

Designing Poisson Integrators Through Machine Learning

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Abstract: This paper presents a general method to construct Poisson integrators, i.e., integrators that preserve the underlying Poisson geometry. We assume the Poisson manifold is integrable, meaning there is a known local symplectic groupoid for which the Poisson manifold serves as the set of units. Our constructions build upon the correspondence between Poisson diffeomorphisms and Lagrangian bisections, which allows us to reformulate the design of Poisson integrators as solutions to a certain PDE (Hamilton-Jacobi). The main novelty of this work is to understand the Hamilton-Jacobi PDE as an optimization problem, whose solution can be easily approximated using machine learning related techniques. This research direction aligns with the current trend in the PDE and machine learning communities, as initiated by Physics-Informed Neural Networks, advocating for designs that combine both physical modeling (the Hamilton-Jacobi PDE) and data.

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1. INTRODUCTION

Due to their persistent presence in science and engineering, Hamiltonian systems have been intensively studied for centuries. Special attention has been given to all the structures able to describe Hamiltonian systems, namely symplectic and Poisson geometry. It is broadly recognized that geometry plays a pivotal role in the dynamical behavior of the aforementioned systems. Nonetheless, since Hamiltonian systems can describe a wide array of systems in nature, they usually show a high level of complexity that hinders their complete understanding. This fact has led several communities to the design of algorithms that seek to produce accurate simulations of Hamiltonian systems as an enabling tool for the analysis of their dynamical behavior and properties.

To tackle this challenge, we follow here the geometric approach. The main observation is that numerical schemes sharing the same geometric properties as the original system usually enjoy better accuracy and more faithful qualitative description of the system compared to non-geometric algorithms. This philosophy has been broadly exploited when the underlying geometry is symplectic, see for instance Sanz-Serna and Calvo (1994); Hairer et al. (2010).

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Nonetheless, when the Hamiltonian system is described using the more general Poisson setting, the situation is more subtle. See Cosserat (2023) and the references therein. This is mainly due to the fact that Poisson geometry is, in a way, singular and irregular when compared to symplectic geometry. Moreover, to the best of the authors’ knowledge, there are no general methods for obtaining Poisson integrators¹, although some recent attempts include those in Cosserat (2023). In cases where the Poisson structure is linear and integrable, the references Ge (1991); Zhong and Marsden (1988); McLachlan et al. (2014); Ferraro et al. (2017) provide methods to generate them. These methods rely on the exploitation of the properties of the symplectic groupoid that integrates the Poisson manifold, or other symplectic realizations. Additionally, the same geometric structure was recently used to develop learning methods that conserve the underlying Poisson structure, as shown in Vaquero et al. (2023). Also in Jin et al. (2023) the authors design Poisson neural networks to learn constant rank Poisson Hamiltonian systems based on the Darboux-Lie theorem, finding first a coordinate change of coordinates that locally transforms the Poisson manifold as the product of a symplectic manifold (with the canonical symplectic structure) and a manifold with the null Poisson bracket (see Weinstein (1983) for a more general result).

In this paper, following the research direction initiated in Vaquero et al. (2023), we propose a step further in the construction of Poisson integrators, combining differ-

¹ By integrator we mean a numerical scheme designed to approximate the dynamics of a system. In this case, of a Hamiltonian vector field on a Poisson manifold.

ential geometry with machine learning techniques. More precisely, we present the following contributions. (1) We introduce a general geometric setting for describing Poisson geometric integrators when the problem evolves on an integrable Poisson manifold. (2) We provide a method for approximating the Hamilton-Jacobi equation using machine learning-inspired techniques. (3) We illustrate our findings using the rigid body as an example.

2. A QUICK REVIEW OF GEOMETRY

2.1 Basic Notions on Symplectic and Poisson Geometry

In this section we introduce the main geometric structures used along the paper. We refer the reader to Crainic et al. (2021) for additional details.

Definition 1. (Symplectic Manifold). A symplectic manifold is a pair (M, Ω) , where M is a manifold and Ω a non-degenerate closed two-form.

