Variational Langevin Integrators

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Abstract: This poster summarizes a collaborative paper with Houman Owhadi that analyzes a new class of structure-preserving Langevin integrators obtained from a Lie-Trotter splitting of the Langevin equations into Hamilton's and Ornstein-Uhlenbeck equations. A variational integrator is used to solve Hamilton's equations and an exact solution is used for Ornstein-Uhlenbeck equations. The composite map is first-order and preserves structure of Langevin equations.

Structure of Langevin Equations

Here are Langevin equations

$$\begin{cases} dq &= \frac{\partial H}{\partial p} dt, \\ dp &= -\frac{\partial H}{\partial q} dt - c\mathbf{C}\frac{\partial H}{\partial p} dt + \sigma \mathbf{C}^{1/2} dW. \end{cases}$$

The stochastic process (q_t, p_t) is ergodic with respect to the Boltzmann-Gibbs (BG) measure. Moreover, we assume it's rate of convergence to equilibrium is geometric.

Roughly, a sufficient condition for geometric ergodicity is definiteness of C and certain regularity on the Hamiltonian.

Lie-Trotter Splitting

Hamilton's equations

$$\begin{cases} dq &= \frac{\partial H}{\partial p} dt \\ dp &= -\frac{\partial H}{\partial q} dt \end{cases}$$

Ornstein-Uhlenbeck equations

$$\begin{cases} dq &= 0 \\ dp &= -c\mathbf{C}\frac{\partial H}{\partial p} dt + \sigma \mathbf{C}^{1/2} dW \end{cases}$$

This splitting is quite natural, but seems to have been only recently introduced in the literature.

