigma & 0 \\ 0 & P_\sigma \end{bmatrix} \mathbf{v}) \\
 &= (P_\sigma P_\sigma \cdot \mathbf{d}, \Gamma_{(\theta_1, \dots, \theta_n)^T} \begin{bmatrix} P_\sigma & 0 \\ 0 & P_\sigma \end{bmatrix} \Gamma_{(\bar{\theta}_1, \dots, \bar{\theta}_n)^T} \begin{bmatrix} P_\sigma & 0 \\ 0 & P_\sigma \end{bmatrix} \mathbf{v}) \\
 &= \Gamma_{(\sigma, (\theta_1, \dots, \theta_n)^T)}(\Gamma_{(\bar{\sigma}, (\bar{\theta}_1, \dots, \bar{\theta}_n)^T)}(\mathbf{d}, \mathbf{v})).
 \end{aligned}$$

9.8 Proof of Proposition 32

Recall that $(\mathbf{d}_1, \mathbf{v}_1)$ and $(\mathbf{d}_2, \mathbf{v}_2)$ lie in the same $(S_n \rtimes_\phi \mathbb{T}^n)$ -orbit if and only if for some $\sigma \in S_n$ and $(\theta_1, \dots, \theta_n) \in \mathbb{T}^n$.

- (i) $d_{2,i} = d_{1,\sigma(i)}$, $i = 1, \dots, n$.
- (ii) $v_{2,i}^2 + v_{2,n+i}^2 = v_{1,\sigma(i)}^2 + v_{1,n+\sigma(i)}^2$.

Clearly, (i) above is equivalent to Proposition 18 (i). Moreover, Proposition 18 (ii) implies that for $k = 0, \dots, n-1$,

$$\begin{aligned}
 \mathbf{v}_1^T \begin{bmatrix} F_{1,k} & 0 \\ 0 & F_{1,k} \end{bmatrix} \mathbf{v}_1 &= (P^T \mathbf{v}_2)^T \begin{bmatrix} F_{1,k} & 0 \\ 0 & F_{1,k} \end{bmatrix} P^T \mathbf{v}_2 \\
 \iff \sum_{i=1}^n F_{1,k}^{(i)} \cdot (v_{1,i}^2 + v_{1,n+i}^2) & \\
 &= \sum_{i=1}^n F_{1,k}^{(i)} \cdot (v_{2,\sigma^{-1}(i)}^2 + v_{2,n+\sigma^{-1}(i)}^2)
 \end{aligned}$$

Now, let $\bar{R}_1 = (R_{1,1}, \dots, R_{1,n})^T$, where $R_{1,i} = v_{1,i}^2 + v_{1,n+i}^2$. Let $\bar{R}_2 = (R_{2,1}, \dots, R_{2,n})^T$, where $R_{2,i} = v_{2,\sigma^{-1}(i)}^2 + v_{2,n+\sigma^{-1}(i)}^2$. Identify the diagonal matrix $F_{1,k}$ as a row vector in \mathbb{R}^n . Then, the above is equivalent to saying that the inner product of $F_{1,k}$ with \bar{R}_1 and \bar{R}_2 are the same for all $k = 0, \dots, n-1$. Rewrite these inner products as matrix multiplication gives

$$\begin{bmatrix} F_{1,0} \\ F_{1,1} \\ \vdots \\ F_{1,n-1} \end{bmatrix} \cdot (\bar{R}_1 - \bar{R}_2) = 0.$$

The determinant of this matrix is $(\prod_{i=1}^n d_i) \cdot (\prod_{1 \leq j < k \leq n} d_j^2 - d_k^2)$. Since there are no repeated symplectic eigenvalues, we must have $\bar{R}_1 = \bar{R}_2$, namely $v_{1,i}^2 + v_{1,n+i}^2 = v_{2,\sigma^{-1}(i)}^2 + v_{2,n+\sigma^{-1}(i)}^2$ for all $i = 1, \dots, n$. Thus, (ii) holds by inverting the permutation σ . The converse is clearly true.

