Deep Learning: Hydrodynamics, and Lie–Poisson Hamilton–Jacobi Theory

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Abstract

The interpretation of deep learning as a dynamical system has gained a considerable attention in recent years as it provides a promising framework. It allows for the use of existing ideas from established fields of mathematics for studying deep neural networks. In this article we present deep learning as an equivalent hydrodynamics formulation which in fact possess a Lie-Poisson structure and this further allows for using Poisson geometry to study deep learning. This is possible by considering the training of a deep neural network as a stochastic optimal control problem, which is solved using mean-field type control. The optimality conditions for the stochastic optimal control problem yield a system of partial differential equations, which we reduce to a system of equations of quantum hydrodynamics. We further take the hydrodynamics equivalence to show that, with conditions imposed on the network, that it is equivalent to the nonlinear Schrödinger equation.

As such systems have a particular geometric structure, we also present a structure-preserving numerical scheme based on the Hamilton–Jacobi theory and its Lie–Poisson version known as Lie–Poisson Hamilton–Jacobi theory. The choice of this scheme was decided by the fact it can be applied to both deterministic and mean-field type control Hamiltonians. Not only this method eliminates the possibility of the emergence of fictitious solutions, it also eliminates the need for additional constraints when constructing high order methods.

1 Introduction

The kinship between deep learning and dynamical systems, discussed thoroughly and lucidly in [102], has gained a considerable attention in recent years as it was studied in a number of papers such as [10, 67, 68]. This comes as a consequence of the increased complexity of deep learning and their success in various real world applications, such as performing outstandingly in recognition tasks for images [30, 62, 99], and speech [42, 93], automated language translation [98], drug discovery [22, 34, 69] and predicting splicing patterns of RNA and their role in genetic diseases [8, 66, 104]. Yet, the inner workings are not well understood and the lack of mathematical framework in which one can analyse the systems. Further, basic tools of linear algebra are not sufficient to explain and analyse the behaviour of complex systems.

This article is part of a series that view deep learning as a hydrodynamics system within the geometric mechanics framework to better understand the behaviour of deep
networks. And here, we introduce a Hamiltonian hydrodynamic system on Poisson manifold which is equivalent to training of deep neural networks. The result is a system of partial differential equations similar to quantum Euler equation, or Madelung equation and this equation can be further transformed into the nonlinear Schrödinger equation. As these equations have special properties, we will also present geometric numerical schemes to be used as training algorithms.

The passage from deep learning to hydrodynamics is not direct and at its core is optimal control interpretation of deep learning. The use of optimal control method for deep learning is not new, in fact, it is used to train residual neural networks [10,67,68,103]. In addition to that, it is a candidate for a framework for studying deep neural networks [10,40]. Besides training this point of view is important as there is an association between optimal control and geometry [13,35,97] and this offers the opportunity to use methods and theories beyond linear and nonlinear algebra to study deep learning. This association is due in part to Pontryagin's Maximum Principle [89] for solving the optimal control problem, where it gives a Hamiltonian function whose associated vector field generates a flow that solves the training problem. In Hamiltonian mechanics, the solutions can be considered as coordinate transformations between two symplectic manifolds known as symplectic transformations, or symplectomorphisms. The underlying geometry allows one to make the transition into continuum mechanics [14,43] and such transition is reminiscent of [9] use of fluid dynamics for solving optimal transport problems. Here, we consider a general case when the deep neural network is stochastic as a way to quantify uncertainties. That said, the training problem becomes a stochastic optimal control problem and there are different ways to solve this problem. The approach chosen here is mean–field type control [11], which casts the problem as a deterministic problem. What is advantageous is that the conditions for optimality can be reduced to an equivalent hydrodynamics system, which is indeed a Lie–Poisson system. The resultant system of partial differential equations has a structure as the one for ideal compressible fluid.

Such formulation for deep learning is novel, and it is presented in this article. Not only it helps in applying Hamilton–Jacobi for Poisson integrators, but also provides a framework for studying and analysing deep learning problems. The said Lie–Poisson system for deep learning presented here has the same structure as the ideal compressible fluids; it allows us to use theories of hydrodynamics to study neural networks. The question of stability can help choosing hyperparameters heuristically and methods such as energy–momentum [94,95], and energy–Casimir both deterministic [45] and stochastic [4] can be used to study the stability of Lie–Poisson systems. That said, the study of stability is reserved for a future article. Here the focus is on employing Hamilton–Jacobi theory and its variants for systems with symmetry for deriving structure–preserving integrators for Hamiltonian systems.

Since these systems are Hamiltonian, one needs to use numerical schemes that are symplectic or Poisson. There are a number of ways one can derive such integrators, such as the partitioned Runge–Kutta method [1], or variational integrators [78] and here we focus on a type that uses generating functions. It relies on the Hamilton–Jacobi theory, which is an alternative formulation of Hamiltonian mechanics in terms of wavefronts and instead of solving for a single path, it generates a family of solutions. At the heart of the Hamilton–Jacobi theory, there is the Hamilton–Jacobi equation, as it appears in geometrical optics [16,19], and the equation for modelling the wave front propagation and
this is considered a passage from quantum mechanics to classical mechanics [53]. The solution of the Hamilton–Jacobi equation, known as generating function, which from the point of view of symplectic geometry, allows to heuristically construct coordinate transformations that preserve a geometric structure known as symplectic structure. This forms a basis for the numerical scheme, as obtaining an approximation of the generating function we can then use it to generate symplectic transformations. In other words, the numerical scheme is a symplectic transformation.

Here, we limit the application of the Hamilton–Jacobi theory to the construction of a structure–preserving numerical scheme, based on the generating function, by projecting a continuous neural network model onto a finite dimensional space while conserves a number of the network’s properties. The second application is more elaborate as it takes into account uncertainties in the network and uses mean–field games interpretation of deep learning and it uses a variant of Hamilton–Jacobi theory known as Lie–Poisson Hamilton–Jacobi theory [107]. As mentioned, the resultant system of partial differential equations has the same Poisson structure as the ideal compressible fluid [76], and because it is defined on semidirect product spaces, it necessitates the derivation of Lie–Poisson Hamilton–Jacobi theory of semidirect products spaces.

Most numerical methods for the class of Lie–Poisson equations for infinite dimensional systems use a discretisation of the vector field on the group of diffeomorphisms and not the group’s elements [29,79] based on the works of [106]. However, it is difficult to discretise the group of diffeomorphisms directly, as it is an infinite dimensional group, and apply Lie–Poisson Hamilton–Jacobi theory. One option is to consider the discretisation of [87] where the group of diffeomorphisms is approximated in finite dimensional space as the Lie group $GL(N)$. Such discretisation comes with its own challenges, such as the introduction of flat operators. For this reason we introduce a discretisation that uses the group of pseudodifferential symbols instead of the group of diffeomorphisms, which is a submanifold of the group of pseudodifferential symbols, and it makes systems on the infinite dimensional space compatible with the Lie–Poisson Hamilton–Jacobi theory. The reward of going to these lengths for numerical integrators is that the scheme preserves important properties such as the coadjoint orbit, meaning that the numerical solution would always belong to the solution set. Figure 1 demonstrates visually the solution of the angular momentum of Hamiltonian system of the SO(3) rigid body obtained by three different numerical schemes. For this rigid body, the coadjoint orbit is a sphere. It is evident the explicit Euler and 4th order Runge–Kutta method yield solutions that do not belong to the set of solutions, whereas the Lie–Poisson Hamilton–Jacobi scheme yields a solution that remains on the surface of the sphere.

The three main reasons for using generating functions to derive numerical schemes are high order integrators, possible lack of hyperregularity and its extension to the stochastic case. The first reason concerns the construction of high-order schemes and using generating functions one can construct high-order methods without the need to resort to carefully select coefficients, such as symplectic Runge–Kutta method [1], or compose a number low order integrators to form a high order one [105]. The second reason is due to the nature of the optimal control Hamiltonian. In Hamiltonian mechanics, the move into the Lagrangian formulation is done by using Legendre transform, however, this transform is not bijective when the Hamiltonian is not hyperregular. One approach to solving Hamiltonian systems numerically is to move into the Lagrangian
Figure 1: The solution of $SO(3)$ Rigid body, which is a Lie–Poisson system, computed using three different numerical methods to highlight the importance of structure–preserving integrators. The equation of motion is $\dot{\Pi} = \Pi \times \Omega$, with $\Pi = \Omega \mathbf{I}$ and $\mathbf{I} = \text{diag}(1, 2, 3)$ is the inertia tensor. In figure 1a, the Euler scheme is used to approximate the solution and it is evident that it does not stay on the sphere. The second scheme used is the 4th order Runge–Kutta method, shown in figure 1b, although it fares better than Euler method, it too does not preserve the structure. The last scheme is structure–preserving scheme that uses Lie–Poisson Hamilton–Jacobi theory of [107], the method is discussed in section 3.1, and the results that it yields, shown in figure 1c, are satisfactory.

2 Preliminaries

2.1 Hamilton–Jacobi Theory

As it plays central role for the derivation of structure–preserving schemes, here, we give a brief summary of the Hamilton–Jacobi theory and the important concepts used throughout this article. One source that we highly recommend is [77]. We consider the space of all possible states of the dynamical system and it is called configuration manifold $Q$ with coordinates $q = (q^1, \ldots, q^n)$, where $n$ is the dimension of $Q$. The tangent space of the configuration bundle is $TQ$ and its dual is the cotangent bundle $T^*Q$, whose generalised coordinates are $(q, p) = (q^1, \ldots, q^n, p^1, \ldots, p^n)$. In mechanics, there are a number of ways to describe the motion of the system and one of these is Newtonian mechanics. Despite the fact that the intuition behind Newtonian mechanics is easier to grasp, when there are physical and geometric constraints, it becomes difficult to model. Lagrangian mechanics was introduced to tackle this and it is a formulation that is widely used for constraint particle motion. Such formulation of mechanics requires $(q, \dot{q}) \in TQ$ to describe the motion of the system. An alternative formulation, and the one used here, is the Hamiltonian formulation which uses position and conjugate momenta $(q, p) \in T^*Q$ to describe evolution of the system. Another important object in Hamiltonian mechanics is the Hamiltonian function $H : T^*Q \rightarrow \mathbb{R}$, which carries all the information of the dynamics of the system. The Hamiltonian, $H$, is related to the energy of the system and, in some cases, it coincides with the total energy. Once we have the Hamiltonian, $H$, and with fixed boundary terms $q(0)$ and $q(T)$, the variational
principle states that
\[ \delta \int_0^T \langle p, \dot{q} \rangle - H(q, p) \, dt = 0, \]
and it yields Hamilton’s equation
\[ \frac{dq}{dt} = \frac{\partial H}{\partial p}(q, p), \quad \text{and} \quad \frac{dp}{dt} = -\frac{\partial H}{\partial q}(q, p). \]

Often, Hamilton’s equation are described as what is known as a Hamiltonian vector field \( X_H = (\frac{\partial H}{\partial p}, -\frac{\partial H}{\partial q}) \) whose flow \( \Phi_{X_H} : (q_0, p_0) \to (q, p) \) , and it maps the initial points \((q_0, p_0) \in T^*Q\) to the final points \((q(t), p(t)) \in T^*Q\) at time \( t \). This mapping leaves the symplectic structure, \( \omega = dq \wedge dp \) invariant, i.e.
\[ (\Phi_{X_H})^* \omega - \omega = 0, \]
and this allows for constructing coordinate transformation that considerably simplifies the equation of motion. The mapping \( (\Phi_{X_H})^* \) is the pull-back of of \( \omega \) by flow of \( X_H \) and (3) can be easily proven by taking the time derivative and using Cartan’s formula for Lie derivatives [77].

In fact, one choice of coordinates \((w, J)\), known as action-angle coordinates, chooses the momentum \( J \) to be a constant of motion and this coordinate system is central to the celebrated Kolmogorov-Arnold-Moser theorem. Meanwhile, the symplectic form can be written as an exact form
\[ \omega = d\theta = dq \wedge dp, \quad \text{where} \quad \theta = pdq \]
where \( d \) is a map from \( k \)-forms on a manifold to \( (k+1) \)-forms on the same manifold known as exterior derivative and it is linear and satisfies the product rule [2]. In coordinates, if a \( k \)-form is given by
\[ \alpha = \alpha_{i_1, \ldots, i_k} dx^{i_1} \wedge \cdots \wedge dx^{i_k}, \]
the exterior derivative is given by
\[ d\alpha = \sum_{j=1}^{k} \frac{\partial \alpha_{i_1, \ldots, i_k}}{\partial x^{j}} dx^{j} \wedge dx^{i_1} \wedge \cdots \wedge dx^{i_k}. \]
It has the properties that \( d^2 = 0 \) and when \( f \) is a scalar function, \( df \) is equal to the differential of \( f \). The relation (4) holds is due to the fact that \( \omega \) is a closed form, i.e. \( d\omega = 0 \). This is important, as it allows us to write
\[ (\Phi_{X_H})^* d\theta - d\theta = d((\Phi_{X_H})^* \theta - \theta) = d^2 S = 0 \]
and it implies there the difference between the one-form and its pullback by the flow of the Hamiltonian system is a closed one-form. This closed one-form is defined as an exterior derivative of the function, \( S : Q \times Q \times \mathbb{R} \to \mathbb{R} \) , and it is known as generating function. The generation of symplectic transformation from \( S \) comes from the relation
\[ dS = pdq - p_0dq_0, \]
which yields
\[ p(t) = \frac{\partial S}{\partial q}(q_0, q(t), t), \quad \text{and} \quad p_0 = \frac{\partial S}{\partial q_0}(q_0, q(t), t). \] (7)

Luckily, the generating function satisfies a partial differential equation
\[ \frac{\partial S}{\partial t} + H(q, \frac{\partial S}{\partial q}) = 0. \] (8)

known as Hamilton–Jacobi equation. Solving Hamilton’s equations and solving Hamilton–Jacobi equation is one and the same thing. The main difference between the two approaches is that the latter deals with functions defined on the configuration manifold, \( Q \), while the former the dynamics belong to the cotangent bundle \( T^*Q \).

