Time Adaptive Variational Integrators: A Space-Time Geodesic Approach

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Marsden number: 1
Time adaptive symplectic integrators

- Motivation for variational integrators (VIs)
- Known results in time adaptive VIs
- Advantages of space-time geodesic formulation
  - Symplectic and energy preservation
- Simulation results
  - Simple pendulum
  - Double well system
  - Chaotic double well
  - Figure eight solution in three body problem

Nair [2011], To Appear in Physica D
Variational Integrators

Hamilton’s principle

- configuration manifold $Q$, tangent bundle $TQ$
- Lagrangian $L : TQ \to \mathbb{R}$
- variational principle
  $\delta \int_{0}^{T} L(q, \dot{q}) \, dt = 0$
- Euler Lagrange equations
  $\frac{d}{dt} \frac{\partial}{\partial \dot{q}} L - \frac{\partial}{\partial q} L = 0$

Marsden & West [2001]
Variational Integrators

Main idea behind VIs

- Discretize the variational principle instead of the underlying ODEs
- Gives exact (discrete) momentum conservation
- Very good long term energy behavior
- Extensions to stochastic Langevin (Bou-Rabee et. al)
- Extensions to PDEs Schkoller, Wulff, ...)

Marsden & West [2001]
Variational Integrators

**Hamilton’s principle**

- configuration manifold $Q$, tangent bundle $TQ$
- Lagrangian $L : TQ \to \mathbb{R}$
- variational principle
  \[ \delta \int_0^T L(q, \dot{q}) \, dt = 0 \]
- Euler Lagrange equations
  \[ \frac{d}{dt} \frac{\partial}{\partial \dot{q}} L - \frac{\partial}{\partial q} L = 0 \]

**discrete Hamilton’s principle**

- 2 copies of configuration manifold $Q \times Q$
- discrete Lag. $L_d : Q \times Q \to \mathbb{R}$
- discrete variational principle
  \[ \delta \sum_{k=0}^{N-1} L_d(q_k, q_{k+1}) = 0 \]
- discrete EL equations
  \[ D_2 L_d(q_{k-1}, q_k) + D_1 L_d(q_k, q_{k+1}) = 0 \]

Marsden & West [2001]
Variational Integrators

- Initial \((q,v)\) constraints are transformed to constraints on \((q_0,q_1)\) via discrete Legendre trans

\[
\text{discrete Legendre transformation } F^\pm L_d : Q \times Q \rightarrow T^* Q
\]

\[
(q_k, q_{k+1}) \mapsto (q_k, p_k^-) = (q_k, -D_1 L_d(q_k, q_{k+1}))
\]

\[
(q_{k-1}, q_k) \mapsto (q_k, p_k^+) = (q_k, D_2 L_d(q_{k-1}, q_k))
\]

- VI preserves momentum and symplectic form
- Good energy behavior in long term simulation
- Preservation of nearby Hamiltonian
  - See *Geometric Numerical Integration* by Hairer, Lubich and Wanner [2006]
Kepler example

\[ L(q, \dot{q}) = \frac{1}{2} m(\dot{x}^2 + \dot{y}^2) - V(q) \text{ with } V(q) = -\frac{mM}{\sqrt{x^2 + y^2}} \]
Kepler example

\[ L(q, \dot{q}) = \frac{1}{2} m(\dot{x}^2 + \dot{y}^2) - V(q) \quad \text{with} \quad V(q) = -\frac{mM}{\sqrt{x^2 + y^2}} \]

\[ h = 0.0025 \]
Kepler example

\[ L(q, \dot{q}) = \frac{1}{2} m(\dot{x}^2 + \dot{y}^2) - V(q) \text{ with } V(q) = -\frac{mM}{\sqrt{x^2 + y^2}} \]

Angular momentum is still preserved
Known Results in Time Adaptivity

Variational structure necessary but not sufficient
  ‣ M. Ortiz [1986], example of nonlinear energy preserving algorithm with diverging solution
Known Results in Time Adaptivity

Variational structure necessary but not sufficient
‣ M. Ortiz [1986], example of nonlinear energy preserving algorithm with diverging solution