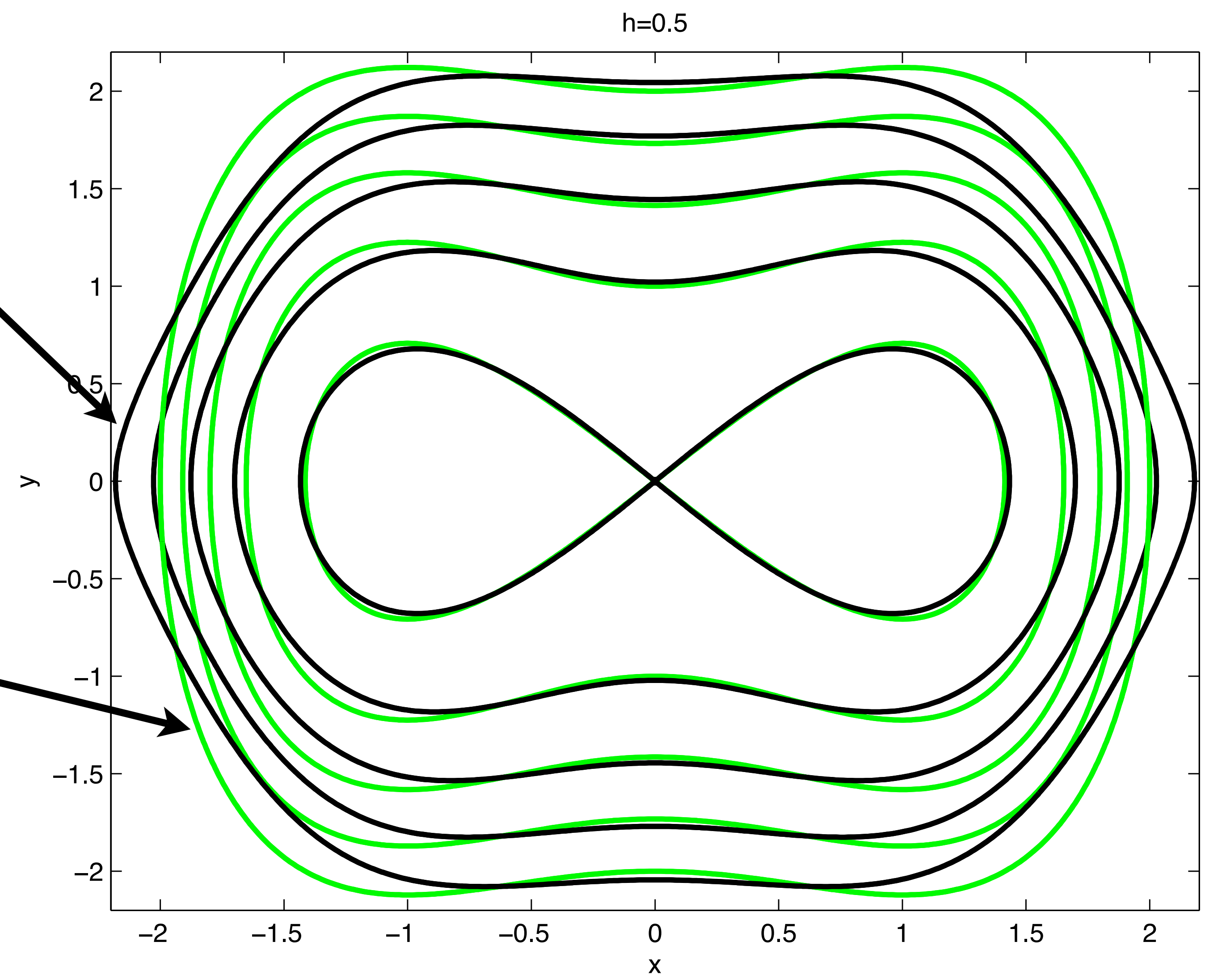
Variational Integrator

We use a variational integrator for Hamilton's equations.

One can show numerical orbits are very nearly interpolated by a global, autonomous Lagrangian system.

Exact Orbits of Cubic Oscillator

Orbits of Nearby Interpolating Lagrangian



Ornstein-Uhlenbeck Integrator

Ornstein-Uhlenbeck equations are linear SDEs

$$\begin{aligned} dp(t) &= -c\mathbf{C}\mathbf{M}^{-1}p(t)dt + \sigma\mathbf{C}^{1/2}dW(t) \\ p(0) &= p, \end{aligned}$$

With solution

$$p(t) = \exp(-c\mathbf{C}\mathbf{M}^{-1}t)p + \sigma\int_0^t \exp(-c\mathbf{C}\mathbf{M}^{-1}(t-s))\mathbf{C}^{1/2}dW(s).$$

Defines map that exactly preserves BG measure

$$\psi_h : (q,p) \mapsto (q, p(h)).$$

Stochastic Variational Integrator

$\theta_h : T^*Q \to T^*Q$
approximates

$$\begin{cases} dq &= \frac{\partial H}{\partial p} dt \\ dp &= -\frac{\partial H}{\partial q} dt \end{cases}$$

$\psi_h : T^*Q \to T^*Q$
approximates

$$\begin{cases} dq &= 0 \\ dp &= -c\mathbf{C}\frac{\partial H}{\partial p} dt + \sigma \mathbf{C}^{1/2} dW \end{cases}$$

$\phi_h = \theta_h \circ \psi_h$
approximates

$$\begin{cases} dq &= \frac{\partial H}{\partial p} dt, \\ dp &= -\frac{\partial H}{\partial q} dt - c\mathbf{C}\frac{\partial H}{\partial p} dt + \sigma \mathbf{C}^{1/2} dW. \end{cases}$$

Remark: Easy to extend to manifolds.

Conventional Accuracy

This method is first-order mean-squared accurate:

$$\|\phi_h^k(q,p) - \varphi_{t_k}(q,p)\|_{ms} \leq Ch.$$

As a consequence, a result due to Mattingly, Stuart, and Highman [2002], shows if the original Langevin process is geometrically ergodic then so is this integrator.

Let μ_h denote the discrete invariant measure associated to ϕ_h

Even though the integrator is first-order accurate, the distance between μ and μ_h is based on order of accuracy of the variational integrator

Near Preservation of BG-measure

Assume that the variational integrator is pth-order accurate.

$$\|\theta_h^N(q,p) - \vartheta_{Nh}(q,p)\| \leq Ch^p.$$

Then, one can prove the following identity by change of variables:

$$\int_{T^*Q} (\mathbb{E}(f(\phi_h)) - f)\, d\mu = \int_{T^*Q} f\left(e^{-\beta\left(H((\theta_h)^{-1}) - H\right)} - 1\right) d\mu$$

change in energy of a variational integrator

Near Preservation of BG measure

Under assumption of geometric ergodicity:

$$\left| \int_{T^*Q} \left[f(\phi_h^N) - f \right] d\mu \right| \leq \mathcal{O}(\log(1/h)\, h^p)$$

Moreover, TV distance of discrete invariant measure satisfies

$$\|\mu - \mu_h\|_{TV} \leq \mathcal{O}(\log(1/h)h^p).$$

NB: Practical sufficient conditions based on regularity of potential energy are provided in the paper.