For certain systems, it is taxing to work with generating function \( S \) that generates a canonical transformation from the old to the new coordinates, \((q_0, p_0)\) and \((q(t), p(t))\) respectively, and for this it is not unwise to consider a combination of old and new coordinates. The said combinations can be constructed using Legendre transformations and one transformation that is widely used is the type-II generating function
\[ S_2(q_0, p(t), t) = S(q_0, q(t), t) + \langle q(t), p(t) \rangle. \] (9)

Substituting \( S \) in terms of \( S_2 \) we obtain a Hamilton–Jacobi equation (8) for each type of generating function.

**Remark 2.1.** For numerical schemes based on generating functions, it is practical to use type-II generating function as it allows for initial condition to be \( S_2(p_0, p(0), 0) = 0 \) and, in the same time, satisfy the identity transformation required by the Hamilton–Jacobi theory.

### 2.2 Optimal Control Theory

In this section, we give a brief overview of optimal control theory and formulating deep learning as an optimal control problem. The reader is invited to read of the following references [3,17,49] for more detailed exposition on the subject. Let \( Q \) be a configuration manifold and a system’s state, on the time interval \([0, T]\), is described by \( q(t) \in Q \). The goal of optimal control is to move the system from the state \( q(0) = q_0 \) to the state \( q(T) = q_T \), where \( q_0, q_T \in Q \) are predetermined states. This is actualised by choosing \( \theta = (u, b) \in U \), where \( U \) is called the space of admissible controls, such that the cost functional
\[ S(q, \theta) = \int_0^T \ell(q(t), \dot{q}(t), \theta(t)) \, dt \] (10)

is maximised/minimised and at the same time \( q(t) \in Q \) satisfies
\[ \frac{d}{dt} q = \sigma (u \cdot q + b), \] (11)

where \( q \in Q, \frac{d}{dt} q \in TQ \) and \( \theta = (u, b) \in U \) and \( \sigma : Q \times U \to \mathbb{R} \). The term \( \ell : TQ \times U \to \mathbb{R} \), in (10), is the loss function or cost Lagrangian. The choice of loss function depends on the application, and it is usually chosen as a measure of how far is the state of the
system, \( q(t) \), from a predetermined target. There are two methods that are widely used to compute \( \theta \): dynamic programming and Pontryagin’s Maximum Principle. The former breaks the problem into a smaller problem on the interval \([t, t + \Delta t]\) and uses the solution of the smaller problem to construct a solution on \([0, T]\) and it yields a solution which satisfies the necessary and sufficient condition for optimality. However, it is not considered in this article and instead we use Pontryagin’s Maximum Principle.

The method in essence is finding a curve on the Pontryagin’s bundle \( T^*Q \times U \), denoted by \((q(t), p(t), \theta(t))\), that minimises (10) and it also satisfies the following Hamilton’s equation:

\[
\frac{dq}{dt} = \frac{\partial H}{\partial p}, \quad \frac{dp}{dt} = -\frac{\partial H}{\partial q}, \quad \frac{\partial H}{\partial \theta} = 0,
\]  

with the Hamiltonian function \( H: T^*Q \times U \to \mathbb{R} \), defined by \( H(q, p, \theta) = \langle p, \sigma(q(t), \theta(t)) \rangle - \ell(q(t), \theta(t)) \). These equations, (12), are the stationary variations of Hamilton’s principle

\[
0 = \delta S = \delta \int_0^T \langle p, \dot{q} \rangle - H(q, p, \theta) \, dt.  
\]

The equation \( \dot{p} = -\frac{\partial H}{\partial q} \) is the costate equation and also known as the adjoint equation and it has gained attention in deep learning research as it is the core of methods such as neural ordinary differential equation [23, 25, 96]. Solving such Hamiltonian system is an arduous task, thus numerical methods are required to approximate the solution. The application of numerical integrators for optimal control problems has been explored in [15, 48, 58, 63, 64] and the key idea is to use a discrete version of the variational principle. On the contrary, in this article, the idea is, instead of applying discrete variational principle, we use the structure-preserving numerical scheme derived using Hamilton–Jacobi theory, given by (82), to approximate the solution of Pontryagin’s Maximum Principle (12). Concerning the initial conditions for \((q(t), p(t))\), we are only given \( q_0 \) and \( q_T \) and for this reason an additional step is needed to find the correct \( p^0 \) that would make \((q^k, p^k, \theta^k)\), where \( k = 0, \ldots, N_t \) satisfy \( q^0 = q_0 \) and \( q^{N_t} = q_T \). There are a number of choices for the extra step, such as the shooting method where \( p^0 \) is chosen at random and then adjusted. The other approach is to use nonlinear programming, and the idea is that it makes the solution of the algebraic expressions (82) and the boundary conditions as the solution of a nonlinear system of equations.

### 2.3 Deep Neural Network Training As Optimal Control Problem

Now considering deep learning, we first need to a representation of the neural networks as a dynamical system. Artificial neural networks can be viewed as a group of simple sub-systems referred to as synapses connected in a specific way. Mathematically, a synapsis is modelled as the following transformation \( Q_k \to Q_{k+1} \), without the loss of generality, in this article we solely consider the case where this transformation is an endomorphism, i.e. a transformation \( Q \to Q \), given by

\[
q^{k+1}_i = F^k(q^k_i, \theta^k), \quad \text{for} \quad k = 0, \ldots, N_t - 1
\]

where \( q^{k+1}_i \) is the \( i \)th synapsis of the \( k + 1 \) layer, \( q^k \in Q, \theta^k = (u^k, b^k) \in U \) is the network’s parameters and the map \( F^k : Q \times U \to Q \) is the state transition map. The
vector \( q^{k+1} = (q^{k+1}_1, \ldots, q^{k+1}_{N_l}) \in Q \subset \mathbb{R}^{N_l} \) constitute a single layer in the network. For general cases, the configuration space \( Q \) need not be vector spaces, they can be Hilbert spaces or differentiable manifold, and in that case (14) can be regarded as a pullback operation from \( Q_k \) to \( Q_{k+1} \). The choice of the state transition map determines the type of network and here we consider a transition of the type

\[
q^{k+1}_i = F(q^k_i, \theta^k) = q^k_i + \alpha \sigma \left( \sum_{j=0}^{N_l} u^k_{i,j} q^k_j + b^k_i \right), \quad \alpha \in \mathbb{R}_{>0},
\]

and this renders (14) as residual neural network, ResNet henceforth. The function \( \sigma : Q \times U \to Q \) is the activation function and it is applied element-wise and few of the most commonly used ones are: linear rectifier, denoted by ReLU, hyperbolic tan, sigmoid function, and softmax. Here, \( u^k_{i,j} \) is the element of the \( i \)th row and \( j \)th column of weight matrix and \( b^k_i \) is the \( i \)th element of bias vector for the \( k \)th layer. We do not specify \( \theta^k = (u^k, b^k) \) for \( k = 0, \ldots, N_l \), before hand, at first, random weights and biases are sampled form a distribution function. Finding the values for \( \theta^k \) to make the neural network model a specific system is the focus of training methods studied in the field of machine learning.

Equation (15) is viewed as Euler discretisation of a continuous dynamical system [23, 26, 27, 91]. The move to the continuous domain can be interpreted as taking the limit when the number of hidden layers approaches infinity, \( N_l \to \infty \). The result is a dynamical system defined on the manifold \( Q \) of the form

\[
\frac{d}{dt} q(t) = \sigma(q(t), \theta(t)), \quad t \in [0, T], \quad \text{and} \quad q(0) = q_0,
\]

where \( q_0 \in Q \).

**Remark 2.2.** In some literature [23, 25], the limit of ResNet, (16), is referred to as neural ordinary differential equation. In this article, we substitute this naming with continuous ResNet.

Training the neural network can be treated as an optimal control problem with (16) as a constraint, and the dataset \( \{(q^{(i)}_0, c^{(i)})\}_{i=0, \ldots, N} \) specifies the initial conditions and the final conditions [67]. We define \( \mathcal{C} \) as the space of target data. Thus, we state the training of continuous ResNet as follows

**Problem 2.3.** Given the training set \( \{(q^{(i)}_0, c^{(i)})\}_{i=0, \ldots, N} \), compute \( \theta = (u, b) \) such that it minimises

\[
S = \int_0^T \ell_d(q(t), \theta(t)) \, dt + \sum_{i=0}^N L(\pi((q(T)^{(i)}), c^{(i)}),
\]

such that it satisfies

\[
\frac{d}{dt} q(t) = \sigma(u(q(t)) + b(t)),
\]

and \( q(0) = q^{(i)}_0 \) and \( \pi(q(T)) = c^{(i)} \) for \( i = 0, \ldots, N \).
Here, where \( \ell : Q \times U \rightarrow \mathbb{R} \) is the cost Lagrangian and in machine learning it acts as a regularisation term. The last term of the functional \( S \) is the terminal condition and it is a metric for measuring how far the output of (57), \( q(T)^{(i)} \), whose starting point is \( q(0) = q_0^{(i)} \), is from the target data \( c^{(i)} \). A suitable candidate is \( \sum_{i=0}^{N} L(\pi(q(T)^{(i)}), c^{(i)}) \), where \( L : C \times C \rightarrow \mathbb{R} \) and the projection \( \pi : Q \rightarrow C \) and in this article it is chosen as \( \pi(x) = \frac{1}{1+e^{-x}} \). As for \( L \), in many classification problems, a common and a suitable choice is the categorical cross entropy loss function.

3 Stochastic Optimal Control for Deep Learning

In this section, we consider a continuous residual neural network that takes into consideration the network’s uncertainties. These uncertainties are accounted for by modelling them as a stochastic process and for the time-being, we only consider Wiener processes. That means the dynamical model for continuous ResNet, given by (16), is now a stochastic differential equation. The addition of stochastic terms not only render the model robust for potential variations, but also it is very rich mathematically as shall we explore in this section.

Similar to the previous sections, we present an algorithm for training deep learning using a generating function for stochastic continuous ResNet. As the dynamical system is now stochastic, the application of the Pontryagin’s Maximum Principle used in this article cannot be done directly. For this we require stochastic optimal control and especially mean–field type optimal control [11], and, in this paradigm, the solution to the optimal control problem satisfies a system of partial differential equations instead of ordinary differential equations. The idea of using stochastic optimal control for deep learning was studied in [27,88], however, the main difference is we use elimination theorem of [24] to reduce the system of partial differential equations to hydrodynamic equation with advected quantity.

One major consequence of mean–field optimal control is that we can no longer utilise the Hamilton–Jacobi theory used in section ???. However, there are two possible ways to construct structure–preserving schemes for optimal control: using multisymplectic integrators and using integrators based on generating functions on Poisson manifolds. In this article, we only focus on the latter, as the former is studied in [32]. The key here is to use Poisson map analogous to the symplectic transformation and we, first, reduce the system of partial differential equations that we obtain by mean–field type optimal control to a hydrodynamics equation. Then we restate the said hydrodynamics equation as a Lie–Poisson equation, which is the same equation but from the Hamiltonian viewpoint. The Poisson geometry counterpart for the Hamilton–Jacobi theory was introduced in [107] and it is known as the Lie–Poisson Hamilton–Jacobi theory.

We give a brief overview of the theory in section 3.1 and we introduce a variant of the theory that concerns semidirect products. In section 3.1.1 we introduce the algebras of pseudodifferential symbols whose dual space is where the Lie–Poisson equation evolves. In section 4.1, we use algebras of pseudodifferential symbols on discrete meshes to derive numerical scheme based on generating function on Poisson space is presented in proposition 4.11.
3.1 Hamilton–Jacobi for Systems with Symmetry

Having demonstrated how Hamilton–Jacobi theory is used as a formulation for Hamiltonian systems on $Q$, here we consider a special case when the Hamiltonian is $G$-invariant.