Example 1. The cotangent bundle of a manifold, say T^*Q , is endowed with the canonical symplectic form $\omega_Q = -d\theta_Q$, where θ_Q is the Liouville one form Abraham and Marsden (1987). In local coordinates (x^i, p_i) , $\omega_Q = dx^i \wedge dp_i$.

Darboux's Theorem guarantees that given a symplectic manifold (M, Ω) there are local coordinates (x^i, y_i) in which the coordinate representation of Ω is $\Omega = dx^i \wedge dy_i$.

Definition 2. (Lagrangian Submanifold). A Lagrangian submanifold L of a symplectic manifold (M, Ω) is a submanifold of dimension half the dimension of M and such that the restriction of Ω to L is zero.

Example 2. Given a manifold Q , $\dim Q = n$, and its cotangent bundle T^*Q , any differentiable function $S : Q \rightarrow \mathbb{R}$ produces a Lagrangian submanifold in T^*Q by just taking $\text{graph}(dS) \subset T^*Q$, this is called a horizontal Lagrangian submanifold. In canonical coordinates, (x^i, p_i) ,

this submanifold is just given by $(x^i, p_i = \frac{\partial S}{\partial x^i}(x))$, where $x \in Q$. The main difficulty is to describe Lagrangian submanifolds which are not horizontal (i.e. the image of dS). It means that one can allow S to be dependent not only on the variables (x^i) , but on mixed set of n -coordinates like (x^a, p_{n-a}) , $1 \leq a \leq m < n$. Of course, this statement holds only locally (see Arnold (1966)).

Definition 3. (Poisson Manifold). A Poisson manifold is a manifold P endowed with a bi-vector Π satisfying $[\Pi, \Pi] = 0$, where $[\cdot, \cdot]$ is the Schouten bracket, see (Crainic et al., 2021, Definition 2.3).

Definition 4. (Casimir function). A function $C : P \rightarrow \mathbb{R}$ is called a Casimir function of a Poisson manifold (P, Π) if it verifies that $\Pi(dC, dg) = 0$ for all function $g : P \rightarrow \mathbb{R}$.

Once we have set the basic objects of our constructions, we introduce the mappings conserving these geometric structures.

Definition 5. (Poisson Mappings). Let (P_1, Π_1) and (P_2, Π_2) be two Poisson manifolds. Then, a mapping $f : P_1 \rightarrow P_2$ is Poisson (resp. anti-Poisson) if $f_*\Pi_1 = \Pi_2$ (resp. $f_*\Pi_1 = -\Pi_2$). See (Crainic et al., 2021, Definition 2.13) for the definition of the pushforward $f_*(\cdot)$.

One of the main uses of Poisson manifolds is the description of Hamiltonian vector fields.

Definition 6. (Hamiltonian Vector Field). Given a Poisson manifold (P, Π) and a function (Hamiltonian) $H : P \rightarrow \mathbb{R}$, we define the associated Hamiltonian vector field, X_H , as the unique vector field satisfying $X_H(g) = \Pi(dH, dg)$ for all functions $g : P \rightarrow \mathbb{R}$, see Crainic et al. (2021).

The flow of the Hamiltonian vector field X_H is denoted by φ_t^H . A basic result in Poisson geometry states that φ_t^H is a Poisson diffeomorphism for all fixed t .

2.2 Poisson manifolds, Symplectic Realizations, and Symplectic Groupoids

Poisson manifolds are singular and difficult to deal with. A common approach in mathematics for analyzing complex structures is to seek "desingularizations". In other words, we aim to obtain a "nicer" geometric structure (symplectic in our case) on a manifold, endowed with a projection over the Poisson manifold under a Poisson mapping. This structure is called a *symplectic realization*, see (Crainic et al., 2021, Ch. 6). The main advantage of this approach is that it allows us to use the better understood and manageable techniques from symplectic geometry. Among them, Lagrangian submanifolds and their generating functions play an instrumental role here.

The motivation for introducing *symplectic groupoids* is twofold: (1) The study of symplectic realizations naturally leads to symplectic groupoids, as described in Coste et al. (1987); Crainic et al. (2021). Symplectic groupoids constitute symplectic realizations when the set of units is a Poisson manifold. Moreover, the structural mappings *sou* and *tar* (described below) become Poisson and anti-Poisson mappings. Remarkably, *sou* and *tar* exhibit a dual pair structure, as detailed in (Crainic et al., 2021, Ch 14) and (Coste et al., 1987, Section III). (2) Lagrangian submanifolds in symplectic groupoids induce Poisson diffeomorphisms in the set of units (see Theorem 9 below).