9.9 Proof of Proposition 33

f is well-defined. Let $(\mathbf{d}_1, \mathbf{v}_1)$ and $(\mathbf{d}_2, \mathbf{v}_2)$ be in the same orbit of the $(S_n \rtimes_{\phi} \mathbb{T}^n)$ -action. This means there exists $\sigma \in S_n$ and $\Theta \in \mathbb{T}^n$ such that $\Gamma_{\sigma}(\mathbf{d}_1) = \mathbf{d}_2$ and $\Gamma_{\Theta}(\Gamma_{\sigma}(\mathbf{v}_1)) = \mathbf{v}_2$. This immediately implies $(\mathbf{d}_1)_{\uparrow} = (\mathbf{d}_2)_{\uparrow}$, as well as $\mathcal{R}(\mathbf{v}_2) = \mathcal{R}(\Gamma_{\sigma}(\mathbf{v}_1))$. Moreover, let $\sigma_i \in S_n$ be the unique permutation such that $\Gamma_{\sigma_i}(\mathbf{d}_i) = (\mathbf{d}_i)_{\uparrow}$, $i = 1, 2$. Then we have,

$$\begin{aligned} \mathbf{d}_2 &= \Gamma_{\sigma_2^{-1}}((\mathbf{d}_2)_{\uparrow}) = \Gamma_{\sigma_2^{-1}}((\mathbf{d}_1)_{\uparrow}) \\ &= (\Gamma_{\sigma_2^{-1}} \circ \Gamma_{\sigma_1})(\mathbf{d}_1) \\ &= \Gamma_{\sigma_2^{-1}\sigma_1}(\mathbf{d}_1). \end{aligned}$$

Since all the entries of \mathbf{d} are distinct, we necessarily have $\sigma = \sigma_2^{-1}\sigma_1$. We want to show $\mathcal{R}(\Gamma_{\sigma_1}(\mathbf{v}_1)) = \mathcal{R}(\Gamma_{\sigma_2}(\mathbf{v}_2))$, but since \mathcal{R} and Γ_{σ} commutes for any $\sigma \in S_n$, this is equivalent to

$$\begin{aligned} \Gamma_{\sigma_1}(\mathcal{R}(\mathbf{v}_1)) &= \Gamma_{\sigma_2}(\mathcal{R}(\mathbf{v}_2)) \\ \iff \Gamma_{\sigma_1}(\mathcal{R}(\mathbf{v}_1)) &= \Gamma_{\sigma_2}(\mathcal{R}(\Gamma_{\sigma}(\mathbf{v}_1))) \\ \iff \Gamma_{\sigma_1}(\mathcal{R}(\mathbf{v}_1)) &= \Gamma_{\sigma_2}(\mathcal{R}(\Gamma_{\sigma_2^{-1}\sigma_1}(\mathbf{v}_1))) \\ \iff \Gamma_{\sigma_1}(\mathcal{R}(\mathbf{v}_1)) &= \mathcal{R}(\Gamma_{\sigma_1}(\mathbf{v}_1)), \end{aligned}$$

which is clearly true.

f is surjective. This is obvious.

f is injective. Now suppose $((\mathbf{d}_1)_{\uparrow}, \mathcal{R}(\Gamma_{\sigma_1}(\mathbf{v}_1))) = ((\mathbf{d}_2)_{\uparrow}, \mathcal{R}(\Gamma_{\sigma_2}(\mathbf{v}_2)))$. This immediately implies the existence of some $\sigma \in S_n$ such that $\Gamma_{\sigma}(\mathbf{d}_1) = \mathbf{d}_2$. On the other hand, since $\mathbf{d}_i = \Gamma_{\sigma_i^{-1}}(\mathbf{d}_i)_{\uparrow}$, $i = 1, 2$, we have $\sigma = \sigma_2^{-1}\sigma_1$ and hence $\mathbf{d}_2 = \Gamma_{\sigma_2^{-1}\sigma_1}(\mathbf{d}_1)$. On the other hand, $\mathcal{R}(\Gamma_{\sigma_1}(\mathbf{v}_1)) = \mathcal{R}(\Gamma_{\sigma_2}(\mathbf{v}_2))$ implies $\mathcal{R}(\Gamma_{\sigma_2^{-1}\sigma_1}(\mathbf{v}_1)) = \mathcal{R}(\mathbf{v}_2)$, which further implies the existence of some $\Theta \in \mathbb{T}^n$ such that $\mathbf{v}_2 = \Gamma_{\Theta}(\Gamma_{\sigma_2^{-1}\sigma_1}(\mathbf{v}_1))$. This concludes that $(\mathbf{d}_1, \mathbf{v}_1)$ and $(\mathbf{d}_2, \mathbf{v}_2)$ lie in the same orbit.