What we mean by that, we consider a configuration manifold $Q$ and when $g \in G$ is a Lie group action acting on the Hamiltonian $H : T^*Q \to \mathbb{R}$, the following holds

$$H(g \cdot q, (g)^*p) = H(q, p), \quad (q, p) \in T^*Q.$$ 

This allows us to perform the Lie–Poisson reduction [77]. We will not cover reduction theory here, the reader is advised to refer to [72,76,77]. In essence, the invariance allows us to choose action such that $T^*Q/G$ and the resultant quotient space is isomorphic to the dual of the Lie algebra $g^*$. For example, when $Q = SO(3)$ and $G = SO(3)$, the quotient space $T^*SO(3)/SO(3)$ is isomorphic to $so^*(3)$, the dual of the Lie-algebra associated to $SO(3)$. In general, the dual of Lie algebra $g^*$ is an example of what is known as a Poisson manifold [76]. A manifold $(P, \{\cdot, \cdot\})$ is said to be a Poisson manifold when a Poisson structure

\begin{equation}
\{f, h\} = \sum_{i=1}^n \left( \frac{\partial f}{\partial q_i} \frac{\partial h}{\partial p_i} - \frac{\partial h}{\partial q_i} \frac{\partial f}{\partial p_i} \right),
\end{equation}

is defined for any function on $C^\infty(P)$, the form is anti-symmetric, satisfies both the Jacobi identity and Leibniz’s rule. The bilinear form $\{\cdot, \cdot\}$ is known as the Poisson structure. Let $(P_1, \{\cdot, \cdot\}_1)$ and $(P_2, \{\cdot, \cdot\}_2)$ be two Poisson manifolds, then a map $\phi : P_1 \to P_2$ that satisfies $\{f \circ \phi, h \circ \phi\}_1 = \{f, h\}_2 \circ \phi$ for any $f, h \in C^\infty(P_2)$ is called a Poisson map. A detailed exposition of reduction is beyond the scope of this article, however, it is only summarised. For the dynamics, whose Hamiltonian is $H : T^*Q \to \mathbb{R}$, its integral curves when projected to a Poisson manifold $P$ using the map $\pi_P : T^*Q \to P$, coincide with the integral curves of dynamics, whose Hamiltonian is $H_P : P \to \mathbb{R}$. We can say that the flow $F$ of the Hamiltonian $H$ and the flow $F_P$ of $H_P$ are related by $\pi_P \circ F = F_P \circ \pi_P$.

The Hamiltonian dynamics on $T^*Q$ induce Lie–Poisson equation on $g^*$

\begin{equation}
\frac{d}{dt} F = \{F, H_P\},
\end{equation}

which is equivalent to

\begin{equation}
\frac{d}{dt} \mu = ad^*_\mu \mu,
\end{equation}

where $ad^* : g \times g^* \to g^*$ is the coadjoint map.

The Lie–Poisson reduction can also be used for the Hamilton–Jacobi theory [107]. Starting with the Hamilton–Jacobi theory

$$\frac{\partial S}{\partial t}(q, q_0) + H(q, \frac{\partial S}{\partial q}) = 0, \quad p_0 = -\frac{\partial S}{\partial q_0}, \quad p(t) = \frac{\partial S}{\partial q},$$

where $S : Q \times Q \to \mathbb{R}$ is the generating function, the Hamiltonian $H : T^*Q \to \mathbb{R}$ is a $G$-invariant Hamiltonian. The generating function yields a canonical transformation
from \((q_0, p_0) \rightarrow (q(t), p(t))\). Let \(S_L(g) = S(q^{-1}q, q^{-1}q_0) = S(e, g)\), where \(g = q^{-1}q_0\), the Lie–Poisson reduction reduces (21) to

\[
\frac{\partial S_L(g)}{\partial t} + H(-J_L \circ \mathsf{d}S_L) = 0, \quad \mu_0 = T\mathsf{L}_g^* \mathsf{d}_g S_L, \quad \mu = T\mathsf{R}_g^* \mathsf{d}_g S_L,
\]

with \(\mu_0, \mu \in \mathfrak{g}^*\). Here we have \(S_L : Q \rightarrow \mathbb{R}, g \in G\) is the Lie group action, \(T\mathsf{L}_g^*\) and \(T\mathsf{R}_g^*\) are the left and right cotangent lift of Lie group action \(g\). The map \(J_L : T^*Q \rightarrow \mathfrak{g}^*\) is the \textit{the momentum map} for the cotangent lift and it is equal to

\[
J_L(\alpha) = T_e R_g^* \alpha,
\]

while \(J_R : T^*Q \rightarrow \mathfrak{g}^*\) is given by

\[
J_R(\alpha) = T_e L_g^* \alpha.
\]

The partial differential equation and two expressions in (22) are known as \textit{Lie–Poisson Hamilton–Jacobi theory} introduced in [107]. In fact, the integrator that was used in figure 1, to showcase one of the advantages of structure–preserving integrators, uses the discrete version (22) on \(SO(3)\).

Now, the generating function \(S_L\), generates a Poisson map \(\phi : \mu_0 \rightarrow \mu\), which is the analogue of symplectic map on the cotangent bundle \(T^*Q\). This reduction is not only valid for semisimple Lie groups such as \(SO(3)\), it can be applied to semidirect products. First, let us recall some basic facts about semidirect products. Let \(S = G \oplus V\) be a semidirect product space with Lie group \(G\) and vector space \(V\). Let \(\zeta : G \rightarrow \text{Aut}(V)\) be the representation of the Lie group \(G\) in \(V\), and \(\zeta' : \mathfrak{g} \rightarrow \text{End}(V)\) is the Lie algebra representation in \(V\). The multiplication of \(S\) is defined as

\[
(g_1, v_1)(g_2, v_2) = (g_1 g_2, v_1 + \zeta(g_1)v_2),
\]

where \((g_1, v_1), (g_2, v_2) \in S\). The corresponding Lie algebra \(\mathfrak{s} = \mathfrak{g} \times V\) has the Lie bracket

\[
[[\xi_1, v_1], [\xi_2, v_2]] = ([\xi_1, \xi_2], \zeta'(\xi_1)v_2 - \zeta'(\xi_2)v_1),
\]

where \((\xi_1, v_1), (\xi_2, v_2) \in \mathfrak{s}\). The left action of \(S\) on to itself is defined as

\[
L_{(g,v)}(h, u) = (gh, v + \zeta(g)u),
\]

and tangent lift of the left action is

\[
T_{(h,u)}L_{(g,v)}(v_h, u, w) = (T_h L_g(v_h, v + \zeta(g)u, \zeta(g)w),
\]

where \((v_h, u, w) \in T_{(h,u)} (G \oplus V)\). The tangent lift at the element \((g, v)(h, u) \in S\) and we are introducing it, so we can define left action momentum map \(J_L\) later.

\[
T_{(g,v)(h,u)}L_{(g,v)}^{-1}(v_{gh}, v + \zeta(g)u, w) = (T_{gh} L_{g^{-1}}(v_{gh}, u, \zeta(g^{-1})w),
\]

for any \((v_{gh}, v + \zeta(g)u, w) \in T_{(g,v)(h,u)} (G \oplus V)\). The cotangent lift is

\[
(T_{(g,v)(h,u)}L_{(g,v)}^{-1})^* (\alpha_h, v, a) = (T_{gh} L_{g^{-1}})^* \alpha_h, u + \zeta(g) v, \zeta_e(g)a,
\]

where \((\alpha_h, v, a) \in T^*_h (G \oplus V)\). On the other hand, the right action of \(S\) on itself is

\[
R_{(g,v)}(h, u) = (hg, u + \zeta(h)v),
\]
and the tangent lift is 

\[ T_{(h,u)}R_{(g,v)}(v_h, u, w) = (T_hL_g(v_h, u + \zeta(h)v, \zeta(h)w), \]

and the lift over the point \((g, v)(h, u) \in S\),

\[ T_{(h,u)(g,v)}R_{(g,v)}^{-1}(v_{hg}, u + \zeta(h)v, w) = (T_{hg}R^{-1}_g(v_{hg}, v, w - T_{hg}\zeta(v_{hg}) \cdot \zeta(g^{-1})v), \]

and the cotangent lift is

\[(T_{(h,u)(g,v)}R_{(g,v)}^{-1})^*(\alpha_h, v, a) = ((T_{hg}R^{-1}_g)^*\alpha_h - df^\tau_{(g^{-1})v}(h), v + \zeta(h)v, a)\]

With that we can write the left momentum map, \(J_L : T^*(G \oplus V) \to \mathfrak{s}_+^*\) and the right momentum map, \(J_R : T^*(G \oplus V) \to \mathfrak{s}_-^*\) by using (28) and (32) with \((g, v) = (g, v)^{-1}\) and \((h, u) = (g, v)\) and that gives

\[ J_L = (T_{(c,0)}R_{(g,v)})^*(\alpha_g, u, a) = ((TeR_g)^*\alpha_g + (\zeta'_v)^*a, a), \]
\[ J_R = (T_{(c,0)}L_{(g,v)})^*(\alpha_g, u, a) = ((TeL_g)^*\alpha_g, \zeta'(g)a). \]

**Theorem 3.1.** Given the left \(G\)-invariant Hamiltonian, \(H\), then the left reduced Lie–Poisson Hamilton–Jacobi equation for semidirect products for a function \(S_L : G \oplus V \times \mathbb{R} \to \mathbb{R}\) is the following:

\[ \partial_t S_L((g, v), t) + H_r (TR^*_g d_g S_L + (\zeta'_v)^*d_v S_L, d_v S_L) = 0 \]

The solution of equation (35), known as **Lie–Poisson Hamilton–Jacobi equation**, generates a Poisson map that defines the flow of the reduced Hamiltonian \(H_r\). The Poisson map transforms the initial momentum map \(\mu_0 \to \mu(t)\), where

\[ (\mu_0, \Gamma_0) = (-TL_g^*d_g S_L, \zeta'(g)d_v S_L), \]
\[ and \quad (\mu(t), \Gamma(t)) = (TR^*_g d_g S_L + (\zeta'_v)^*d_v S_L, d_v S_L), \]

where \(g \in G\) and \(v \in V\).

For construction of a numerical scheme, the steps followed are similar to the ones taken in section 4. First, the equation is approximated numerically in time, using a numerical scheme, such as Euler method or Runge–Kutta method, while maintaining that it is parameterised in \((g, v)\). For example, a first order in \(t\) approximation is given by

\[ S_L((g, v)) \approx S_0((g, v)) + \Delta t H (TR^*_g d_g S_0 + (\zeta'_v)^*d_v S_0, d_v S_0), \]

where \(S_0\) is the initial condition of \(S_L\) and it is chosen such that it satisfies the identity mapping. The next step is to then use this approximation of \(S_L\) and substitute it into equation (36) and it allows to obtain the group action \((g, v)\) that would result in \((\mu_0, \Gamma_0)\). Once the action \((g, v)\) is found, it is then used in (37) to compute \((\mu(t), \Gamma(t))\).
3.1.1 Lie Algebra of Pseudodifferential Symbols

Here we give a brief overview of the basics of Lie groups whose Lie algebras are pseudodifferential symbols. A profound study of such groups is not required at the moment as we only require the basics. For detailed exposition on this topic, the reader can refer to [12, 56, 57]. This Lie algebra is required as it allows for the application of Lie–Poisson Hamilton–Jacobi to Lie–Poisson partial differential equations.

We begin by defining what we mean by an operator of order \( m \),

\[
P = \sum_{|\alpha| \leq m} a_{\alpha}(x) D^{\alpha},
\]

where \( D \) is a differential operator and \( \alpha \) is a multiindex and \( a_{\alpha} \in H^s(\mathbb{R}) \). The symbol of the operator \( P \) is a polynomial in \( \xi \) variable

\[
p(x, \xi) = \sum_{|\alpha| \leq m} a_{\alpha}(x) \xi^{\alpha}.
\]

In this section we denote the algebra of pseudodifferential symbols by \( \Psi DS_{m} \), where the \( m \) subscript indicates the order. The union of such algebras \( \Psi DS = \bigcup_{k} \Psi DS_{k} \) and it is closed under multiplication defined by

\[
U(x, \xi) \circ M(x, \xi) = \sum_{n \geq 0} \frac{1}{n!} \left( \frac{d^n}{d\xi^n} U(x, \xi) \right) \left( \frac{d^n}{dx^n} M(x, \xi) \right),
\]

where \( U \in \Psi DS_{m} \) and \( M \in \Psi DS_{n} \). The multiplication, \( U(x, \xi) \circ M(x, \xi) \), belongs to the group \( \Psi DS_{n+m} \subset \Psi DS \), i.e. multiplication is a closed group operation. The Lie bracket of the Lie algebra \( \Psi DS \) is given by

\[
[U, M] = U \circ M - M \circ U = \sum_{n \geq 0} \frac{1}{n!} \left\{ \left( \frac{d^n}{d\xi^n} U(x, \xi) \right) \left( \frac{d^n}{dx^n} M(x, \xi) \right) - \left( \frac{d^n}{dx^n} U(x, \xi) \right) \left( \frac{d^n}{d\xi^n} M(x, \xi) \right) \right\}.
\]

The algebra \( \Psi DS \) can be written as the direct sum of two other subalgebras, i.e.

\[
\Psi DS = \Psi DS_{DO} \oplus \Psi DS_{INT},
\]

where

\[
\Psi DS_{DO_{m}} := \left\{ \sum_{\alpha=0}^{m} a_{\alpha}(x) \partial^{\alpha} \right\}, \quad \text{and} \quad \Psi DS_{INT_{m}} := \left\{ \sum_{\alpha=-m}^{-1} u_{\alpha}(x) \partial^{\alpha} \right\},
\]

and \( \Psi DS_{DO} = \bigcup_{m \geq 0} \Psi DS_{DO_{m}} \) and \( \Psi DS_{INT} = \bigcup_{m \geq 0} \Psi DS_{INT_{m}} \).

