Symplectic integration of learned Hamiltonian systems

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Question

How to predict motions and phase portraits of Hamiltonian systems based on discrete trajectory observations?

Message of this poster

Do *not* learn the flow map directly. Do *not* learn the exact Hamiltonian and integrate the learned system. Instead, learn a modified structure adapted to your favourite geometric integrator.

Background

Hamiltonian system. A Hamiltonian system on the phase space $M = \mathbb{R}^{2n}$ is a differential equation of the form

$$\dot z = J^{-1}\nabla H(z), \quad J = \begin{pmatrix} 0 & -I_n \\ I_n & 0 \end{pmatrix}, \tag{1}$$

where $H\colon M \to \mathbb{R}$ and I_n is an n-dimensional identity matrix. Hamiltonian systems arise in classical mechanics, plasma physics, electrodynamics, sampling problems (Hamiltonian Monte Carlo methods) and many other applications. Trajectories of Hamiltonian systems conserve H (energy) and the dynamical system has no attractors.

Symplectic transformations. The flow map $\phi_t\colon M \to M$ to a Hamiltonian system is *symplectic*, i.e. it fulfils

$$\phi_t'(z)^\top J \phi_t'(z) = J \qquad \forall z \in M, \tag{2}$$

where $\phi_t'(z)$ denotes the Jacobian matrix of ϕ_t at z. Symplecticticity of the flow is related to further qualitative properties of the system such as volume preservation and a favourable interaction with symmetries (Noether's theorem).

Geometric Integrator / Symplectic Integrator. A discretisation scheme for Hamilton's equations such that the numerical flow is a symplectic transformation is called *Geometric Integrator* or *Symplectic Integrator*. Example: *Symplectic Euler scheme:*

$$\begin{pmatrix} q_n \\ p_n \end{pmatrix} = \begin{pmatrix} q_{n-1} \\ p_{n-1} \end{pmatrix} + hJ^{-1}\nabla H((q_n, p_{n-1})). \tag{3}$$

Here h is the timestep. The numerical flow $\psi_h(q_{n-1}, p_{n-1}) = (q_n, p_n)$ is a symplectic transformation.

(Inverse) modified Hamiltonian. The numerical flow map ψ_h of a symplectic integrator preserves a *modified Hamiltonian* $\widetilde{H}$ (up to exponentially small errors in h). The *inverse modified Hamiltonian* $\overline{H}$ is a Hamiltonian such that an application of a symplectic integrator to $\dot z = J^{-1}\nabla \overline{H}(z)$ yields the exact flow map ϕ_h (in the sense of formal power series [6]).

$$\begin{tikzcd}
\dot z = J^{-1}\nabla \overline{H}(z) \arrow[r, "\text{BEA}"] \arrow[dr, "\text{Integrator}"'] & \dot z = J^{-1}\nabla H(z) \arrow[d, "\text{exact flow}"] \arrow[r, "\text{BEA}"] \arrow[dr, "\text{Integrator}"'] & \dot z = J^{-1}\nabla \widetilde{H}(z) \arrow[d, "\text{exact flow}"] \\
& z_n = \phi_h(z_{n-1}) & z_n = \psi_h(z_{n-1})
\end{tikzcd}$$

What is Symplectic Shadow Integration?

Problem

Predict the motion of a dynamical system of the form (1). The Hamiltonian H and the Hamiltonian vector field $J^{-1}\nabla H$ are not explicitly known and the prediction must be made based on data consisting of discrete trajectory observations.

Procedure of Symplectic Shadow Integration.

1. *Preparation.* Chose a symplectic integrator and a step size h compatible with the trajectory data.
2. *Inverse system identification.* Learn the inverse modified Hamiltonian $\overline{H}$ from trajectory data.
3. *Integration.* Apply the symplectic integrator to the inverse modified Hamiltonian system $\dot z = J^{-1}\nabla \overline{H}(z)$ to obtain a flow map.
4. *System identification (Bonus).* Compute H from $\overline{H}$.

Advantages of Symplectic Shadow Integration

Strategy 1: Learn the flow map directly.

One could use established learning techniques, such as artificial neural networks or Gaussian processes, to learn the flow map of the system directly. However, Symplectic Shadow Integration has the following advantages over this approach.

- The Hamiltonian structure can be incorporated into the learned system. This guarantees important qualitative aspects of the prediction such as energy conservation, preservation of phase space volume and topological properties of the phase portrait.
- Further conservation laws, such as (angular) momentum conservation, can be incorporated via a combination with symmetric learning, for instance using symmetric kernels in case of Gaussian processes [5]. The conservation laws are then guaranteed by a discrete Noether theorem (future work).
- Only a real valued map $\overline{H}$ needs to be learned rather than the flow map, reducing the dimension of the learning problem and data requirements.
- Hamiltonian structure is identified during the process. It provides physical insight into the dynamics and can be used for verification.