9.10 Proof of Theorem 34

Proof of part (i). Say we are given a latent system

$$\begin{cases} \dot{\mathbf{z}} = \mathbb{J}_n Q \mathbf{z} + B u \\ y = B^T Q \mathbf{z}, \end{cases} \quad (31)$$

where $\mathbb{J}_n = \begin{bmatrix} 0 & \mathbb{I}_n \\ -\mathbb{I}_n & 0 \end{bmatrix}$, $B \in \mathbb{R}^{2n}$ and Q a $2n$ by $2n$ symmetric, positive-definite matrix. Consider the matrix

$$\begin{bmatrix} \mathbb{J}_n & 0 \\ 0 & \mathbb{J}_{m-n} \end{bmatrix} = \begin{bmatrix} 0 & \mathbb{I}_n & 0 & 0 \\ -\mathbb{I}_n & 0 & 0 & 0 \\ 0 & 0 & 0 & \mathbb{I}_{m-n} \\ 0 & 0 & -\mathbb{I}_{m-n} & 0 \end{bmatrix}.$$

There exists a conjugate transform by an orthogonal matrix that turns this matrix into \mathbb{J}_m , since only elementary row(column) permutation matrices are involved, and these elementary matrices are themselves orthogonal. That is, there exists $OO^T = O^T O = \mathbb{I}_{2m}$ such that $O \begin{bmatrix} \mathbb{J}_n & 0 \\ 0 & \mathbb{J}_{m-n} \end{bmatrix} O^T = \mathbb{J}_m$. Now, consider the following linear port-Hamiltonian system in normal form

$$\begin{cases} \dot{\tilde{\mathbf{z}}} = \left(O \begin{bmatrix} \mathbb{J}_n & 0 \\ 0 & \mathbb{J}_{m-n} \end{bmatrix} O^T \right) \left(O \begin{bmatrix} Q & 0 \\ 0 & \mathbb{I}_{2m-2n} \end{bmatrix} O^T \right) \tilde{\mathbf{z}} + O \begin{bmatrix} B \\ 0 \end{bmatrix} u \\ = \mathbb{J}_m \left(O \begin{bmatrix} Q & 0 \\ 0 & \mathbb{I}_{2m-2n} \end{bmatrix} O^T \right) \tilde{\mathbf{z}} + O \begin{bmatrix} B \\ 0 \end{bmatrix} u \\ y = \left(O \begin{bmatrix} B \\ 0 \end{bmatrix} \right)^T \left(O \begin{bmatrix} Q & 0 \\ 0 & \mathbb{I}_{2m-2n} \end{bmatrix} O^T \right) \tilde{\mathbf{z}} \\ = [B^T Q \quad 0] O^T \tilde{\mathbf{z}} \end{cases}$$

with the change of variable $\mathbf{z} = O^T \tilde{\mathbf{z}}$, which is equivalent to

$$\begin{cases} \dot{\mathbf{z}} = \begin{bmatrix} \mathbb{J}_n Q & 0 \\ 0 & \mathbb{J}_{m-n} \end{bmatrix} \mathbf{z} + \begin{bmatrix} B \\ 0 \end{bmatrix} u \\ y = [B^T Q \quad 0] \mathbf{z}, \end{cases}$$

which, restricted to the upper subspace, coincides with (31). Moreover, the matrix $O \begin{bmatrix} Q & 0 \\ 0 & \mathbb{I}_{2m-2n} \end{bmatrix} O^T$ is again symmetric positive-definite by construction.