Usually for Lie algebras, there’s an associated Lie group and to map the Lie algebra to the Lie group an exponential map is used. The map needs to be bijective and here is defined as the solution of the following differential equation

\[
\frac{d}{ds} G(x, s) = U \circ G(s),
\]

13
where $G$ is the group element and $U$ belongs to the Lie algebra, and the initial condition is chosen as $G(0) = I_d$. The differential equation (44) actually yields a system of differential equations, in most cases it is a triangular system, for each coefficients of symbols of $G$ and solving this system is required to obtain the coefficients of the group element $G$ [57]. Here we use the $\Psi G$ as the group whose vector fields at the identity are the $\Psi DS$ symbols. Basically, $\Psi G$ is a group whose elements are solutions of (44). The reasoning behind not considering it a full Lie group is that the full algebra of symbols $\Psi DS$ does not have a corresponding Lie group nor its subalgebra $\Psi DS_{DO}$. However, for the subalgebra $\Psi DS_{INT}$ does have an associated Lie group $G_{INT}$ and the exponential map is bijective $\exp : g_{INT} \to G_{INT}$. We denote the algebra $\Psi DS_{INT}$ by $g_{INT}$ henceforth.

The pairing between the Lie algebra $g_{INT}$ and its dual $g_{INT}^*$, $\langle \cdot, \cdot \rangle : g_{INT} \times g_{INT}^* \to \mathbb{R}$, is defined by

$$\langle M, U \rangle = \text{Tr} (M \circ U) = \int \text{res} (M \circ U), \quad U \in g_{INT}, \ M \in g_{INT}^*. \quad (45)$$

and we actually find that $g_{INT}^* \simeq g_{DO}$, where $g_{DO}$ denotes the Lie algebra of differential operators $\Psi DS_{DO}$. For Hamiltonian systems, we need to compute functional derivatives. Let $M$ be an element of $g_{INT}$, and consider the functional $F : g_{INT} \to \mathbb{R}$, its functional derivative is obtained using the following pairing

$$DF(M) : M = \left\langle \frac{\delta F}{\delta M}, M \right\rangle = \sum_i \int \delta F \frac{\delta m_i}{m_i} dx, \quad (46)$$

thus we obtain,

$$\frac{\delta F}{\delta M} = \sum_{i=1}^m \frac{\delta F}{\delta m_i} \xi^{-i}. \quad (47)$$

Using the functional derivatives, one can define the Lie–Poisson bracket by

$$\{F, H\} (M) = \left\langle M, \left[ \frac{\delta F}{\delta M}, \frac{\delta H}{\delta M} \right] \right\rangle = \int \text{res} \left( M \circ \left[ \frac{\delta F}{\delta M}, \frac{\delta H}{\delta M} \right] \right), \quad (48)$$

where $H$ and $F$ are functionals that depend on the coefficients of the pseudodifferential symbols.

To apply theorem 3.1, for deep learning, we first need to compute the cotangent lifts of the action on the dual of the Lie algebra. Let $A$ be an element of the group $G_{INT}$. The multiplication operator is defined by (41) and to compute the tangent lift, let $B \in \Psi G_{INT}$ such that $\left. \frac{d}{ds} \right|_{s=0} B(s) = X$, where $X \in g_{INT}$. Multiplying $A$ with $B$ and taking the derivative with respect to $s$ and evaluate at $s = 0$, we have

$$TL_A X = \left. \frac{d}{ds} \right|_{s=0} A(t) \circ B(s) = A(t) \circ X, \quad (49)$$

and

$$TR_A X = \left. \frac{d}{ds} \right|_{s=0} B(s) \circ A(t) = X \circ A(t). \quad (50)$$
To compute the cotangent lifts, $TL^*_A$ and $TR^*_A$, are computed by pairing the tangent lifts to an element $\alpha \in g^*_\text{INT}$, the pairing is done using the trace operator, i.e
\[
\text{Tr} (TL^*_A \alpha \circ X) = \text{Tr} (\alpha \circ TL_A X) = \int \text{res} (\alpha \circ A(t) \circ X),
\] (51)
and
\[
\text{Tr} (TR^*_A \alpha \circ X) = \text{Tr} (\alpha \circ TR_A X) = \int \text{res} (\alpha \circ X \circ A(t)).
\] (52)

These yield the following cotangent lift of the left and right action
\[
TL^*_A \alpha = \alpha \circ A(t),
\] (53)
\[
TR^*_A \alpha = A(t) \circ \alpha.
\] (54)

### 3.2 Hydrodynamics Formulation of Deep Learning

From the basic iterative relation of deep neural networks, we can interpret them, in the language of geometric mechanics, as applying a pullback to a curve on a manifold. It is very reminiscent of the particle relabeling symmetry of fluids labels, i.e the action of the group of diffeomorphism, denoted by $\text{Diff}(Q)$, on the Lagrangian labels [7, 28].

The vector field associated with $\text{Diff}(Q)$ is denoted by $X(Q)$. The neurons of the hidden layers can be viewed as Lagrangian labels
\[
dt q(x,t) = \sigma (u \circ q(x,t)),
\] (55)
where $q \in \text{Diff}(Q)$ and $u \in \mathfrak{X}(Q)$, and each time they propagate through to the next layer, a transformation is applied to the labels. Let $(\Omega, \mathcal{F}, \mathbb{P})$ be the probability space, with $\Omega$ the sample space, and $\mathcal{F}$ is $\sigma$-algebra of measurable events of $\Omega$ and $\mathbb{P}$ is the probability measure on $(\Omega, \mathcal{F})$. We consider the stochastic differential equation for continuous ResNet
\[
dt q(t) = (u \circ q) dt + \nu dW_t, \quad q(0) = q_0, \quad \text{and} \quad q(T) = q_T,
\] (56)
where $u \in \mathfrak{X}(Q)$ is a vector field that plays the role of network parameters, and $\xi_k \in \mathfrak{X}(Q)$ are vector fields that couple the Brownian motion $W^k_t$ to $\mathfrak{X}(Q)$ and $\nu \in \mathbb{R}$. Notice in (56) the activation function was removed because it is redundant in this form. Here, the network parameters are specified to be a vector field on the group of diffeomorphisms on $Q$ and can be viewed as a combination of the weight matrix and activation function. Since the system is stochastic, the cost functional (57) cannot be used in its current form, instead, we use its expected value. Thus, we can state the training problem of stochastic continuous ResNet as follows:

**Problem 3.2.** Let $(\Omega, \mathcal{F}, \mathbb{P})$ and given the training set $\{(q_0^{(i)}, c^{(i)})\}_{i=0,\ldots,N}$, compute $u \in$ such that it minimises
\[
S = \int_Q \int_0^T \rho(x,t) \ell_d (u(t)) \ dt \ dx + \sum_{i=0}^N \int_Q \rho(x,t) L(\pi((q(T)^{(i)}), c^{(i)})) \ dx,
\] (57)
where $\rho(x,t)$ is the probability density function. The solution should make $q(t)$ satisfy
\[
d_t q = u \circ q \ dt + \nu \sum_k \xi_k dW^k_t,
\] (58)
and $q(0) = q_0^{(i)}$ and $\pi(q(T)) = c^{(i)}$ for $i = 0, \ldots, N$. 

15
The solution method for this optimal control problem is mean–field optimal control, described in [11]. Instead of controlling (58), the equation for the evolution of probability density function associated with \( q(t) \), known as the Fokker–Planck equation,

\[
\frac{\partial \rho(x,t)}{\partial t} + \nabla \cdot (u(x,t)\rho(x,t)) - \frac{\nu^2}{2} \nabla \cdot (\nabla \rho(x,t)) = 0, \quad \rho(x,0) = \rho_0(x).
\]

This way, we can apply Pontryagin’s Maximum Principle in a similar way to the deterministic optimal control problems. The result is the mean–field games system

\[
\frac{\partial \rho(x,t)}{\partial t} + \nabla \cdot (u(x,t)\rho(x,t)) - \frac{\nu^2}{2} \nabla \cdot (\nabla \rho(x,t)) = 0
\]

\[
\partial_t \rho(x,t) + u(x,t) \nabla \rho(x,t) - \nu^2 \nabla \cdot (\nabla \rho(x,t)) = 0
\]

\[
\partial_t \lambda(x,t) + u(x,t) \nabla \lambda(x,t) + \nu^2 \nabla \cdot (\nabla \lambda(x,t)) = \ell_d
\]

where it is basically a coupled system of Fokker–Planck equation, (61), and stochastic Hamilton–Jacobi–Bellman equation, (62). In [32], the network parameter \( u \) is substituted by \( u = \omega + \nu^2 \nabla \log(\rho) \) and this is done to reduce the system of equations (60), (61) and (62) to the following equation

\[
\frac{\partial \delta \ell_d}{\partial \omega} + \frac{\partial}{\partial \omega} \rho \nabla \delta \ell_d = \rho \nabla \delta \ell_d - \frac{\partial \rho}{\partial \rho}
\]

\[
\partial_t \rho + \nabla \cdot (\omega \rho) = 0
\]

where \( \text{ad}^* : \mathfrak{X} \times \mathfrak{X}^* \rightarrow \mathfrak{X}^* \) is the coadjoint map and in this case it is defined in coordinates of \( \mathbb{R}^N \) as

\[
\left( \text{ad}^* \frac{\delta \ell_d}{\delta \omega} \right)_i = \left( \partial_{x^j} \left( \frac{\delta \ell_d}{\delta \omega} \right)_i \omega^j \right) + \left( \frac{\delta \ell_d}{\delta \omega} \right)_i \partial_{x^j} \omega^j.
\]

One thing to note that the approach of [32] relies on the Lagrangian formulation of mechanics and we cannot apply Hamilton–Jacobi theory directly, but in order to do so, we need to translate it into the Hamiltonian point of view.

**Remark 3.3.** It is worth pointing out that when \( \nu \rightarrow 0 \) in (63), it is in effect the celebrated hydrodynamics formulation of the Monge–Kantorovitch mass problem of optimal transport [9]. And for the optimal control problem, with \( \nu \rightarrow 0 \) in (60), (61) and (62), it was shown that it reduces to a Euler’s fluid equation in [14].

### 3.3 Deep Learning as a Lie-Poisson System

In this section, we formulate the reduced mean–field games (63) to a Lie–Poisson system, and in doing so, we translate it into the language of Lie–Poisson Hamilton–Jacobi theory. This allows us to construct a Poisson mapping from the target of the training dataset to the initial conditions.

This first problem that we need to overcome is that the Hamiltonian for the mean–field games (60), (61) and (62) is a covariant Hamiltonian and theorem 3.1 is not adapted for such Hamiltonians. For covariant Hamiltonians, there has been attempt to introduce
a general Hamilton–Jacobi theory, such as the work done in [47, 80, 101]. An alternative approach in [100], where boundary integrals of the variational principle are used to derive generating functions for partial differential equations. Having said that, the route taken here is to expand the work with a larger configuration manifold, that is, the group of pseudospectral symbols instead of the group diffeomorphism. In order to use Lie–Poisson Hamilton–Jacobi theory, we discretise the group of pseudospectral symbols in space only. This is inspired by the work of [87] where the group of diffeomorphisms is discretised as $GL(N)$ and EPDiff equation is written in terms of vector fields on dual of the discretised Lie algebra which is a subalgebra of $\mathfrak{g}l(N)$.

For the deep learning problem, the Hamiltonian for the system (63) is

$$
H = \frac{1}{2} \int_Q \rho \| \omega \|^2 d\text{Vol}(x) + \frac{\nu^2}{2} \int_Q \rho \langle \omega, \nabla \log(\rho) \rangle d\text{Vol}(x)
+ \frac{\nu^4}{8} \int_Q \rho \| \nabla \log(\rho) \|^2 d\text{Vol}(x)
$$

and $H$ is a function defined on the dual of the Lie algebra of a semidirect product $s^* = g_{\text{INT}} \oplus \text{Dens}(Q)$. The corresponding group is $S = G_{\text{INT}} \oplus \text{Dens}(Q)$. From the definitions of group actions on itself, tangent and cotangent lifts defined in section 3.1, here $G_{\text{INT}}$ acts on $\text{Dens}(Q)$ by (push-forward), i.e.

$$
\zeta(g)\rho = (g)^*\rho, \quad g \in G_{\text{INT}}
$$

Another important map that we need to define is the algebra $g_{\text{INT}}$ representation on $\text{Dens}(Q)$, denoted by $\zeta' : g_{\text{INT}} \to \text{End}(\text{Dens}(Q))$, is given by

$$
\zeta'(U)\rho = -\mathcal{L}_U \rho,
$$

where $U \in g_{\text{INT}}$ and $\mathcal{L}_U$ denotes the Lie derivative along the direction of $U$, and in coordinates $\zeta'(U)\rho = \text{div}(\rho U)$. Once we have the representation on the Lie algebra, we derive the representation of the dual of the Lie algebra $g_{\text{INT}}^*$, i.e. the mapping $(\zeta')^* : \text{Dens}(Q)^* \to g_{\text{INT}}^*$. It is obtained by using the pairing and for any $\rho \in \text{Dens}(Q)$, $\eta \in \text{Dens}(Q)^*$ and $U \in g_{\text{INT}}$ we have

$$
\langle \eta \diamond \rho, U \rangle = \langle (\zeta')^* \rho, U \rangle = -\langle \eta, \zeta U \rho \rangle = -\int \eta \nabla \cdot (U \rho) \, dx = -\int \rho \nabla \eta \cdot U \, dx,
$$

and this means $\eta \diamond \rho = (\zeta')^* \rho = \rho \nabla \eta$. The operator $\diamond : \text{Dens}(Q) \times \text{Dens}(Q)^* \to g_{\text{INT}}^*$ is often used in describing motion of various hydrodynamics, introduced in [46], and it used to map Clebsch variables to the dual of Lie algebra [44].