Definition 7. (Groupoid). A *groupoid* (G) consists of the following components:

- (1) Two Sets:
 - A set of objects (or units), denoted (G_0) .
 - A set of arrows (or morphisms), denoted (G_1) .
- (2) Source and Target Maps:
 - A source map $\text{sou} : G_1 \rightarrow G_0$ assigning to each arrow an object called its source.
 - A target map $\text{tar} : G_1 \rightarrow G_0$ assigning to each arrow an object called its target.
- (3) Composition Law: A partially defined composition (or multiplication) operation $m : G_1 \times_{G_0} G_1 \rightarrow G_1$, where $G_1 \times_{G_0} G_1$ is the set of all pairs of arrows (g, h) such that the target of h is the source of g (i.e., $\text{tar}(h) = \text{sou}(g)$). The result of the composition $m(g, h)$ is an arrow from the source of h to the target of g .
- (4) Associativity: The composition of arrows is associative where defined. That is, for any three arrows f, g, h in G_1 , if $f \cdot (g \cdot h)$ and $(f \cdot g) \cdot h$ are defined, then $f \cdot (g \cdot h) = (f \cdot g) \cdot h$.
- (5) Identity Elements: For each object x in G_0 , there exists an identity arrow e_x in G_1 such that $\text{sou}(e_x) = x$, $\text{tar}(e_x) = x$, and for any arrow g with $\text{sou}(g) = x$ or $\text{tar}(g) = x$, the compositions $e_x \cdot g$ and $g \cdot e_x$ are defined and equal to g .

- (6) Inverses: For each arrow g in G_1 , there exists an inverse arrow g^{-1} in G_1 such that $sou(g^{-1}) = tar(g)$, $tar(g^{-1}) = sou(g)$, and the compositions $g \cdot g^{-1}$ and $g^{-1} \cdot g$ are defined and equal to the identity arrows of $tar(g)$ and $sou(g)$, respectively.

Definition 8. (Symplectic Groupoid). A symplectic groupoid is a groupoid G equipped with a symplectic structure (a non-degenerate, closed 2-form) on its space of arrows G_1 , such that the graph of the multiplication map $m : G_1 \times_{G_0} G_1 \rightarrow G_1$ is a Lagrangian submanifold of $G_1 \times G_1 \times \overline{G_1}$ (here $\overline{G_1}$ denotes G_1 with minus the given symplectic structure).

When there is no room for confusion, we identify the set of arrows G_1 and the groupoid itself, G . Although there are known geometric obstructions to obtaining global symplectic groupoids whose set of units is a given Poisson manifold, it is possible to obtain a local symplectic groupoid, as discussed in Cabrera (2022). We would like to emphasize that local existence is sufficient for our constructions, as they are inherently local in nature.

Example 3. Let \mathfrak{h} a Lie algebra with Lie bracket $[\cdot, \cdot]$ and H a Lie group integrating it. Consider the Poisson manifold $(G_0 = \mathfrak{h}^*, \Pi_{LP})$ where Π_{LP} is the induced Lie-Poisson structure.

$$\Pi_{LP}(dg_1, dg_2)(\mu) = -\mu([dg_1(\mu), dg_2(\mu)])$$

where $g_1, g_2 : \mathfrak{h}^* \rightarrow \mathbb{R}$ and $\mu \in \mathfrak{h}^*$. In this particular case, we can take G_1 as T^*H where the source and target maps are given by

$$\begin{aligned} sou : T^*H &\longrightarrow \mathfrak{h}^* \\ (\mu_h) &\longmapsto sou(\mu_h) = J_L(\mu_h), \\ tar : T^*H &\longrightarrow \mathfrak{h}^* \\ (\mu_h) &\longmapsto tau(\mu_h) = J_R(\mu_h). \end{aligned} \tag{1}$$

where

$\langle J_L(\mu_h), \xi \rangle = \langle \mu_h, T_e \mathcal{R}_h(\xi) \rangle$, $\langle J_R(\mu_h), \xi \rangle = \langle \mu_h, T_e \mathcal{L}_h(\xi) \rangle$ for all $\xi \in \mathfrak{h}$. Here, \mathcal{R}_h and \mathcal{L}_h denote the right and left translations on the Lie group H , respectively. See more details and examples in Marle (2005); Ferraro et al. (2017).

