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Symplectic Gaussian process regression of maps in Hamiltonian systems

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Discrete representations of Hamiltonian systems require structure-preserving properties in order to preserve invariants of motion and orbit topology in phase space. Here, we investigate mapping techniques that rely on given orbit data over a period of time. In contrast to (geometric) numerical integration, the mapping time step is not necessarily required to be small compared to the periods of motion of the system. It is even possible to construct the map between Poincaré sections of interest. We use multi-output Gaussian process regression with derivative observations of the generating function of a canonical transformation and enforce the symplectic property via the choice of the matrix-valued covariance function. The approach supports unstructured orbit data on irregular domains without the explicit knowledge of the Hamiltonian. Once the map is constructed, it is used to compute evolving system states over long periods of time and can thus be used to construct fast emulators for numerical orbit tracers. The method is tested on the pendulum and the standard map where the correct reproduction of chaotic diffusion is shown. In addition, the Jacobian is directly available from the emulator model and can be used to calculate local Lyapunov exponents that give insight into the local predictability of the dynamical system. Combined with a Bayesian classifier, the structure-preserving GP model can be used for early classification of chaotic versus regular trajectories.