Going back to training of deep neural networks on Poisson manifolds and for this particular problem we choose the symbol to be

$$
U(x, \xi) = u(x) \xi^{-1} \in g_{\text{INT}},
$$

and we require that the dual space $g_{\text{INT}}^*$ should be the space of pseudodifferential symbols of order 2, i.e.

$$
M(x, \xi) = \sum_{i=0}^{2} m_i(x) \xi^i
$$
The importance of these conditions on the Lie algebra is that for the functionals $F$ and $H$ substituting them into the Lie–Poisson bracket (48), we obtain

$$
\{ F, H \} = \int m(x) \left[ \frac{\delta F}{\delta m} \nabla \left( \frac{\delta H}{\delta m} \right) - \frac{\delta H}{\delta m} \nabla \left( \frac{\delta F}{\delta m} \right) \right] \, dx.
$$

(71)

The Lie–Poisson bracket of functionals on the dual of the Lie algebra of semidirect product $s^* = g^*_\text{INT} \oplus \text{Dens}(Q)^*$ is

$$
\{ F, H \}_\pm (M, \rho) = \pm \left\langle M, \left[ \frac{\delta F}{\delta M}, \frac{\delta H}{\delta M} \right] \right\rangle \mp \left\langle \rho, \mathcal{L}_{\frac{\delta F}{\delta \rho}} \frac{\delta H}{\delta \rho} - \mathcal{L}_{\frac{\delta H}{\delta \rho}} \frac{\delta F}{\delta \rho} \right\rangle,
$$

(72)

where $F, H : s^* \to \mathbb{R}$ and the first term of the Lie–Poisson bracket is given by (48). In explicit terms,

$$
\{ F, H \}_\pm (M, \rho) = \pm \int_Q m(x) \left[ \frac{\delta F}{\delta m} \nabla \left( \frac{\delta H}{\delta m} \right) - \frac{\delta H}{\delta m} \nabla \left( \frac{\delta F}{\delta m} \right) \right] \, dx
$$

$$
\mp \int_Q \rho \left[ \left( \frac{\delta H}{\delta m} \cdot \nabla \right) \frac{\delta F}{\delta \rho} - \left( \frac{\delta F}{\delta m} \cdot \nabla \right) \frac{\delta H}{\delta \rho} \right] \, dx.
$$

(73)

**Remark 3.4.** This Lie–Poisson bracket is the same bracket for ideal compressible fluid [75, 76].

Since the Lie–Poisson bracket is in terms of $(M, \rho) \in s^*$, and that necessitates the need to write the Hamiltonian (65) in those coordinates and for that we use $M = \rho \omega$,

$$
H(M, \rho) = \frac{1}{2} \int_Q \frac{\|M\|^2}{\rho} \, d\text{Vol}(x) + \frac{\nu^2}{2} \int_Q \langle M, \nabla \log(\rho) \rangle \, d\text{Vol}(x)
$$

$$
+ \frac{\nu^4}{8} \int_Q \rho \|\nabla \log(\rho)\|^2 \, d\text{Vol}(x).
$$

(74)

Plugging in $F = (M, \rho)$, we obtain the Lie–Poisson on semidirect product space

$$
\partial_t M = \{ M, H \}_+,
$$

$$
\partial_t \rho = \{ \rho, H \}_+,
$$

(75)

or in coordinates od $\mathbb{R}^N$, it is written as

$$
\partial_t m_i = m_i \partial_x \left( \frac{\delta H}{\delta m_i} \right) + \partial_x \left( m_i \frac{\delta H}{\delta m_i} \right) + \rho \partial_x \left( \frac{\delta H}{\delta \rho} \right) \text{ for } i = 1, \ldots, N
$$

$$
\partial_t \rho = -\partial_x \left( \rho \frac{\delta H}{\delta \rho} \right),
$$

(76)

where $\text{ad}^* : g^*_\text{INT} \times g^*_\text{INT} \to g^*_\text{INT}$ and it is the same as in (64).

**Proposition 3.5.** The deep learning dynamics can be written in Lie–Poisson form

$$
\partial_t M = \pm \text{ad}^*_{\frac{\delta H}{\delta \rho}} M \pm \frac{\delta H}{\delta \rho} \cdot \rho
$$

$$
\partial_t \rho = \pm \mathcal{L}_{\frac{\delta H}{\delta \rho}} \rho,
$$

(77)

where $\text{ad}^* : g^*_\text{INT} \times g^*_\text{INT} \to g^*_\text{INT}$ and it is the same as in (64).
Proof. Let \((\eta, \varrho), (u, a) \in s\) and \((M, \rho) \in s^*\), from the definition of the coadjoint map and the diamond operator, we then have

\[
\langle (\text{ad}_u^* M - a \diamond \rho, -L_u \rho), (\eta, \varrho) \rangle = \langle \text{ad}_u^* M - a \circ \rho, \eta \rangle + \langle -L_u \rho, \varrho \rangle
\]

\[
= \langle M, \text{ad}_u \eta \rangle + \langle \rho, L_u \eta - L_u a \rangle
\]

\[
= \langle M, [u, \eta] \rangle + \langle \rho, L_u \eta - L_u a \rangle
\]

\[
= \langle \{M, u\}, \eta \rangle + \langle \rho, L_u \rho \rangle
\]

\[
= \langle \{M, u\}, \langle \rho, u \rangle, (\eta, \varrho) \rangle.
\]

From the equation we get

\[
(\text{ad}_u^* M - a \circ \rho, -L_u \rho) = \langle \{M, u\}, \{\rho, u \} \rangle
\]

and thus we can write equation (75) as

\[
\partial_t M = \pm \text{ad}_u^* \frac{\delta H}{\delta M} M - \text{ad}_u^* \frac{\delta H}{\delta \rho} \circ \rho
\]

\[
\partial_t \rho = \mp \text{L} \frac{\delta H}{\delta \rho} \rho.
\]

Now, we can apply the Lie–Poisson Hamilton–Jacobi theory for semidirect products as

\[
\partial_t S_L((A, \rho)) + h \left( TR_A^* d_A S_L + (\zeta_u')^* d_\rho S_L, d_\rho S_L \right) = 0
\]

(78)

The solution of equation (35) generates a Poisson map that defines the flow of the reduced Hamiltonian \(h\). The Poisson map transforms the initial momentum map \(\mu_0 \to \mu(t)\), where

\[
(\mu_0, \rho_0) = (-d_A S_L \circ A, \zeta(A)^* d_\rho S_L), \quad \text{and} \quad (\mu(t), \rho(t)) = (A \circ d_A S_L + (\zeta_u')^* d_\rho S_L, d_\rho S_L).
\]

(79)

Now we decipher the two previous equations in (79). The first component \(d_A S_L \circ A\) is the multiplication in \(\Psi DS\) and the second, as mentioned, is the action of \(\Psi G\) acting on \(\text{Dens}(Q)\) by pullback. The term \((\zeta_u')^* d_\rho S_L\) is the diamond operator defined in (68).

The terms \((d_A S_L, d_u S_L)\) can be eliminated from the second equation in (79), by taking the left action of \((A, u)^{-1}\) of \((\mu_0, \rho_0)\). This results in

\[
(\mu(t), \rho(t)) = (-A \circ \mu_0 \circ A^{-1} + (\zeta_u')^* \rho_0 (A \circ x), \rho_0 (A \circ x))
\]

\[
= \text{Ad}_{(A,u)^{-1}}^* (\mu_0, \rho_0),
\]

where \(\text{Ad}_{(A,u)^{-1}}^*: S \times s^\ast \to s^\ast\) is the coadjoint operator.

Despite the Lie–Poisson Hamilton–Jacobi theory introduces a level of complexity to the matter; the power of the method comes out when it is employed for constructing numerical algorithms. Up until now, we have worked exclusively with continuous-time representation of deep learning, but for it to applicable we need to discretise it. The discrete Lie–Poisson Hamilton–Jacobi theory would yield an \(N\) dimensional system that preserves the geometric structure of the continuous equations. Furthermore, the flow or solution trajectories, generated by the Hamiltonian vector-field corresponding to (73)
belong to the coadjoint orbit. The coadjoint orbit, \( O_{(\mu, \rho)} \), is the set of elements of \( s^* \) that are moved by the elements of the group \( S = \Psi G \times \text{Dens}(Q) \), or mathematically,
\[
O_{(\mu, \rho)} := \left\{ \text{Ad}^*_A - 1(\mu, \rho) \mid (A, u) \in \Psi G \right\},
\]
and \((\mu, \rho) \in s^*\). The coadjoint orbit is in fact a sub-manifold of \( s^* \) and it is endowed with a symplectic structure [73]. The Lie–Poisson Hamilton–Jacobi constructs a numerical solution that naively belongs to \( O_{(\mu, \rho)} \) and this makes it worth studying. The preservation of the coadjoint orbit was further looked at in [74].

What is interesting regarding the discrete equations is that they are also a Hamiltonian system and this is a consequence of applying reduction to generating function on cotangent bundle. In [33] it was shown how to derive the modified Hamiltonian for the discrete equations obtained from Lie–Poisson Hamilton–Jacobi theory, albeit the systems considered in [33] are stochastic. However, the same steps can be followed for the deterministic case.

The fact that mean–field games system (60), (61) and (62) is written as a coadjoint motion, then according to theorem 2.7 in [35], the optimal solution is restricted to \( O_{(\mu, \rho)} \). This means \((\mu_0, \rho_0)\) as well as \((\mu_T, \rho_T)\) are on the same coadjoint orbit \( O_{(\mu, \rho)} \) and that means the curve \((\mu(t), \rho(t)) \in s^*\) is a minimising curve of the functional and it also connects the two densities \(\rho_0\) and \(\rho_T\).

## 4 Hamilton–Jacobi Integrators for Deep Learning

In this section we show the application of generating function in constructing a structure–preserving integrator for training deep neural network. Symplectic transformations, that are generated by the solution of the Hamilton–Jacobi equation, preserve the structure and it is the basis for construction of the numerical scheme. This is done by applying a numerical method for solving the Hamilton–Jacobi equation and then use that with (7) to obtain the approximated solution. From Pontryagin’s Maximum Principle, the necessary conditions for optimality of the solution of an optimal control problem satisfy a Hamiltonian system (12). Thus, it is fitting that a geometric integrator is used to solve optimal control problem to guarantee that the numerical solution is representative of the control system. First, we describe how optimal is used to formulate the training of deep neural network in section 2.3 and, here, we adhere to the approach of [10, 20, 67]. The resultant Hamilton’s equations are then solved numerically using structure–preserving integrator.

The idea of using generating functions for numerical integrators was first introduced in [21, 52]. Recall that the solution of a Hamiltonian system is a symplectomorphism and one time-step integration is also a symplectic transformation \((q^k, p^k) \rightarrow (q^{k+1}, p^{k+1})\) generated by the solution of Hamilton–Jacobi equation at time \(\Delta t\). Using a generating function of type-II and (7), we obtain the following numerical scheme
\[
q^{k+1} = q^k + \frac{\partial S_2}{\partial p}(q^k, p^{k+1}, \Delta t), \quad p^{k+1} = p^k - \frac{\partial S_2}{\partial q}(q^k, p^{k+1}, \Delta t)
\]
and such scheme preserves the symplectic form \(\omega = dq^k \wedge dp^k = dq^{k+1} \wedge dp^{k+1}\). The generating function, \(S_2\) is the approximation of solution of Hamilton–Jacobi equation.
and it can be expressed as a truncated power series

\[ S_2(q, p, t) = \sum_{i=1}^{m} t^i S_{2,i}(q, p, t), \quad (83) \]

where the coefficients of the power series are functions in term of the Hamiltonian \( H \) and its partial derivatives

\[ S_{2,1} = H(q, p), \quad S_{2,2} = \frac{1}{2} \left( \frac{\partial H}{\partial q}, \frac{\partial H}{\partial p} \right), \quad S_{2,3} = \ldots \]

The order of scheme (82) is determined by the number of terms, \( m \), in the approximation (83).