3. LAGRANGIAN BISECTIONS AND POISSON DIFFEOMORPHISMS: THE HAMILTON-JACOBI EQUATION

Let $(P \equiv G_0, \Pi)$ be a given Poisson manifold and assume there exists a symplectic groupoid, G , having G_0 as its set of units. This assumption is always valid locally, so there is no loss of generality. Let $H : G_0 \rightarrow \mathbb{R}$ be a Hamiltonian. Our goal is to design methods to accurately approximate φ_t^H . Towards this end, the stepping stone of our constructions is the following observation.

Key Observation: Poisson diffeomorphisms in G_0 , like φ_t^H , can be described through Lagrangian submanifolds in the symplectic groupoid G .

In this context, the next result is at the core of our construction of Poisson integrators.

Theorem 9. (Coste et al. (1987)). Let G be a symplectic groupoid. Let L be a Lagrangian submanifold of G such that $sou|_L : L \rightarrow G_0$ is a (local) diffeomorphism (a Lagrangian bisection). Then

- (1) $tar|_L : L \rightarrow G_0$ is a (local) diffeomorphism as well.
- (2) The mapping $\hat{L} = sou \circ tar|_L^{-1} : G_0 \rightarrow G_0$ is a (local) Poisson diffeomorphism.

Motivated by this result, a natural question is how to characterize and find the Lagrangian submanifold L , inducing the transformation φ_t^H . The answer leads directly to a geometric version of the Hamilton-Jacobi equation, as discussed in Ferraro et al. (2017). Due to space constraints, we provide here only a local description of the Hamilton-Jacobi equation. Consider a symplectic groupoid (G, Ω) with Darboux coordinates, (x^i, p_i) such that Ω reads as $dx^i \wedge dp_i$. We examine the extended space $\mathbb{R}^2 \times G$ with coordinates (t, p_t, x^i, p_i) , where we think of p_t as the dual variable to t . In this context, we consider the 2-form with local expression $dt \wedge dp_t + dx^i \wedge dp_i$, which turns $\mathbb{R}^2 \times G$ into a symplectic manifold. Below, we define a generalized solution of the Hamilton-Jacobi equation.

Definition 10. A Lagrangian submanifold L in $\mathbb{R}^2 \times G$ is a generalized solution to the Hamilton-Jacobi equation if

$$(p_t + H \circ sou)|_L = \text{constant}. \tag{Gen. HJ}$$

When a generating function, say S , is used to describe the Lagrangian submanifold L , then equation (Gen. HJ) takes the usual PDE form. For simplicity in this paper, we only consider the case where the generating function depends on (t, p_i) . This approach is applicable to the Lie-Poisson case treated below. Then, the Hamilton-Jacobi equation reads as follows

$$\frac{\partial S}{\partial t}(t, p_i) + H(sou(\frac{\partial S}{\partial p}(t, p_i), p_i)) = \text{constant}. \tag{2}$$

Proposition 11. (Ferraro et al. (2017)). The Lagrangian submanifold satisfying the Hamilton-Jacobi equation induces the Hamiltonian flow, φ_t^H , up to an initial condition. That is, we can recover $\varphi_t^H \circ f$ where f is a Poisson diffeomorphism. If $S(0, p_i)$ induces the identity on P , then we recover exactly φ_t^H .