Proof of part (ii). According to the system morphism conditions, we just need to check

$$\begin{cases} L\mathbb{J}_n Q = \mathbb{J}_m O \begin{bmatrix} Q & 0 \\ 0 & \mathbb{I}_{2m-2n} \end{bmatrix} O^T L \\ LB = O \begin{bmatrix} B \\ 0 \end{bmatrix} \\ B^T Q = [B^T Q \quad 0] O^T L. \end{cases}$$

The first condition is

$$\begin{aligned} L\mathbb{J}_n Q &= \mathbb{J}_m O \begin{bmatrix} Q & 0 \\ 0 & \mathbb{I}_{2m-2n} \end{bmatrix} \begin{bmatrix} \mathbb{I}_{2n} \\ 0 \end{bmatrix} \\ &\iff O^T L\mathbb{J}_n Q = O^T \mathbb{J}_m O \begin{bmatrix} Q & 0 \\ 0 & \mathbb{I}_{2m-2n} \end{bmatrix} \begin{bmatrix} \mathbb{I}_{2n} \\ 0 \end{bmatrix} \\ &\iff \begin{bmatrix} I_{2n} \\ 0 \end{bmatrix} \mathbb{J}_n Q = \begin{bmatrix} \mathbb{J}_n & 0 \\ 0 & \mathbb{J}_{m-n} \end{bmatrix} \begin{bmatrix} Q & 0 \\ 0 & \mathbb{I}_{2m-2n} \end{bmatrix} \begin{bmatrix} \mathbb{I}_{2n} \\ 0 \end{bmatrix} \\ &\iff \begin{bmatrix} \mathbb{I}_{2n} \\ 0 \end{bmatrix} \mathbb{J}_n Q = \begin{bmatrix} \mathbb{J}_n Q \\ 0 \end{bmatrix}. \end{aligned}$$

The second and third conditions are clear with $L = O \begin{bmatrix} \mathbb{I}_{2n} \\ 0 \end{bmatrix}$

9.11 Proof of Proposition 35

f is well-defined. Given $(Q_1, B_1) \sim_{sys} (Q_2, B_2)$, there exists an invertible $L \in \mathbb{R}^{2n}$ such that (14) is satisfied. Let $L' = O \begin{bmatrix} L & 0 \\ 0 & \mathbb{I}_{2m-2n} \end{bmatrix} O^T$. Check that L' satisfies the conditions (14) together with (Q'_1, B'_1) and (Q'_2, B'_2) . Therefore, $(Q'_1, B'_1) \sim_{sys} (Q'_2, B'_2)$.

f is surjective. This is clear from definition of (Q', B') .

f is injective. Given $(Q'_1, B'_1) \sim_{sys} (Q'_2, B'_2)$, it means there exists an invertible $L' \in \mathbb{R}^{2m}$ such that L' satisfies the conditions in (14) together with (Q'_1, B'_1) and (Q'_2, B'_2) . Write the matrix $O^T L' O$ in the form $\begin{bmatrix} L_1 & L_2 \\ L_3 & L_4 \end{bmatrix}$, where $L_1 \in \mathbb{R}^{2n}$. Then check L_1 satisfies the conditions (14) together with (Q_1, B_1) and (Q_2, B_2) . Therefore, $(Q_1, B_1) \sim_{sys} (Q_2, B_2)$.

9.12 Proof of Proposition 36

Clearly, Q' is also symmetric and positive-definite. Thus, again by Williamson's theorem, $Q' = (S')^T \begin{bmatrix} D' & 0 \\ 0 & D' \end{bmatrix} S'$.