**Remark 4.1.** When \( m = 1 \), i.e. \( S = \Delta t H \), the scheme (82) becomes the symplectic Euler scheme

\[ q^{k+1} = q^k + \Delta t \frac{\partial H}{\partial p}(q^k, p^{k+1}, \Delta t), \quad p^{k+1} = p^k - \Delta t \frac{\partial H}{\partial q}(q^k, p^{k+1}, \Delta t) \]

The application of structure–preserving integrators based on generating function can be used to approximate the solution of optimal control problem, now we use that to solve problem 2.3. Using Pontryagin’s Maximum Principle, the control Hamiltonian \( H : T^*Q \times U \rightarrow \mathbb{R} \) is

\[ H(q_0, \ldots, q_N, p_0, \ldots, p_N, \theta) = \sum_{i=0}^{N} \langle p_i, \sigma(q_i, \theta) \rangle - \frac{\gamma}{2} \| \theta \|^2 \quad (84) \]

where \( \gamma \in \mathbb{R}_{\geq 0} \) and the last term is the regularisation term. We also require that

\[ \frac{\delta H}{\delta \theta} = \frac{1}{\gamma} \sum_{i=0}^{N} p_i \frac{\partial \sigma}{\partial z} q_i^T - \theta = 0 \]

and substitute the expression for \( \theta \) into \( H \), we obtain a Hamiltonian in terms of canonical coordinates \( (q, p) \) on cotangent bundle \( T^*Q \). Then the Hamiltonian, \( H : T^*Q \rightarrow \mathbb{R} \), becomes a function defined on the cotangent space rather than the Pontryagin’s bundle and it is given by

\[ H(q_0, \ldots, q_N, p_0, \ldots, p_N, t) = \sum_{i=0}^{N} \left( p_i, \sigma \left( q_i, \frac{1}{\gamma} \sum_{j=0}^{N} p_j \frac{\partial \sigma}{\partial z} q_j^T \right) \right) - \frac{1}{2\gamma} \left\| \sum_{j=0}^{N} p_j \frac{\partial \sigma}{\partial z} \right\|^2 \quad (85) \]

**Problem 4.2.** Given the training set \( \{(q_0^{(i)}, c_N^{(i)})\}_{i=0, \ldots, N} \), compute the sequence \( (q^k, p^k) \) such that it satisfies

\[ q_i^{k+1} = q_i^k + \Delta t \sigma \left( \frac{1}{\gamma} \sum_{j=0}^{N} \frac{\partial \sigma}{\partial z} p_j^{k+1} (q_j^k)^T q_i^k + \frac{1}{\gamma} \sum_{j=0}^{N} \frac{\partial \sigma}{\partial z} p_j^{k+1} \right), \quad (86) \]

\[ p_i^{k+1} = p_i^n - \frac{\Delta t}{\gamma} \frac{\partial \sigma}{\partial z} \left( \sum_{j=0}^{N} \frac{\partial \sigma}{\partial z} p_j^{k+1} (q_j^k)^T \right) \]
The accuracy of the neural networks predictions is shown in figures 2a and 2c, for the two spirals and two circles datasets respectively, over 5000 training iterations. On the other hand, the residual, computed by

$$\sum_{i=0}^{N} \| \pi(q^{(50)}_{i}) - c_{i} \|^2,$$

is shown in figures 2b and 2d, for the two spirals and two circles datasets respectively.

In order to iterate through (86), we require \( p_{0} \), however at this point, it is not available. Further, the value of \( p_{0} \) must ensure that \( q_{0}^{(i)} = q_{0}^{(i)} \) and \( \pi(q^{N_{t}}) = c^{(i)} \) for each \( i = 0, \ldots, N \).

$$\pi(q^{N_{t}}) = c^{(i)}$$

for \( k = 0, \ldots, N_{t} - 1 \) and the boundary conditions \( q_{0} = q_{0}^{(i)} \) and \( \pi(q^{N_{t}}) = c^{(i)} \) for each \( i = 0, \ldots, N \).

In order to iterate through (86), we require \( p_{0} \), however at this point, it is not available. Further, the value of \( p_{0} \) must ensure that \( q_{0}^{(i)} = q_{0}^{(i)} \) and \( \pi(q^{N_{t}}) = c^{(i)} \). There are a number of ways in which one can choose a suitable initial value for the costate equation and one of them is shooting method [61]. The idea is to pick an arbitrary \( p_{0} \) and then evaluate how different \( \pi(q^{N_{t}}) \) from \( c^{(i)} \) and use this error to modify \( p_{0} \). The process is then iterated to refine the choice of \( p_{0} \). An alternative approach is to use the fact that we can derive the \( p^{N_{t}} \) from the cost functional. Once we have that, we can use that to define (86) as the Karush–Kuhn–Tucker condition for nonlinear programming. For such constraint optimisation problems, iterative methods such as sequential quadratic programming [41], or even using Newton’s iterative method.

To evaluate the numerical scheme presented in this section, we train the network for two separate classification problems: two spirals, and two concentric circles classification. That said, this is just a toy example as a sanity check. Both datasets contain data from only two classes, that means for all classification space \( C = \{0, 1\} \). The two spirals dataset contains 2000 data points for training and 2000 other data points for testing. Whereas, the two concentric circles dataset uses, for each training and testing, 1000 data points. The number of layers used for both datasets is \( N_{t} = 50 \) and \( \Delta t = 0.075 \). The training was done over 5000 iterations.
Figure 3: The transformation of two spirals training set \( \{(q^{(i)}_0, c^{(i)}_N)\}_{i=0,...,N} \) with \( N = 2000 \) at the 20th layer (the second column from the left), 30th layer (the third column from the left), and the final layer (rightmost column). Figure 3a, shows the network discretised using Euler scheme, while figure 3b, shows the results obtained using 4th order Runge–Kutta method. Finally, figure 3c is when the symplectic method using Euler scheme for the generating function. The solid black line separates between the two classes/categories.

In order to put the structure–preserving scheme into perspective, other numerical schemes for ordinary differential equations are used for neural networks: Euler method, and fourth order explicit Runge–Kutta method. The methods are compared using the error function in (57), \( L = \sum_{i=0}^{N} \| \pi((q(50))^{(i)}) - c^{(i)} \|^2 \), and the accuracy at each training steps. The accuracy and residuals for the two datasets are shown in figure 2. Figure 3 shows snap shots of the data, only for the two spirals dataset, propagating through the layers of each discretisation of the continuous ResNet. At the final layer, we see that, for all implementations, the majority of data points of each class are carried in a way they become sorted. Figure 4, shows the trajectories that each data point takes for all three discretisations.
Figure 4: The trajectories of the two spirals data are plotted, where the solid dots are the initial data and the hollow circles are the final data. The light coloured lines are the individual paths each data point followed when iterated through the discretised continuous residual network. Figure 4a shows the paths when the network is discretised using Euler scheme, while figure 4b and 4c show the trajectories of the 4th order Runge–Kutta and symplectic integrator, respectively.

4.1 Deep Neural Networks as Discrete Lie-Poisson System

Before discretising (79), we first need to review a particular discretisation compatible with the Lie–Poisson Hamilton–Jacobi theory. The discretisation is done on the algebra of pseudodifferential symbols \( \Psi\text{DS} \) instead of discretising the Hamilton–Jacobi equation. The philosophy here is similar to [84, 87], where the volume preserving group of diffeomorphisms is discretised and approximated as a subgroup of \( GL(N) \) Lie group instead.

Let \( Q \) denote a smooth manifold, its discrete analogue is denoted by

\[
Q := \{(x_1^i, x_2^i, \ldots, x_N^i) : i = 0, \ldots, N_t, \ (x_1^i, x_2^i, \ldots, x_N^i) \in Q\},
\]

and in this discretisation, the space between each point in each dimension is a constant \( D_x \). Consider the pseudodifferential operator (39), when applied to a function \( u \in C^\alpha(Q) \), and instead of evaluating the Fourier transform on \( Q \), it is evaluated on \( Q \).

With out the loss of generality, in 1 dimensions, the pseudodifferential operator on \( u \) can be written as

\[
P_d u(x_j) = \frac{1}{(2\pi)^n} \sum_{j,k} \int e^{i(x_k - x_j)\xi} a_k(x_j)\xi^k u_j d\xi, \quad (87)
\]

From the previous expression, the following polynomial

\[
p(x_j, \xi) = \sum_{k \leq m} a_{k,j}\xi^k, \quad (88)
\]
where \( a_{k,j} = a_k(x_j) \), is called discrete symbol of order \( m \). We denote the algebra of pseudodifferential symbols of order \( m \) on \( Q \) by \( \Psi DS_{d,m} \). Basic operations and definitions carry also to pseudodifferential operators on \( Q \).

**Definition 4.3.** Let \( A \in \Psi DS_d \) and \( B \in \Psi DS_{d,n} \), then the multiplication of \( A \circ B \) on \( Q \) is the operator \( C \) with symbol of order \( m + n \) defined by

\[
c_j(\xi) = \sum_{|\alpha| < N} \frac{1}{\alpha!} \partial^{\alpha}_{\xi} a_j(\xi) D^\alpha_x b_j(\xi)
\]

where \( D^\alpha_x \) is the discrete difference operator in the \( x \) direction of order \( \alpha \).

**Definition 4.4.** Let \( A \in \Psi DS_d \) and \( B \in \Psi DS_{d,n} \), the commutator bracket for the \( \Psi DS_d \) is

\[
[A, B](x_j) = \sum_{n \geq 1} \frac{1}{\alpha!} \partial^{\alpha}_{\xi} a_j(\xi) D^\alpha_x b_j(\xi) - D^\alpha_x a_j(\xi) \partial^{\alpha}_{\xi} b_j(\xi)
\]

Another important map that is used extensively is the trace map \( \text{Tr} : \Psi DS_d \rightarrow \mathbb{R} \), and here for \( A \in \Psi DS_{d,m} \), it is defined by

\[
\text{Tr}(A) = \sum_k a_{-1,k}.
\]

Having defined the trace mapping, this enable us to define the pairing between the algebra \( \Psi DS_d \) and its dual \( \Psi DS^*_d \) defined as a map \( \langle \cdot , \cdot \rangle : \Psi DS_d \times \Psi DS^*_d \rightarrow \mathbb{R} \) described by

\[
\langle A, B \rangle = \text{Tr}(A \circ B),
\]

where \( A \in \Psi DS_d \), and \( B \in \Psi DS^*_d \).

**Remark 4.5.** This is useful when the the space \( \Psi DS_d \) is decomposed into two subspaces as in (43) to help identify the the Lie algebra with its dual.

To directly apply Lie–Poisson Hamilton–Jacobi theory of proposition 3.1, we first need to give the explicit expression for the group action and its cotangent lift on pseudodifferential algebra on \( Q \). As we are only interested in a subalgebra of \( \Psi DS_d \), we only state the algebraic expressions of the subalgebra of interest. From this point onwards, we use the notation \( g_{\text{INT}}(Q) \) to denote the algebra of pseudodifferential integral operators on the discrete set \( Q \) and \( g_{\text{INT}}^*(Q) \) its dual. Analogous to the continuous case, the Lie algebra \( g_{\text{INT}}(Q) \) has an associated Lie group \( G_{\text{INT}}(Q) \) and elements of this Lie group, \( g_j(s) \), satisfy the following differential equation

\[
\frac{d}{ds} g_j(s) = A_j \circ g_j(s),
\]

where \( A_j \in g_{\text{INT}}(Q) \) and \( g_j(0) = \text{Id} \). The subscript \( j \) denotes that action is evaluated at \( x_j \in Q \).

Computing the tangent and cotangent lifts the actions of \( G_{\text{INT}}(Q) \) on \( g_{\text{INT}}(Q) \) and \( g_{\text{INT}}^*(Q) \) for all orders is beyond the scope of this project. However, we only consider the order \( -1 \) of pseudodifferential symbols, because it is the symbol that would yield the desired Lie–Poisson bracket (73).
Using interpolation of the probability density function then in (80), the action is appears in Lagrangian coordinates, but the discrete setting hydrodynamics \[82\], where the elements of \(\text{Dens}(\cdot)\) in the continuity equation in (75). For the former, it is inspired by smoothed particle \(G\) and the tangent lift of the right action on \(G\) is

\[
\text{TL}_{g_j} P_j = p_{1,j} \xi^{-1} + p_{2,j} \xi^{-2} + (u_{1,j} p_{1,j} + p_{3,j}) \xi^{-3} + (u_{1,j} p_{2,j} - 2u_{1,j} D_x p_{1,j} + u_{2,j} p_{1,j}) \xi^{-4} + \mathcal{O}(\xi^{-5}),
\]

and the tangent lift of the right action on \(P_j\) is

\[
\text{TR}_{g_j} P_j = p_{1,j} \xi^{-1} + p_{2,j} \xi^{-2} + (u_{1,j} p_{1,j} + p_{3,j}) \xi^{-3} + (u_{1,j} p_{2,j} + u_{2,j} p_{1,j} - p_{1,j} D_x u_{1,j}) \xi^{-4} + \mathcal{O}(\xi^{-5}).
\]

Meanwhile, the cotangent lift of the action of \(G_{\text{INT}}(\mathbb{Q})\) on \(g_{\text{INT}}^*(\mathbb{Q})\) are computed according to (53) and (53).