Strategy 2: Learn the exact Hamiltonian and then use a symplectic integrator.

Techniques have been developed to learn Hamiltonians from data [1]. Symplectic Shadow Integration has the following advantages over learning the exact Hamiltonian H and applying a symplectic integrator to (1).

- The numerical integrator introduces a discretisation error. The discretisation error is in addition to uncertainty in the Hamiltonian due to limited training data and is *not* inevitable.
- Step-size selection is decoupled from accuracy requirements. This is beneficial if the learned Hamiltonian and its gradient are expansive to evaluate.
- Symplectic Shadow Integration uses the trajectory data directly. There is no need to approximate data of the underlying vector field.

Example

The Henon–Heils system is a Hamiltonian system on $M = \mathbb{R}^2 \times \mathbb{R}^2$ with

$$H(q,p) = \frac{1}{2}\|p\|^2 + V(q), \quad V(q) = \frac{1}{2}\|q\|^2 + \mu\left(q_1^2 q_2 - \frac{q_2^3}{3}\right).$$

The system has bounded as well as unbounded motions. Preserving the energy level of a trajectory under discretisation of (1) makes sure that numerical trajectories cannot escape if its initialisation point lies on a bounded energy level set. We set $\mu = 0.8$. We obtain training data by integrating (1) to high accuracy. Now we follow the steps outlined in **Procedure of Symplectic Shadow Integration.**

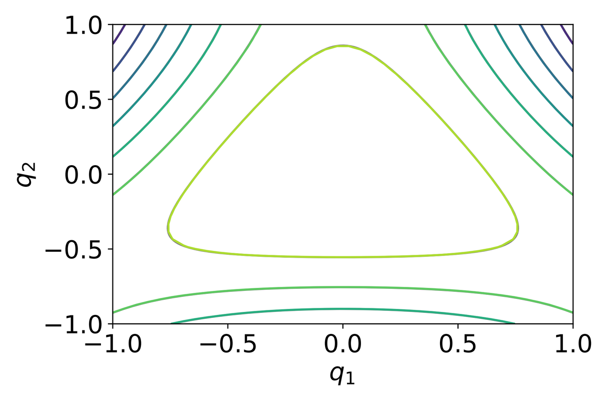

Figure 1: The level sets of the exact potential V and the level sets of the potential recovered from the learned data using Symplectic Shadow Integration are not visually distinguishable.

1. *Preparation.* We chose the Symplectic Euler method (3) with step size $h = 0.1$.
2. *Inverse system identification.* We use Gaussian Process regression with radial basis functions to model $\overline{H}$. We use the Symplectic Euler scheme

$$\begin{pmatrix} q_n \\ p_n \end{pmatrix} = \begin{pmatrix} q_{n-1} \\ p_{n-1} \end{pmatrix} + hJ^{-1}\nabla \overline{H}((q_n, p_{n-1})) \tag{4}$$

to obtain data on the gradient $\nabla \overline{H}$. (There is *no* approximation involved in this step. Equation (4) is exactly fulfilled[1] by the inverse modified Hamiltonian.)

3. *Integration.* We apply the Symplectic Euler method to $\dot z = J^{-1}\nabla \overline{H}$ with step size $h = 0.1$. This is compared to predictions from strategy 1, to learn the flow map directly, and strategy 2, to learn the exact system and apply a symplectic integrator[2] in Figure 2 and 3.
4. *System identification.* We apply the (classical) backward error analysis formula for the Symplectic Euler Scheme [2] to $\overline{H}$

$$\widetilde{\overline{H}} = \overline{H} + \frac{h}{2}\overline{H}_q^\top \overline{H}_p + \frac{h^2}{12}\left(\overline{H}_q^\top \overline{H}_{pp}\overline{H}_q + \overline{H}_p^\top \overline{H}_{qq}\overline{H}_p + 4(\overline{H}_p^\top \overline{H}_{qp}\overline{H}_q)\right) + \dots \tag{5}$$

and use a truncation of $\widetilde{\overline{H}}$ after second order terms as an approximation to H. Figure 1 shows that level sets of the recovered potential and the exact potential are indistinguishable.

