Co-funded by
the European Union

Degenerate Variational Integrators 𝄞 Variations on a Motif

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Acknowledgements: Joshua Burby, Leland Ellison, Omar Maj, Hiroaki Yoshimura, ...

Outline

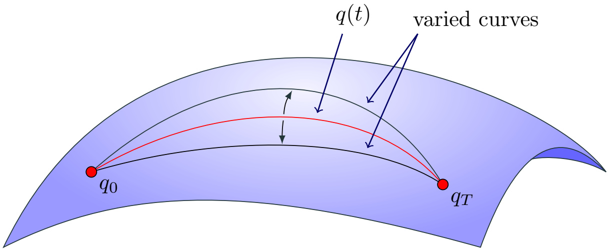
Degenerate Lagrangian Systems

Hamilton's Principle of Stationary Action

- Physical equations are often derived from an action principle

- The action $\mathcal{A}$ is a functional of a trajectory $q : [0, T] \to \mathbb{R}^m$

$$\mathcal{A}[q] = \int_0^T L\big(q(t), \dot{q}(t)\big)\, dt$$



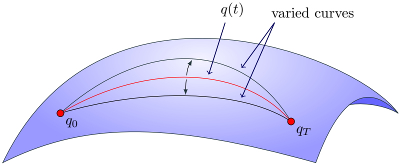
Hamilton's principle of stationary action

Among all possible trajectories connecting q_0 and q_T, the physical trajectory makes the action integral $\mathcal{A}$ stationary.

Hamilton's Principle of Stationary Action

- computing variations

$$\delta\mathcal{A}[q] = \int_0^T \left[\frac{\partial L}{\partial q}\cdot\delta q + \frac{\partial L}{\partial \dot q}\cdot\delta\dot q\right] dt = 0 \text{ for all } \delta q$$



- integration by parts (endpoints fixed: $\delta q(0) = \delta q(T) = 0$)

$$\delta\mathcal{A}[q] = \int_0^T \left[\frac{\partial L}{\partial q} - \frac{d}{dt}\left(\frac{\partial L}{\partial \dot q}\right)\right]\cdot\delta q\, dt + \underbrace{\cancel{\left[\frac{\partial L}{\partial \dot q}\cdot\delta q\right]_0^T}}_{0} = 0 \text{ for all } \delta q$$

- requiring stationarity of the action leads to the Euler-Lagrange equations of motion

$$\frac{\partial L}{\partial q}(q,\dot q) - \frac{d}{dt}\left(\frac{\partial L}{\partial \dot q}(q,\dot q)\right) = 0$$

Regular Lagrangians

- for regular Lagrangians, the velocity space Hessian M is invertible for each $(q, \dot{q})$

$$M_{ij}(q, \dot{q}) = \frac{\partial^2 L}{\partial \dot{q}^i \, \partial \dot{q}^j}(q, \dot{q})$$

- this implies that the Euler–Lagrange equations are a system of m 2nd-order ODEs

$$\ddot{q}^i = M_{ij}^{-1} \left(\frac{\partial L}{\partial q^j} - \frac{\partial^2 L}{\partial \dot{q}^j \, \partial q^k} \, \partial \dot{q}^k \right)$$

following from

$$\frac{d}{dt} \left(\frac{\partial L}{\partial \dot{q}^i}(q, \dot{q}) \right) = M_{ij} \ddot{q}^j + \frac{\partial^2 L}{\partial \dot{q}^i \, \partial q^k} \, \partial \dot{q}^k$$

- the solution of this system of equations requires $2m$ initial conditions

Phasespace Lagrangians

- in the following, we consider phasespace Lagrangians, which have the general form

$$L(q, \dot{q}) = \vartheta(q) \cdot \dot{q} - H(q)$$

- as L is linear in velocities the velocity-space Hessian is zero everywhere

- the Euler-Lagrange equations are first order ordinary differential equations

$$\frac{d}{dt}\vartheta(q) = \nabla\vartheta(q) \cdot \dot{q} - \nabla H(q) \qquad \text{or} \qquad \dot{q}^i \omega_{ij}(q) = \frac{\partial H}{\partial q^i}(q)$$

  with the $m \times m$ noncanonical symplectic matrix ω given by

$$\omega_{ij} = \frac{\partial \vartheta_i}{\partial q^j} - \frac{\partial \vartheta_j}{\partial q^i}$$

- the solution of this system of equations requires m initial conditions

Variational Integrators

Discrete Variational Principle

- discrete action and discrete Lagrangian with discrete trajectory $q_d = \{q_n\}_{n=0}^{N}$

$$\mathcal{A}_d[q_d] = \sum_{n=0}^{N-1} L_d(q_n, q_{n+1}) \qquad \text{e.g.} \qquad L_d(q_n, q_{n+1}) = h\, L\left(\frac{q_n + q_{n+1}}{2}, \frac{q_{n+1} - q_n}{h} \right)$$