Definition 4.7. Consider the discrete symbol \(\alpha_j = \alpha_{1,j} \xi + \alpha_{2,j} \xi^2\) on the dual space of \(g_{\text{INT}}^*(\mathbb{Q})\), then the cotangent lift of the left group action \(g_j(s) = 1 + u_{1,j}(s) \xi^{-1} + u_{2,j}(s) \xi^{-2}\) on \(\alpha_j\) is

\[
\text{TL}^*_{g_j} \alpha_j = \alpha_{2,j} \xi^2 + (u_{1,j} \alpha_{2,j} + \alpha_{1,j}) \xi + u_{1,j} \alpha_{1,j} + u_{2,j} \alpha_{2,j} + 2\alpha_{2,j} D_x u_{1,j} + (u_{2,j} \alpha_{1,j} + 1.0 \alpha_{2,j} D_x u_{1,j} + 2\alpha_{2,j} D_x u_{2,j}) \xi^{-1} + (\alpha_{1,j} D_x u_{2,j} + 1.0 \alpha_{2,j} D_x^2 u_{2,j}) \xi^{-2} + \mathcal{O}(\xi^{-3}),
\]

in parallel, the cotangent lift of the right action is

\[
\text{TR}^*_{g_j} \alpha_j = \alpha_{2,j} \xi^2 + (u_{1,j} \alpha_{2,j} + \alpha_{1,j}) \xi + u_{1,j} \alpha_{1,j} - u_{1,j} D_x \alpha_{2,j} + u_{2,j} \alpha_{2,j} + (-u_{1,j} D_x \alpha_{1,j} + 1.0 u_{1,j} D_x^2 \alpha_{2,j} + u_{2,j} \alpha_{1,j} - 2u_{2,j} D_x \alpha_{2,j}) \xi^{-1} + (u_{1,j} D_x^2 \alpha_{1,j} - 2u_{2,j} D_x \alpha_{1,j} + 3.0 u_{2,j} D_x^2 \alpha_{2,j}) \xi^{-2} + \mathcal{O}(\xi^{-3}).
\]

In addition to the tangent and cotangent lifts, we need to define the discrete version of the representation of the action of \(G_{\text{INT}}(\mathbb{Q})\) on \(\text{Dens}(\mathbb{Q})\). One issue that arises is then in (80), the action is appears in Lagrangian coordinates, but the discrete setting is based on the Eulerian point of view. There are two ways we can resolve this issue: Using interpolation of the probability density function \(\rho\) and numerically integrating the continuity equation in (75). For the former, it is inspired by smoothed particle hydrodynamics [82], where the elements of \(\text{Dens}(\mathbb{Q})\) are approximated by

\[
\rho(x, t) \approx \sum_j \rho_j(t) W_j(x).
\]

Here, \(W_j(x)\) are weights functions and one possible candidate of \(W_j(x)\) is the Gaussian function

\[
W_j(x) = e^{-\alpha \|x-x_j\|^2}, \quad \text{with} \quad \alpha \in \mathbb{R}_{>0}.
\]

The second approach is to use a numerical scheme for approximating \(\rho(x, t)\), where the (75) is solved in the interval \([t, t + \Delta t]\).

Definition 4.8. Consider \(g_j(s) \in G_{\text{INT}}(\mathbb{Q})\) on \(\text{Dens}(\mathbb{Q})\), the function (66), the map \(\zeta : G_{\text{INT}}(\mathbb{Q}) \to \text{Dens}(\mathbb{Q})\) defined by

\[
\zeta(g_j) \rho = \rho_0(g_j \circ x) = \sum_j \rho_j(t) W_j \left( x + \int_0^t u_j \, dt \right).
\]
On the other hand, it can be defined as one time iteration of the Fokker–Planck equation
\[ \zeta(g_j) \rho = \rho^k + (\Delta t) D_x \left( \rho^k u_j \right). \]  

(95)

### Remark 4.9.
From a numerical standpoint, using the pullback operator given in definition (96) is more stable and suitable to the continuity equation, however, the one given by definition (95) guarantees that we recover the continuity equation when taking \( \rho^{k+1} - \rho^k \).

The final term needed to explicitly apply the discrete Lie–Poisson Hamilton–Jacobi theory is the representation of the Lie group action on the dual of the Lie algebra.

### Definition 4.10.
Consider \( g_j(s) \in \Psi G_d \) on \( \text{Dens}^*(Q) \), the discrete version of the map \((\zeta')^* : g_{\text{INT}}(Q) \rightarrow \text{Dens}^*(Q) \) defined by
\[ (\zeta')^* \rho = \rho^k D_x f, \]  

(96)

for all \( f \in \text{Dens}(Q) \).

### Proposition 4.11.
The Hamiltonian system (75), written in the Lie–Poisson Hamilton–Jacobi form (79), is solved numerically by
\[ S_L = S_0 + \Delta t H \left( TL^*_A d_A S_0, d_\rho S_0 \right) \]  

(97)
\[ (\mu^k, \rho^k) = \left( \xi + u_j \xi^{-1} + D_x u_j \xi^{-2} + (\Delta t) \frac{\delta H}{\delta A} \xi + (\Delta t) u_j \frac{\delta H}{\delta A} \xi^{-1} \right. \]  
\[ \left. + (\Delta t) \frac{\delta H}{\delta A} D_x u_j \xi^{-2}, \rho_k - (\Delta t) D_x (\rho_{k,j} u_j) + (\Delta t) \frac{\delta H}{\delta \rho} \right), \]  

(98)
\[ (\mu^{k+1}, \rho^{k+1}) = \left( \xi + u_j \xi^{-1} + (\Delta t) \frac{\delta H}{\delta A} \xi + (\Delta t) u_j \frac{\delta H}{\delta A} \xi^{-1} - 2(\Delta t) u_j D_x \frac{\delta H}{\delta A} \xi^{-2} \right. \]  
\[ \left. + 3(\Delta t) u_j \Delta^2_x \frac{\delta H}{\delta A} \xi^{-3} + \rho_{k+1,j} D_x f, \rho + (\Delta t) \frac{\delta H}{\delta \rho} \right), \]  

(99)

with the initial condition \( S_0 = \text{res}(A) + \| \rho \|^2 \).

One thing that needs to be pointed out, that this formulation introduces a number of open problems regarding the inputs and target data. The use of probability density functions eliminates the role of inputs and targets and requires us to find suitable initial and final joint distributions in order to incorporate the training set in learning. Nevertheless, one application which does not require picking suitable joint distributions is normalizing flow \[90\]. In statistical inference, one requires to sample random data from various distributions and sometimes such distributions are complicated, thus renders standard techniques inefficient. In [90], it was proposed invertible maps, implemented using neural networks, to be applied successively as a way of mapping the target distribution to a simpler one, such as the normal Gaussian distribution. Once that is finished, sampling from the target distribution is done by simply sampling from the simple distribution and then map the sample points using the learned transformation to points that belong to the target distribution. The formulation of presented here lends itself to such application. Indeed, in [32], a stochastic ResNet whose parameters satisfy (77) was used to learn four different non-Gaussian distributions and the results are shown in figure 5. Although, the numerical scheme used in [32] uses a class of structure-preserving integrators known as multisymplectic variational integrators.
Figure 5: This numerical experiment is reproduction of the result in [90]. A stochastic ResNet is used for a normalizing flow example. The idea is to find network parameters which would map a normal Gaussian distribution to a target distribution, that is not necessarily Gaussian. Each row is a separate distribution and the left most column is the target distribution. The other columns are snapshots of the progression a normal distribution through the layers of the stochastic ResNet. A mean-field control is used to solve the stochastic optimal control problem used to train the network and the parameters evolve according to (77). A multisymplectic numerical scheme for deep learning that solves (77), presented in [32], was used to obtain this reproduction.

5 Connection to Integrable Partial Differential Equations

In many cases, substituting the optimality condition $\partial_u H = 0$ into the Pontryagin’s Hamiltonian yields, an integrable system [50,51]. This line of investigation is interesting for deep learning, as it can be beneficial for studying various behaviours. Apart from knowing the solution of the integrable systems, they do posses interesting properties, such as the bi-Hamiltonian structure. The existence of such structure means that the problem has another Hamiltonian function and according to Magri’s lemma [71], we can construct an infinite number of conservation laws by simply knowing the two Poisson structures.

Here, we use Lie–Poisson formulation to show that deep learning training, with certain conditions on the neural network’s parameters, is equivalent to solving the nonlinear Schrödinger equation. One very interesting fact regarding the Hamilton–Jacobi equation is that it works as a bridge from classical to quantum mechanics [36]. This is done by writing the generating function in terms of the wave function, $\psi$, i.e.

$$\lambda(x, t) = \frac{1}{k} \log \psi(x, t),$$  \hspace{1cm} (100)$$

and substituting it into the Hamilton–Jacobi equation and the result is the Schrödinger equation. For the system of equations (60), (61) and (62), instead of (100), the following
wave function is used

\[ \psi = \sqrt{\rho(x,t)} e^{i\lambda(x,t)} \]  

(101)

where \( \rho \) satisfy (61) and \( \lambda \) satisfy (62), and this transformation is called Madelung transformation and it casts the nonlinear Schrödinger equation as the quantum Euler equation [70]. This transformation has gained attention in recent years [31, 54, 55] as it defines a symplectic transformation from the Hilbert space of complex-valued wave functions \( H^\infty(\mathbb{R}^n, \mathbb{C}) \) to the dual of semidirect product Lie algebra \( \mathfrak{X}^*(\mathbb{R}^n) \times H^\infty(\mathbb{R}^n) \).

**Theorem 5.1.** Consider the family of Schrödinger equations

\[ i\hbar \partial_t \psi + \frac{\hbar^2}{2m} \Delta \psi + f(|\psi|^2) \psi, \]  

(102)

where \( \hbar \) is the Planck’s constant, \( m \) is the mass and \( f : \mathbb{R}_{>0} \to \mathbb{R} \) and whose Hamiltonian on the Hilbert space for complex-valued wave functions \( H_{NLS} : H^\infty(Q, \mathbb{C}) \to \mathbb{R} \) is given by

\[ H(\psi) = \frac{\hbar}{2m} \|\nabla \psi\|^2 + \int_Q F(|\psi|^2) \, dx. \]  

(103)

With \( f = 0 \), it is equivalent to the training of deep residual neural networks

\[ J(\theta) = \int_0^T \ell_d(q(t), \theta(t)) \, dt + \sum_{i=0}^N L(\pi((q(T)^{(i)}), c^{(i)}), \]  

(104)

constrained to

\[ d_t q^{(i)}(t) = \theta(t) \circ q^{(i)}(t) \, dt + \nu dW_t, \quad q^{(i)}(0) = q_0^{(i)}, \quad \pi(q^{(i)}(T)) = c^{(i)}, \]  

(105)

with \( i = 1, \ldots, N \), where \( (q_0^{(i)}, c^{(i)}) \) form the dataset used in supervised training. The main assumption imposed here is that

\[ \text{div}(\theta) - \frac{\nu^2}{2} \text{div}(\nabla \log(\rho)) = 0 \]  

(106)

**Proof.** The direct equivalence between the two problems is not direct, so the first step of the proof is to cast the training problem as a mean–field games problem. Instead of controlling (113), the probability density function is controlled. The dynamical constraint for the probability density function is the Fokker–Planck equation

\[ \partial_t \rho + \text{div}(\rho \sigma(x, \theta)) - \frac{\nu^2}{2} \Delta \rho = 0, \]  

(107)

with \( \rho(x,0) = \rho_0 \) and \( \rho(x,T) = \rho_T \). Before solving the optimal control problem for the probability density, as mentioned in section 3.2, a change of variable is performed. The network parameters are decomposed into

\[ \theta(x,t) = \omega(x,t) + \frac{\nu^2}{2} \nabla \log \rho, \]  

(108)
and substituting it into (107), we obtain the continuity equation
\[ \partial_t \rho + \text{div} (\rho \omega(x,t)) = 0. \] (109)

The Pontryagin’s Hamiltonian then becomes
\[ H(\rho, \lambda) = \frac{1}{2} \int_Q \rho \|\omega\|^2 \text{dVol}(x) + \frac{\nu^2}{2} \int_Q \rho \langle \omega, \nabla \log(\rho) \rangle \text{dVol}(x) + \frac{\nu^4}{8} \int_Q \rho \|\nabla \log(\rho)\|^2 \text{dVol}(x) \]

From the assumption (106) we have the condition that \( \text{div} \omega = 0 \) as a result, the Hamiltonian further simplifies to
\[ H(\rho, \lambda) = \frac{1}{2} \int_Q \rho \|\omega\|^2 \text{dVol}(x) + \frac{\nu^4}{8} \int_Q \rho \|\nabla \log(\rho)\|^2 \text{dVol}(x). \] (110)

The Hamiltonian function (110) is obtained by substituting the Madelung transformation (101), which is a mapping from \( H^\infty(Q, \mathbb{C}) \) to \( X^*(Q) \times \text{Dens}(Q) \), into the Hamiltonian, \( H_{\text{NLS}} \), for the Schrödinger equation (102), we have
\[ H(\lambda, \rho) = \frac{\hbar}{2m} \left( \frac{\nabla \rho}{\sqrt{\rho}} e^{i\frac{\lambda}{\hbar}} + i \frac{\sqrt{\rho}}{\sqrt{\hbar}} \nabla \lambda \sqrt{\rho} e^{i\frac{\lambda}{\hbar}} \right) \]
\[ = \frac{\hbar}{8} \frac{\|\nabla \rho\|^2}{\rho} + \frac{1}{2} \rho \|\nabla \lambda\|^2 \] (111)

if \( \hbar = \nu^4 \) and using (60), i.e. \( \nabla \lambda = \omega \), we obtain the Hamiltonian (110). \( \square \)

**Corollary 5.2.** Consider the deep neural network training problem
\[ J(\theta) = \int_0^T \ell(q(t), \theta(t)) \, dt + \sum_{i=0}^N L(\pi((q(T)^{(i)}) \cdot c(i)), \] (112)

constrained to the ensemble of stochastic differential equations
\[ dq^{(i)}(t) = \theta(t) \circ q^{(i)}(t) \, dt + \nu dW_t, \quad q^{(i)}(0) = q_0^{(i)}, \quad \pi(q^{(i)}(T)) = c(i), \] (113)
and the pair of initial and final conditions are the training dataset \((q_0^{(i)}, c(i))\), where \( i = 1, \ldots, N \). The stochastic control problem is equivalent to the Lie–Poisson system with Hamiltonian \( H : \Psi DS(\mathbb{C})^* \to \mathbb{R} \) given by
\[ H(L) = \frac{i}{3} \text{Tr}(L^3), \] (114)

where \( L \in \Psi DS(\mathbb{C})^* \) is defined as
\[ L = \partial_x + \psi \partial_x^{-1} \psi^*. \] (115)

With the Hamiltonian defined on \( \Psi DS(\mathbb{C})^* \), the dual algebra of complex-valued pseudodifferential symbols, we can simply apply theorem 3.1.