As before, we have

$$\begin{aligned}
 & (\lambda^2 + d_1'^2) \cdots (\lambda^2 + d_m'^2) \\
 &= \det \left(\lambda \mathbb{I}_{2m} - \begin{bmatrix} 0 & D' \\ -D' & 0 \end{bmatrix} \right) \\
 &= \det \left(\lambda \mathbb{I}_{2m} - (S')^{-1} \begin{bmatrix} 0 & D' \\ -D' & 0 \end{bmatrix} S' \right) \\
 &= \det \left(\lambda \mathbb{I}_{2m} - \mathbb{J}_m (S')^T \begin{bmatrix} D' & 0 \\ 0 & D' \end{bmatrix} S' \right) \\
 &= \det(\lambda \mathbb{I}_{2m} - \mathbb{J}_m Q') \\
 &= \det \left(\lambda \mathbb{I}_{2m} - \mathbb{J}_m O \begin{bmatrix} Q & 0 \\ 0 & \mathbb{I}_{2m-2n} \end{bmatrix} O^T \right) \\
 &= \det \left(\lambda \mathbb{J}_m + \mathbb{J}_m O \begin{bmatrix} Q & 0 \\ 0 & \mathbb{I}_{2m-2n} \end{bmatrix} O^T \mathbb{J}_m^T \right) \\
 &= \det \left(\lambda \mathbb{J}_m + \mathbb{J}_m O \begin{bmatrix} Q & 0 \\ 0 & \mathbb{I}_{2m-2n} \end{bmatrix} (\mathbb{J}_m O)^{-1} \right) \\
 &= \det \left(\lambda (\mathbb{J}_m O)^{-1} \mathbb{J}_m (\mathbb{J}_m O) + \begin{bmatrix} Q & 0 \\ 0 & \mathbb{I}_{2m-2n} \end{bmatrix} \right) \\
 &= \det \left(\lambda O^T \mathbb{J}_m O + \begin{bmatrix} Q & 0 \\ 0 & \mathbb{I}_{2m-2n} \end{bmatrix} \right) \\
 &= \det \left(\begin{bmatrix} \lambda \mathbb{J}_n & 0 \\ 0 & \lambda \mathbb{J}_{m-n} \end{bmatrix} + \begin{bmatrix} Q & 0 \\ 0 & \mathbb{I}_{2m-2n} \end{bmatrix} \right) \\
 &= \det(\lambda \mathbb{J}_{m-n} + \mathbb{I}_{2m-2n}) \cdot \det(\lambda \mathbb{J}_n + Q) \\
 &= (\lambda^2 + 1)^{m-n} \cdot \det(\lambda \mathbb{I}_{2n} - \mathbb{J}_n Q) \\
 &= (\lambda^2 + 1)^{m-n} (\lambda^2 + d_1'^2) \cdots (\lambda^2 + d_n'^2)
 \end{aligned}$$

If we fixed the order of symplectic eigenvalues \mathbf{d}' according to $\mathbf{d}' = (d_1, \dots, d_n, 1, \dots, 1)$, then

$$\begin{aligned}
 Q' &= O \begin{bmatrix} Q & 0 \\ 0 & \mathbb{I}_{2m-2n} \end{bmatrix} O^T \\
 &= O \begin{bmatrix} S^T \begin{bmatrix} D & 0 \\ 0 & D \end{bmatrix} S & 0 \\ & \mathbb{I}_{2m-2n} \end{bmatrix} O^T \\
 &= O \begin{bmatrix} S^T & 0 \\ 0 & \mathbb{J}_{m-n} \end{bmatrix} \left[\begin{array}{c|c} \begin{bmatrix} D & 0 \\ 0 & D \end{bmatrix} & 0 \\ \hline 0 & \begin{bmatrix} \mathbb{I}_{m-n} & 0 \\ 0 & \mathbb{I}_{m-n} \end{bmatrix} \end{array} \right] \begin{bmatrix} S & 0 \\ 0 & \mathbb{J}_{m-n} \end{bmatrix} O^T \\
 &= O \begin{bmatrix} S^T & 0 \\ 0 & \mathbb{J}_{m-n}^T \end{bmatrix} O^T \left[\begin{array}{c|c} \begin{bmatrix} D & 0 \\ 0 & \mathbb{I}_{m-n} \end{bmatrix} & 0 \\ \hline 0 & \begin{bmatrix} D & 0 \\ 0 & \mathbb{I}_{m-n} \end{bmatrix} \end{array} \right] O \begin{bmatrix} S & 0 \\ 0 & \mathbb{J}_{m-n} \end{bmatrix} O^T
 \end{aligned}$$