The Kepler problem
‣ Preto & Tremaine [1999], Blanes & Budd [2004]
etc
‣ Fictitious time evolution obeys a power law
‣ Exploits scale invariance of Kepler problem

\[
\text{Kepler} \rightarrow \text{ST} \rightarrow \text{LC/KS} \\
(\text{fictitious time})
\]
Known Results in Time Adaptivity

Assuming integrability, separability, reversibility

› Hairer [2005], Blanes & Budd [2004], Hairer & Soderlind [2005], Barenblatt [1996] etc

› Assumes kinetic and potential part are integrable

› Diophantine condition on frequencies (not satisfied by Kepler)
Known Results in Time Adaptivity

Assuming integrability, separability, reversibility
- Assumes kinetic and potential part are integrable
- Diophantine condition on frequencies (not satisfied by Kepler)

No structural assumptions
- Kane, Marsden and Ortiz [1999], Kharevych et. al. [2009]
- No trajectory error control
- Singularity at turning points
- Time varying (not really adaptive)
Variational Integrators

- Need a time *adaptive* VI scheme to handle high velocity regions
- Time *varying* VI schemes
  - Does not treat space and time variables equally
  - Lagrangian quadratic in velocity and linear in time

\[
S = \int_{\tau_1}^{\tau_2} \left[ \left( \frac{1}{2}v^2 - V(q) \right)N - E(\dot{t} - N) + p(\dot{q} - vN) \right] d\tau,
\]
Variational Integrators

- Need a time *adaptive* VI scheme to handle high velocity regions
- Time *varying* VI schemes
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  - Lagrangian quadratic in velocity and linear in time

Our contribution: Reformulation of the variational principle which allows for time adaptivity with equal emphasis on space and time variable
Potential free particle

› Consider a particle in potential free environment

\[ \delta \int T(q, q_t) dt = 0 \quad \delta \int \sqrt{T(q, q_t)} d\lambda = 0. \]

› Not invariant w.r.t nonlinear re-parametrization

› Invariant w.r.t nonlinear re-parametrization

Can one see an arbitrary Lagrangian system as a potential free system?
Motivation for space-time geodesic

\[ L_{GR} = \frac{1}{2} \left( \left(1 - \frac{r_s}{r}\right) c^2 t'^2 - \frac{r'^2}{(1 - \frac{r_s}{r})} - r^2 \phi'^2 \right) \]

\[ \tilde{L}_N = \frac{1}{2} (\dot{r}^2 + r^2 \dot{\phi}^2) - \tilde{V}(r) \]

\[ \tilde{V}(r) = -\frac{GM}{r} + \frac{L^2}{2mr^2} - \frac{GMI^2}{c^2mr^3} \]
Space-time geodesic

\[ L = \frac{1}{2} \dot{x}^2 - V(x) \]

\[ \ddot{x} = -\frac{\partial V}{\partial x} ; \quad x_0 = x(0), \dot{x}_0 = \dot{x}(0) \quad (12) \]

Proposition 1. Let \( x(t) \) solve (12) for some time interval \( t \in [0 \ T] \). Consider the Lagrangian

\[ \tilde{L} = \frac{1}{2} x'^2 + \frac{1}{2V} t'^2 \quad (13) \]

with Euler-Lagrange equations and initial conditions

\[ x'' = -\frac{1}{2V^2} \frac{\partial V}{\partial x} t'^2 \quad ; \quad x_0 = x(0), x'_0 = \dot{x}_0 t'_0 \quad (14a) \]
\[ t'' = \frac{1}{V} \frac{\partial V}{\partial x} t' x' \quad ; \quad t(0) = 0, t'(0) = \alpha V(x_0) \quad (14b) \]

If \( \tilde{x}(\lambda), t(\lambda) \) solves (14) for some time interval \( \lambda \in [0 \ \tilde{T}] \), then \( \tilde{x}(\lambda) = x(t/\beta) \) for as long as both sides are defined. Here, \( \beta \) is a constant given by \( \sqrt{\alpha} \). Therefore, the solutions for \( x \) and \( \tilde{x} \) differ only by a constant rescaling of time.
Space-time geodesic

- We can now exploit nonlinear parametrization invariance
- Extension to multidimensional nonlinear metric
  - Solve a metric PDE
- Preserves the underlying physics (as opposed to GR setting)
- Resulting time coordinate is not the physical time
  - Physical time reconstructed by imposing conservation of physical Hamiltonian
We can now exploit nonlinear parametrization invariance