The nonlinear Schrödinger equation is not only integrable equation that arises from deep learning, in fact, when equation (77), when \( \nu \to 0 \), and the network’s parameters regularising norm \( \ell \) is chosen as \( H^1 \) Sobolev norm, the equation becomes
\[ \partial_t m = \pm \text{ad}_u^* m, \]
\[ m = u - \alpha \partial_x^2 u \]
or when expressed in coordinates on $\mathbb{R}^N$, it becomes
\[\partial_t m_i + \partial_x \left( m_i u^j \right) + \left( m_j \right) \partial_x u^j = 0 \]
and it is the dispersionless Camassa–Holm equation [18] and it is an example of a Lie–Poisson system. An interesting property of this partial differential equation is that its weak solution is also a Hamiltonian system
\[H(q, p, t) = \sum_{i=0, k=0}^{N_b N_b} p^{(i)} p^{(k)} e^{-\frac{1}{2} \|q^{(i)} - q^{(k)}\|^2} \]
(117)

The physics that are described by this Hamiltonian is an approximation to the N-particle solution, or peakon train, of Euler–Poincaré equation with $H^1$ Sobolev norm [60, 81]. What is meant by the peakon or peaked soliton is the a type of soliton, but with a discontinuity or a cusp at the crest of the wave. For the actual peakon train, the Gaussian in the Hamiltonian (117), is replaced by Green’s function $G(x, y) = e^{-|x-y|}$ for shifted Poisson differential operator $I_d - \partial^2_x$.

Further, the Hamilton’s equation for the peakon train do have a Lax pair, and it is an example of an integrable system.

\[\frac{d}{dt}L = [L, P], \]
(118)

where $L$ an $N \times N$ matrix, known as Lax matrix, with entries $L_{i,j} = \sqrt{p^{(i)} p^{(k)}} e^{-|q^{(i)} - q^{(k)}|}$ and $P$ is also an $N \times N$ matrix and its entries are $P_{i,j} = -2 \sqrt{p^{(i)} p^{(k)}} \text{sign}(q^{(i)} - q^{(k)}) e^{-|q^{(i)} - q^{(k)}|}$. One advantage of knowing the Lax matrix is that taking trace of its power, i.e. $\text{Tr}(L^k)$ for $k = 2, \ldots, N$, results in the constant of motion [18].

6 Conclusion & Future Direction

We have introduced, in this paper, an equivalent formulation of deep learning as a hydrodynamics system. This made possible by substituting the deep neural network by an ordinary differential equation and formulating the training of deep learning as an optimal control problem as it is equivalent to solving a Hamiltonian system. First, it was the use of mean–field type control for the stochastic optimal control problem and that approach allows for the application of Pontryagin’s Maximum Principle. The Hamilton’s equations that are the optimality condition for deep learning, in this case, are partial differential equations, and instead of using them directly, we have used an equivalent system of equations that is similar to quantum fluid equation. Here we have demonstrated that this optimality condition is a Lie–Poisson system. Interestingly, the Poisson structure for deep learning coincides with the Poisson structure for the ideal compressible fluid.

What is interesting about the Lie–Poisson formulation is that it links deep learning with equations from fluid dynamics, in some specific cases, to the nonlinear Schrödinger equation. Such connection have not been well studied, and it is a future research direction as the nonlinear Schrödinger equation, in one-dimension at least, has a hierarchy of

31
integrable equations. Potentially, this could help deriving conserved quantities for deep learning. The importance of conserved quantities is they allow us to better analyse the performance of the system and construct Lyapunov functions for studying the stability of the system; this approach forms the basis of Arnold’s method for stability.

Despite the fact Lie–Poisson systems are Hamiltonian and with a Poisson structure, it is challenging to solve numerically and for this structure–preserving integrators are required. One type of structure–preserving integrators we have explored in this paper is integrators based on the Hamilton–Jacobi theory and its symmetry reduced version the Lie–Poisson Hamilton–Jacobi theory. The main reason for this choice is it can be used for both Hamiltonian systems on symplectic cotangent bundles and Poisson manifolds. Moreover, one of the advantages of this approach is that can be easily be made high-order without the need to impose additional constraints to enforce the conservation of the symplectic structure. This forms the basis of a training algorithm, and we have shown the algorithm behaves such similar methods using Euler method and 4th order Runge–Kutta method.

The application is not straightforward and as a result there has been a number of modifications are needed. On top of that, the underlying dynamics are defined on infinite dimensional semidirect product space. For that reason, we have extended the Lie–Poisson Hamilton–Jacobi theory to accommodate semidirect product space and we have also formulated the hydrodynamics problem on the group of pseudodifferential symbols. The last step is required as it allows us to apply Lie–Poisson Hamilton–Jacobi theory directly to the quantum fluid equation for deep learning and derive structure–preserving numerical schemes.

**Stability of Deep Learning:** As mentioned, the Arnold’s method of stability can be applied to the nonlinear Schrödinger equation as a surrogate way to study the stability of deep learning, however, other methods that reply on the geometry of the problem can be used. One of such methods is the energy–Casimir method of [5,45], where it is used to study the nonlinear stability of Lie–Poisson systems’ relative equilibria and it is applied to various ideal compressible fluid and even plasma physics. The notion of nonlinear stability for a trajectory \((M(t),\rho(t)) \in \mathfrak{s}^*\) is that there exists \(\epsilon > 0\) such that \(\| (M_0,\rho_0) \| < \epsilon\), then \(\| ((M(t) - M_0,\rho(t) - \rho_0)) \| < \delta\) for all of \(t\), where \(\delta > 0\). In other words, the trajectory, whose initial condition belongs to a specific set, would remain close to the set of initial values. The main ingredient is the Casimir function, which is a map \(C : \mathfrak{s}^* \rightarrow \mathbb{R}\) such that it is the centre of the Lie algebra meaning for every function \(F : \mathfrak{s}^* \rightarrow \mathbb{R}\), the Lie–Poisson bracket is equal to zero, i.e. \(\{C,F\} = 0\). The Hamiltonian is then augmented with the Casimir function to form a new Hamiltonian \(H_C = H + \Phi(C)\) and first variation of the Hamiltonian is evaluated at the equilibrium and then equated to zero. From there we find the function \(\Phi\). The next step is to determine the convexity of the second variation of the Hamiltonian \(H_C\). Once all criteria are met, one can determine the nonlinear stability of the system.

The major challenge with the energy–Casimir method is that it requires a knowledge of the Casimir function, and this motivated the development of energy–momentum method of [95]. Instead, the augmented Hamiltonian is \(H_\xi = H + \langle J,\xi \rangle\), where \(J : T^*Q \rightarrow \mathfrak{s}^*\) and \(\xi \in \mathfrak{s}\). The Lie algebra element \(\xi\) plays the role of the vector field associated with the relative equilibria and it renders the first variation \(\delta H_\xi = 0\).
as energy–Casimir method, the definiteness of $\delta^2 H_\xi$ indicates the stability of the system.

Another route for studying stability of Hamiltonian systems is to find the action-angle variables, denoted by $(I_1, \ldots, I_n, \theta_1, \ldots, \theta_n)$ In this coordinate system, the Hamiltonian $H$ depends only on the actions $I_1, \ldots, I_n$ and the result of that is the configuration manifold is an $n$-torus $\mathbb{T}^n$. These variables are needed in order to study the perturbation of the Hamiltonian and we can assess the stability by KAM theory [6,59,83]. That said, KAM theory works on integrable systems and, at this point it is yet to be investigates, it is not known whether or not the deep learning system is integrable or not. What we know is that for a specific case, we can the Hamiltonian obtained from Pontryagin’s Maximum Principle is integrable, which leads us to the next possible research direction.

**Generating Function For Optimal Control:** The issue with using structure-preserving integrators and gradient methods is that they require an initial guess for the costate and control parameters. Such guesses can affect the behaviour of the Hamiltonian system and convergence in general and in addition, iterative schemes for such problems can be time consuming and computationally taxing. A different approach that is related to dynamic programming was proposed in [37] and further investigated in [38,39,86,92]. The key ingredient is to compute the generating function for symplectomorphism that maps between the initial and final conditions. This further makes it possible to find the solution of the costate in terms of training dataset, thus sidestepping the need to guess the initial/final condition for the costate. Such research direction is worth investigating for training of deep neural networks.

The idea is to treat initial and terminal conditions, $q(0) = q_0 \in Q$ and $q(T) = q_T \in Q$ respectively, as old and new coordinates, $(q_0, p_0)$ and $(q_T, p_T)$. To see how generating functions and optimal transport are related, we start by looking at dynamic programming approach to optimal control. Given the cost functional

$$S(q) = \int_0^T \ell(\theta) dt + \Phi(q(T), q_T),$$

we define the **value function** as

$$V(q(t), t) = \min_{\theta} \left\{ V(q(t + dt), t + dt) + \int_t^{t+dt} \ell(\theta) dt \right\},$$

and it satisfies the **Hamilton–Jacobi–Bellman equation**, which can be regarded as a generalisation of the Hamilton–Jacobi equation. As shown in (Park), the value function is

$$V(q(t), t) = -S(q(t), q_T, t) + \Phi(q(T), q_T)$$

which mean that it can be obtained by solving the Hamilton–Jacobi equation for $S$. That said, one small technical issue: it is not practical to use $S$ directly and that is because at $t = 0$ it is hard to find initial conditions that satisfy the identity transformation. For this reason, we use type-II generating function $S_2$, or type-III generating function $S_3$ instead. Once $V$ is known, the parameters that would train the network are then given by

$$\theta = \arg \max_{\theta^*} \left( H \left( q, \frac{\partial V}{\partial q}, \theta^*, t \right) \right)$$
That said, finding a solution for the generating function is challenging on its own right, however, in [37] it was shown that it can be solved using power series expansion of generating function whose coefficients are obtained by solving a system of ordinary differential equations. The derivation of the system of ordinary differential equations is done by applying the Taylor expansion to the Hamiltonian and the generating function. Once that is done, both expansions are substituted into the Hamilton–Jacobi equation and as a result we obtain a power series whose coefficients are differential equations. Setting the coefficients of the combined series to be equal to zero, we obtain the system of equations whose solution is the coefficients of the generating function $S$.

The $N$ terms Taylor expansion of the Hamiltonian, around the null point of $T^*Q$, is given by

$$
\tilde{H}(q,p,t) = \sum_{i_{q_1}=0}^{N} \cdots \sum_{i_{q_n}=0}^{N} \frac{(q_1)^{i_{q_1}} \cdots (q_n)^{i_{q_n}} (p_1)^{i_{p_1}} \cdots (p_n)^{i_{p_n}}}{i_{q_1}! \cdots i_{p_1}!} \left( \frac{\partial^{i_{q_1}+\cdots+i_{p_n}}}{\partial q_1^{i_{q_1}} \cdots \partial p_n^{i_{p_n}}} H \right)(0, \ldots, 0, t),
$$

likewise, the generating function, is written as a polynomial with $N$ terms,

$$
F(q,P,t) = \sum_{i_{q_1}=0}^{N} \cdots \sum_{i_{q_n}=0}^{N} \frac{(q_1)^{i_{q_1}} \cdots (q_n)^{i_{q_n}} (p_1)^{i_{p_1}} \cdots (p_n)^{i_{p_n}}}{i_{q_1}! \cdots i_{p_1}!} F_{i_{q_1},\ldots,i_{p_n}}(t),
$$

where $F_{i_{q_1},\ldots,i_{p_n}}(t) \in C(Q)$ are the coefficients of polynomial $F$ and they are differentiable functions on $Q$. Substituting the expansions $F(q,P,t)$ and $\tilde{H}(q,p,t)$ into the Hamilton–Jacobi equation, we obtain a system of differential equations for the coefficients of $F(q,P,t)$. Once the solution is obtained, that yields the generating function $F(q,P,t)$, which is then used to obtain (121), which in turn allows us to obtain the weights of the network (122).

This formulation is in the continuous-time space and for large systems, it is practical to use discrete time formulation. Mirroring the approach in the previous section, a discrete version of the generating function approach for solving two-boundary point problems could be beneficial. The Hamilton–Jacobi equation becomes a discrete one and it was introduced in [85]. Given the set of discrete points of the generating function $\{S^k\}_{k=1}^N$ which satisfy the discrete Hamilton–Jacobi equation

$$
S^{k+1}(q_{k+1}) = S^k(q_{k+1}) + D_2 S^{k+1}(q_{k+1}) \cdot q_{k+1} + H^+_d(q_k,D_2 S^{k+1}(q_{k+1})),
$$

with the symplectic mapping $(q_k,p_k) \to (q_{k+1},p_{k+1})$ defined by

$$
q_{k+1} = q_k + D_1 S^{k+1}(q_{k+1}),
$$

$$
p_{k+1} = p_k - D_2 S^{k+1}(q_{k+1}).
$$

Once $\{S^k\}_{k=1}^N$ are obtained, we can then use (121) to obtain $V$ and from it $\theta$ of (122).

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