Now, we check the matrix $O \begin{bmatrix} S & 0 \\ 0 & \mathbb{J}_{m-n} \end{bmatrix} O^T$ is symplectic, that is,

$$\begin{aligned} & \left(O \begin{bmatrix} S & 0 \\ 0 & \mathbb{J}_{m-n} \end{bmatrix} O^T \right)^T \mathbb{J}_m \left(O \begin{bmatrix} S & 0 \\ 0 & \mathbb{J}_{m-n} \end{bmatrix} O^T \right) \\ &= O \begin{bmatrix} S^T & 0 \\ 0 & \mathbb{J}_{m-n}^T \end{bmatrix} (O^T \mathbb{J}_m O) \begin{bmatrix} S & 0 \\ 0 & \mathbb{J}_{m-n} \end{bmatrix} O^T \\ &= O \begin{bmatrix} S^T & 0 \\ 0 & \mathbb{J}_{m-n}^T \end{bmatrix} \begin{bmatrix} \mathbb{J}_n & 0 \\ 0 & \mathbb{J}_{m-n} \end{bmatrix} \begin{bmatrix} S & 0 \\ 0 & \mathbb{J}_{m-n} \end{bmatrix} O^T \\ &= O \begin{bmatrix} \mathbb{J}_n & 0 \\ 0 & \mathbb{J}_{m-n} \end{bmatrix} O^T = \mathbb{J}_m. \end{aligned}$$

Therefore, $O \begin{bmatrix} S & 0 \\ 0 & \mathbb{J}_{m-n} \end{bmatrix} O^T$ is a symplectic matrix diagonalizing Q' in Williamson's theorem. Then, we deduce

$$\mathbf{v}' = S'B' = O \begin{bmatrix} S & 0 \\ 0 & \mathbb{J}_{m-n} \end{bmatrix} O^T O \begin{bmatrix} B \\ 0 \end{bmatrix} = O \begin{bmatrix} SB \\ 0 \end{bmatrix} = O \begin{bmatrix} \mathbf{v} \\ 0 \end{bmatrix}.$$

9.13 Proof of Proposition 37

Similar to the proof of Theorem 22, simply replace Q with $O \begin{bmatrix} Q & 0 \\ 0 & \mathbb{I}_{2m-2n} \end{bmatrix} O^T$, B with $O \begin{bmatrix} B \\ 0 \end{bmatrix}$, S with $O \begin{bmatrix} S & 0 \\ 0 & \mathbb{J}_{m-n} \end{bmatrix} O^T$, D with $\begin{bmatrix} D & 0 \\ 0 & \mathbb{I}_{m-n} \end{bmatrix}$, $\mathbf{v} = \begin{bmatrix} \mathbf{v}_{upper} \\ \mathbf{v}_{lower} \end{bmatrix}$ with $\bar{\mathbf{v}} = \begin{bmatrix} \mathbf{v}_{upper}^T & 0_{m-n} & \mathbf{v}_{lower}^T & 0_{m-n} \end{bmatrix}^T$.

9.14 A note on the design of discrete integrators on the transformed space

Even though we used just a simple Euler integration scheme in the numerical illustration, structure-preserving integration algorithms could have been used. In particular, we could have used an implicit midpoint rule which is symplectic (see Marsden and West (2001)), that is, it preserves the symplectic form $d\mathbf{q} \wedge d\mathbf{p}$. Recall that if $L_{Lag}(\mathbf{q}, \dot{\mathbf{q}})$ is the Lagrangian function of the system of interest, then the midpoint integrator is obtained by using the discrete Lagrangian

$$L_d^\alpha(\mathbf{q}_0, \mathbf{q}_1, h) = h L_{Lag}((1-\alpha)\mathbf{q}_0 + \alpha\mathbf{q}_1, \frac{\mathbf{q}_1 - \mathbf{q}_0}{h}),$$

with $\alpha = \frac{1}{2}$ to approximate the exact discrete Lagrangian

$$L_d^E(\mathbf{q}_0, \mathbf{q}_1, h) = \int_0^h L_{Lag}(\mathbf{q}_{0,1}(t), \dot{\mathbf{q}}_{0,1}(t)) dt.$$

Explicitly, the midpoint integrator for a linear autonomous Hamiltonian system is

$$\mathbf{z}_{n+1} - \mathbf{z}_n = h \cdot \mathbb{J}Q \left(\frac{\mathbf{z}_{n+1} + \mathbf{z}_n}{2} \right),$$

which in terms of the controllable Hamiltonian representation reads

$$L(\mathbf{s}_{n+1} - \mathbf{s}_n) = \frac{h}{2} \mathbb{J}QL(\mathbf{s}_{n+1} + \mathbf{s}_n) = \frac{h}{2} L \cdot g_1^{ctr}(\mathbf{d})(\mathbf{s}_{n+1} + \mathbf{s}_n), \quad (32)$$

where the second equality holds by the construction of L in the proof of Theorem 7 part (i).