3.1 Approximating the Hamilton-Jacobi Equation

Since obtaining an analytical solution to the Hamilton-Jacobi equation is challenging, approximation methods must be considered. A classical approach involves obtaining a Taylor expansion of the generation function S in the t -variable and deriving a recurrence relationship that enables the determination of a solution to a desired arbitrary high order (see Ferraro et al. (2017)). The main contribution of this paper is to present an alternative strategy based on recent developments and tools in machine learning, which involves viewing the PDE as an optimization problem. To do this, we consider a neural network with weights W parametrizing candidate functions, $S(t, p_i; W)$. Then, we select a set of points $\{(p_i)_j\}_{1 \leq j \leq N}$, where the Hamilton-Jacobi equation is evaluated. These points can be obtained using different means: for instance, through uniform sampling in the region where we aim to build the approximation to the Hamilton-Jacobi equation. Then, we enforce the Hamilton-Jacobi equation at the points $(p)_{1 \leq j \leq N}$ through the minimization of the mean-square error loss (or any other loss function), and consider the problem:

$$\min_W \frac{1}{N} \sum_j \left(\frac{\partial S}{\partial t}(t, (p_i)_j; W) + H(sou(\frac{\partial S}{\partial p}(t, (p_i)_j; W), (p_i)_j)) \right)^2. \tag{3}$$

This problem penalizes scenarios where the Hamilton-Jacobi equation is not satisfied. To approximately solve it, we can use the recent advancements in machine learning, including backpropagation to compute gradients and efficient optimization algorithms such as SGD, Nesterov, ADAM and others. See Goodfellow et al. (2016) for a detailed description of these topics.

4. NUMERICAL SIMULATIONS

In this section, we illustrate our findings by applying the described methodology to the rigid body, a benchmark system of Poisson dynamics. We consider the usual Lie-Poisson structure on $\mathfrak{so}^*(3)$, as discussed in Marsden and Ratiu (1994), along with the Hamiltonian

$$H = \frac{1}{2} \left(\frac{x^2}{1.5} + \frac{y^2}{2} + \frac{z^2}{2.5} \right).$$

It can be shown that $T^*SO(3)$ is a symplectic groupoid having $\mathfrak{so}^*(3)$ as its set of units, and therefore constitutes a symplectic realization (see Ferraro et al. (2017)). We uniformly sampled 80,000 points around $(0, 0, 0)$, each coordinate varying between -3 and 3 and used ADAM (10,000 iterations with a learning rate of 10^{-4}) to approximately solve (3). We employed a feed-forward neural network of four layers with 500–250–250–250 neurons and activation function tanh, using Pytorch for Python. We used uniform Xavier initialization for the weights. Two different initial conditions were chosen to showcase the outcomes when the obtained integrators are used, as seen in Fig. 1. The qualitative behaviour of the simulated trajectories is very similar to that of the original system. In both cases, we observe a nice conservation of the Hamiltonian throughout the simulated trajectories, even for very long simulations. As expected, the Casimir is conserved in both cases up to round-off error. The evolution of the Hamiltonian, Casimir and the difference from the original dynamics for a long trajectory (10,000 iterations with stepsize 0.1) is illustrated in Figure 2.

5. CONCLUSIONS AND FUTURE WORK

In this paper, we delved into the geometric setting presented previously in Vaquero et al. (2023). The framework introduced possesses several properties that make it compelling for the design of Poisson integrators: it fully respects the underlying Poisson geometry and it is highly flexible, making it amenable to various modifications and improvements. Here, we describe a couple of research directions that we plan to pursue.

General Poisson Structures: When the symplectic groupoid is not readily available, several means can be used to approximate it. Two main constructions (Cabrera, 2022) have been proposed to produce local symplectic groupoids that can integrate (locally) any Poisson manifold. An ongoing research direction aims to exploit these constructions to extend the presented framework to any Poisson manifold.

Combination with Data: In some situations, trajectories of the system are available. These trajectories might have been obtained through other (geometric or non-geometric) integrators or might correspond to actual measurements.