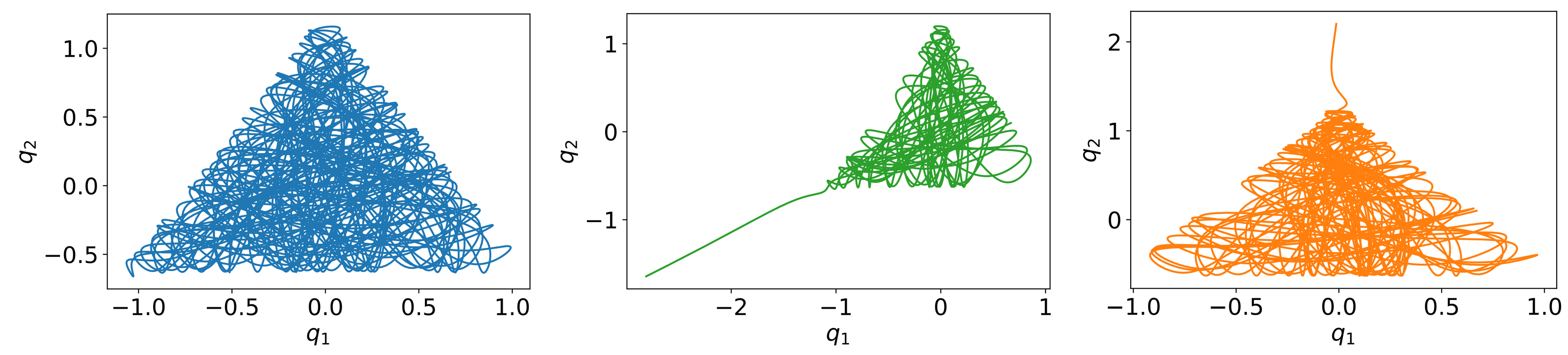

Figure 2: Left: The long term behaviour of a motion is correctly captured by the Symplectic Shadow Integrator. Motions computed using strategy 1 (centre) and 2 (right) incorrectly leave the energy level leading to desastrous errors.

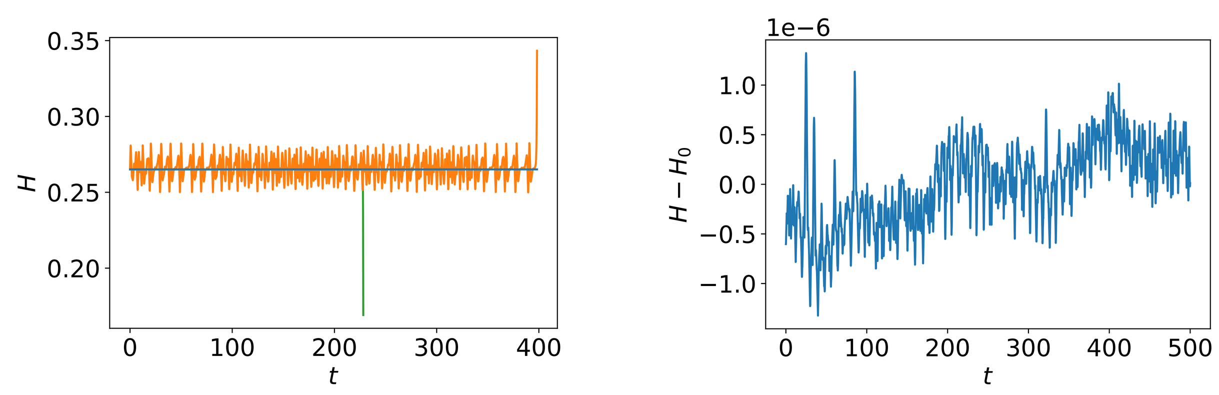

Figure 3: Energy is preserved to high accuracy by the symplectic shadow integration (blue) in comparition with strategy 1 (green) and strategy 2 (orange).

Further remarks

The procedure of Symplectic Shadow Integration is a framework which can be used in combination with several learning techniques and with different symplectic integrators. More details, experiments, and verifications can be found in the corresponding preprint [3]. See [4] for source code.

Conclusion

Symplectic Shadow Integration provides a way to learn the flow map of a Hamiltonian system from trajectory observations. Prior knowledge of the presence of Hamiltonian structure is incorporated, which greatly improves the learned flow map compared with learning the flow map directly. The flow map is symplectic and has excellent energy conservation properties. The technique relies on learning an inverse modified Hamiltonian, which is then integrated using a geometric integrator. Compared with integrating a learned approximation to the exact Hamiltonian system, discretisation errors are eliminated.

References

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[6] Aiqing Zhu, Pengzhan Jin, and Yifa Tang. Inverse modified differential equations for discovery of dynamics, 2020. arXiv:2009.01058.

[1] in the sense of formal power series – optimal truncation results are available in the setting of regular backward error analysis [2]

[2] In the experiment we compare Symplectic Shadow Integration to an application of the Symplectic Euler method to the exact system with the same step size h as the Symplectic Shadow Integrator. This corresponds to strategy 2 in the infinite data limit.