Thus, for the symplectic structure to be preserved in the original space, we can merely integrate by requiring $\mathbf{s}_{n+1} - \mathbf{s}_n = \frac{h}{2} g_1^{ctr}(\mathbf{d})(\mathbf{s}_{n+1} + \mathbf{s}_n)$, where $g_1^{ctr}(\mathbf{d})$ as we have seen, takes the form

$$\begin{bmatrix} 0 & 1 & 0 & \dots & 0 \\ 0 & 0 & 1 & \dots & 0 \\ \vdots & \vdots & \ddots & & \vdots \\ 0 & 0 & 0 & \dots & 1 \\ -a_0 & -a_1 & -a_2 & \dots & -a_{2m-1} \end{bmatrix}_{2m \times 2m}.$$

Therefore, the integrator is given by

$$\mathbf{s}_{n+1} = (\mathbb{I}_{2n} - \frac{h}{2}g_1^{ctr}(\mathbf{d}))^{-1}(\mathbb{I}_{2n} + \frac{h}{2}g_1^{ctr}(\mathbf{d})) \cdot \mathbf{s}_n,$$

where the matrix inverse is well-defined for sufficiently small time step h . Indeed, the integrator can be defined on the quotient space of L , since by (32), we may as well choose \mathbf{s}_{n+1} such that

$$\mathbf{s}_{n+1} - \mathbf{s}_n = \frac{h}{2}g_1^{ctr}(\mathbf{d})(\mathbf{s}_{n+1} + \mathbf{s}_n) + \mathbf{s}_{ker}$$

for an arbitrary $\mathbf{s}_{ker} \in \ker(L)$.

By a similar argument, the midpoint rule in terms of observable Hamiltonian representation reads

$$\mathbf{s}_{n+1} - \mathbf{s}_n = L(\mathbf{z}_{n+1} - \mathbf{z}_n) = \frac{h}{2}L\mathbb{J}Q(\mathbf{z}_{n+1} + \mathbf{z}_n) = \frac{h}{2}g_1^{obs}(\mathbf{d})(\mathbf{s}_{n+1} + \mathbf{s}_n), \quad (33)$$

where the last equality holds by construction of L from Theorem 7 Part (ii).

Therefore, the integrator is

$$\mathbf{s}_{n+1} = (\mathbb{I}_{2n} - \frac{h}{2}g_1^{obs}(\mathbf{d}))^{-1}(\mathbb{I}_{2n} + \frac{h}{2}g_1^{obs}(\mathbf{d})) \cdot \mathbf{s}_n.$$

In the case of port-Hamiltonian system, if the system is driven by some fiber-preserving external force f_H , that is, some input as in our case, then the discrete Lagrange-d'Alembert Principle can be used to construct variational integrators so that all the correspondence relationships and error analysis of standard variational integrators still hold (see Marsden and West (2001)). For example, the midpoint rule applied to the controllable Hamiltonian representation becomes

$$\begin{aligned} \mathbf{z}_{n+1} - \mathbf{z}_n &= h \cdot \mathbb{J}Q\left(\frac{\mathbf{z}_{n+1} + \mathbf{z}_n}{2}\right) + \left[\begin{array}{c} 0 \\ f_H\left(\frac{\mathbf{z}_n + \mathbf{z}_{n+1}}{2}\right) \end{array} \right] \\ \Rightarrow L(\mathbf{s}_{n+1} - \mathbf{s}_n) &= \frac{h}{2}L \cdot g_1^{ctr}(\mathbf{d})(\mathbf{s}_{n+1} + \mathbf{s}_n) + \left[\begin{array}{c} 0 \\ f_H\left(\frac{L(\mathbf{s}_{n+1} + \mathbf{s}_n)}{2}\right) \end{array} \right]. \end{aligned}$$

Note that this structure-preserving integrator is not explicit in general.