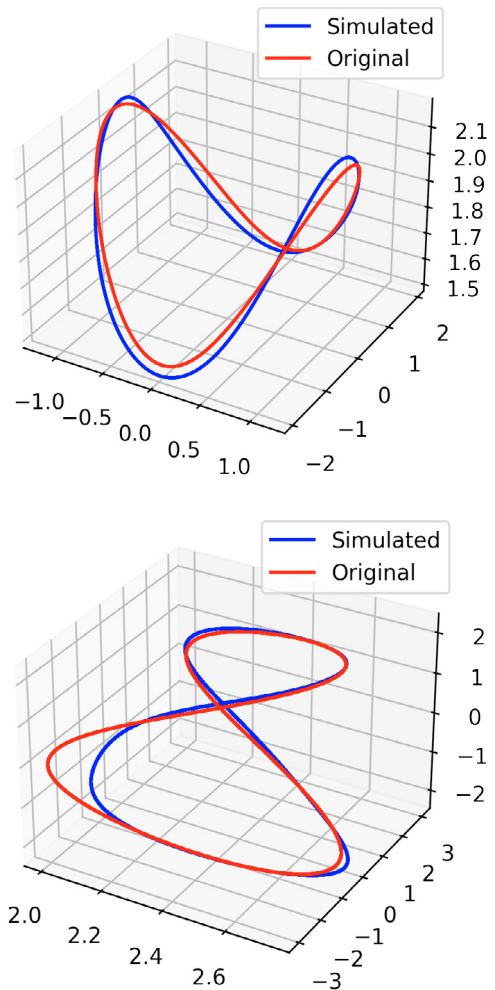


Fig. 1. Comparison of the simulated dynamics (blue) and the real trajectory (red) when the initial condition are the points $(1, 1, 2)$ (top plot) and $(3, 2, 0)$ (bottom plot).

In these cases, we envision a blended approach that combines both the data and the Hamilton-Jacobi equation. In this fashion, we follow the spirit of PINNs as described by Raissi et al. (2019), designing integrators though finding the Lagrangian submanifold that minimizes an objective function of the type $loss = loss_{HJ} + loss_{data}$. In this objective function $loss_{HJ}$ ensures that the Hamilton-Jacobi equations is satisfied to a certain degree, following the same pattern as in (3). The term $loss_{data}$ would make the Lagrangian submanifold L induce a Poisson transformation that matches the given data.

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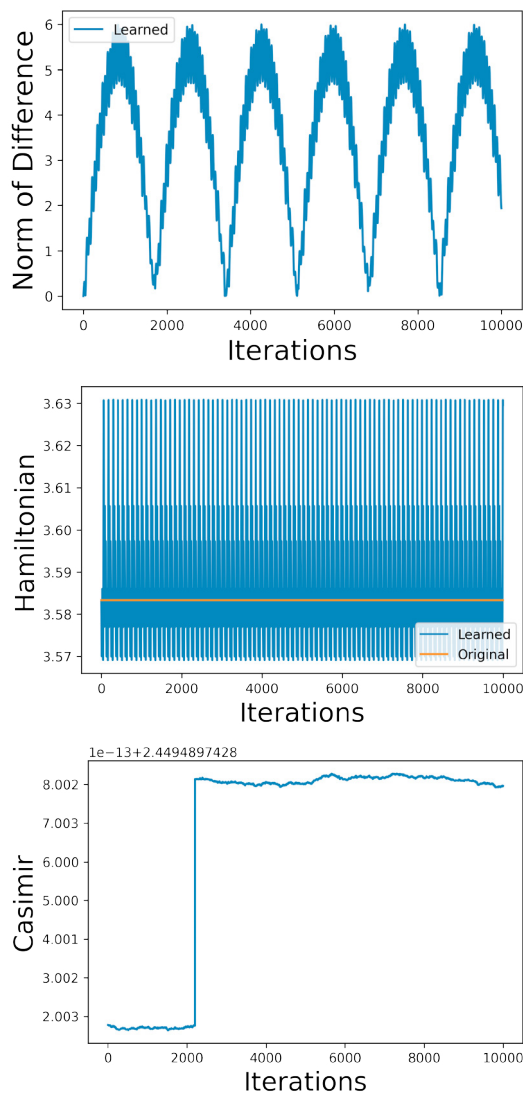


Fig. 2. *Top*: Evolution of the norm of the difference between the simulated and the real trajectories for 10,000 iterations with stepsize 0.1. The difference stays bounded due to the conservation of the underlying geometry. *Middle*: Evolution of the Hamiltonian when evaluated on the simulated trajectory. The Hamiltonian is almost conserved even for very long trajectories. *Bottom*: Evolution of the Casimir. The Casimir function is conserved up to rounding error.

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