Extension to multidimensional nonlinear metric
  Solve a metric PDE

Preserves the underlying physics (as opposed to GR setting)

Resulting time coordinate is not the physical time
  Physical time reconstructed by imposing conservation of physical Hamiltonian
Application to VI

Let

\[ L^p = \frac{1}{2} \dot{x}^2 - V(x) \]
\[ L^{st} = \frac{1}{2} x'^2 + \frac{1}{2V} t'^2 \]

Solve discrete space-time Lagrangian

Constant stepping

\[ \Omega = dx \wedge dp_x + dt \wedge dp_t \]

Adaptive stepping

\[ \Omega_{st}^L = dx \wedge dp_x + dt \wedge dp_t + dL^{st} \wedge d\lambda \]

\((x_0, t_0), \ldots, (x_n, t_n)\)

t’s are not physical time

\[ h_0 D_2 L^p_d(x_0, x_1, h_0) + h_1 D_1 L^p_d(x_1, x_2, h_1) = 0 \]
\[ E^p_d(x_0, x_1, h_0) - E^p_d(x_1, x_2, h_1) = 0 \]

Physical time reconstruction
Pendulum VI simulation

\[ L = \frac{1}{2} \dot{\theta}^2 - V(\theta) \]

Potential energy

\[ V(\theta) = -\cos(\theta). \]

Lagrangian

\[ \dot{\theta} = \omega \]
\[ \dot{\omega} = -\sin(\theta) \]

Euler-Lagrange equations

\[ t_{i+1} - t_i = \begin{cases} 
0.05 & \text{if } |\theta_i| \leq 0.2, \\
0.2 & \text{if } |\theta_i| > 0.6, \\
0.1 & \text{otherwise}
\end{cases} \]

Time adaptive VI

Smaller time steps in high velocity regions

\[ t \text{ is not physical time} \]
Pendulum simulation
Double well potential

\[ L = \frac{1}{2} \dot{x}^2 - V(x) \]

\[ V(x) = \frac{1}{2}(x^4 - x^2) \]
Chaotic Double well potential

\[ L = \frac{1}{2} (x^2 + y^2) - V(x) - \frac{1}{2} y^2 + \epsilon xy \]

\[ V(x) = \frac{1}{2} (x^4 - x^2) \]

\[ \lambda_i = \begin{cases} 
0.01 & \text{if } |x - 0.67| < 0.1 \\
0.01 & \text{if } |x - 0.74| < 0.1 \\
0.001 & \text{otherwise}
\end{cases} \]
Figure Eight Solution for 3 Body Problem

\[ L(x_1, y_1, x_2, y_2, x_3, y_3, \dot{x}_1, \dot{y}_1, \dot{x}_2, \dot{y}_2, \dot{x}_3, \dot{y}_3) = \frac{1}{2} \sum_{i=1}^{3} (\dot{x}_i^2 + \dot{y}_i^2) - V(x_1, y_1, x_2, y_2, x_3, y_3) \]  

where

\[ V(x_1, y_1, x_2, y_2, x_3, y_3) = - \sum_{1 \leq i < j \leq 3} \frac{1}{\sqrt{(x_i - x_j)^2 + (y_i - y_j)^2}} \]  

\[ \lambda_i = \begin{cases} 
0.15 & \text{if } V > -2.6 \\
0.1 & \text{otherwise} 
\end{cases} \]
Figure Eight Solution for 3 Body Problem

\[ \lambda_i = \begin{cases} 
0.15 & \text{if } V > -2.6 \\
0.1 & \text{otherwise} 
\end{cases} \]

\[ h = 0.15 \]
Figure Eight Solution for 3 Body Problem

\[
\lambda_i = \begin{cases} 
0.15 & \text{if } V > -2.6 \\
0.1 & \text{otherwise}
\end{cases}
\]

\[ h = 0.1 \]
Conclusion and Future Work

- Showed equivalence of an arbitrary Lagrangian system to a space-time kinetic energy Lagrangian.
- Demonstrated use of space-time formulation to generate time adaptive VIs.
  - No turning point singularities.
- No assumptions on integrability, separability.
- Individual trajectory error analysis required.
  - Tradeoff with computation cost.
- Extensions to PDE required.
Thank You