- requiring stationarity of the discrete action,

$$\delta \mathcal{A}_d[q_d] = \delta \sum_{n=0}^{N-1} L_d(q_n, q_{n+1}) = 0 \quad \text{for all} \quad \delta q_n,$$

with $\delta q_0 = \delta q_N = 0$, leads to the discrete Euler-Lagrange equations

$$D_2 L_d(q_{n-1}, q_n) + D_1 L_d(q_n, q_{n+1}) = 0 \quad \text{for all} \quad n$$

Discrete Variational Principle

- provided the discrete Hessian

$$\mathrm{M}_{ij}(q_n, q_{n+1}) = \frac{\partial L_d}{\partial q_n^i \, \partial q_{n+1}^j}(q_n, q_{n+1})$$

  is invertible, the discrete Euler-Lagrange equations define a mapping

$$\Psi_{L_d} : (q_{n-1}, q_n) \mapsto (q_n, q_{n+1}^*(q_{n-1}, q_n))$$

- solving the discrete Euler–Lagrange equations requires $2m$ initial conditions

$\rightarrow$ same number of initial conditions required to solve the continuous Euler–Lagrange equations for a regular Lagrangian

Discrete Variational Principle and Phasespace Lagrangians

- for phasespace Lagrangians

$$L(q, \dot{q}) = \vartheta(q) \cdot \dot{q} - H(q)$$

  the mapping

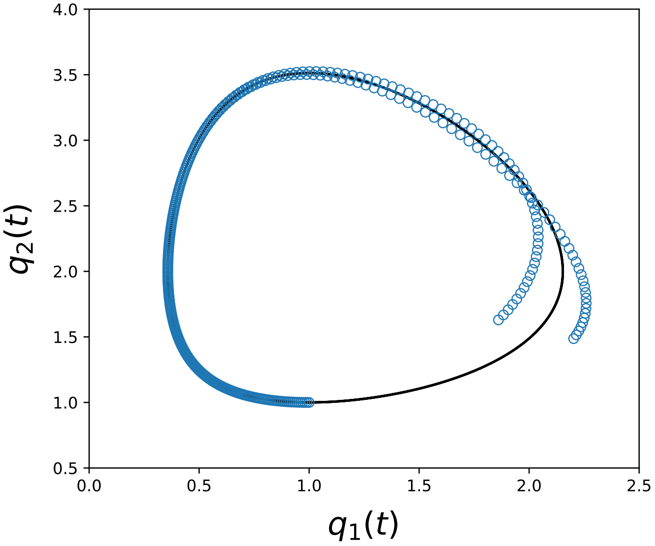
$$\Psi_{L_d} : (q_{n-1}, q_n) \mapsto (q_n, q^*_{n+1}(q_{n-1}, q_n))$$

  corresponds to a multi-step variational integrator

$\rightarrow$ the variational integrator requires $2m$ initial conditions even though the continuous Euler–Lagrange equations (being first order ODEs) require only m initial conditions

$\rightarrow$ susceptible to parasitic modes driving simulations unstable

Lotka–Volterra System with Variational Integrator



Discrete Variational Principle and Phasespace Lagrangians

Problem

Most discrete Lagrangians L_d approximating a phasespace Lagrangian have an invertible discrete Hessian M.

Degenerate Variational Integrators

Special Phasespace Lagrangians

- consider the special phasespace Lagrangian

$$L(q, \dot{q}) = \vartheta(q) \cdot \dot{q} - H(q), \qquad q \in \mathbb{R}^{2d},$$

where $d = m/2$ of the components of ϑ vanish, in particular

$$\vartheta_\mu = 0 \qquad \text{for} \qquad \mu = d+1, \dots, 2d$$

- for clarity sake we will consider a phasespace Lagrangian with $d = 1$

$$L(q^1, q^2, \dot{q}^1, \dot{q}^2) = \vartheta_1(q^1, q^2)\, \dot{q}^1 - H(q^1, q^2)$$

Degenerate Variational Integrators

- consider the discrete degenerate Lagrangian

$$L_d(q_n, q_{n+1}) = h\left[\vartheta_1(q_n^1, q_n^2)\,\frac{q_{n+1}^1 - q_n^1}{h} - H(q_n^1, q_n^2)\right] = 0$$

- the discrete Hessian is degenerate (rank $d = 1$)
- discrete Euler–Lagrange equations look like a multi-step method

$$\frac{\vartheta_1(q_n^1, q_n^2) - \vartheta_1(q_{n-1}^1, q_{n-1}^2)}{h} = D_1\vartheta_1(q_n^1, q_n^2)\,\frac{q_{n+1}^1 - q_n^1}{h} + D_1 H(q_n^1, q_n^2)$$

$$\text{for } n = 1, \dots, N-1,$$

$$0 = D_2\vartheta_1(q_n^1, q_n^2)\,\frac{q_{n+1}^1 - q_n^1}{h} + D_2 H(q_n^1, q_n^2)$$

$$\text{for } n = 0, \dots, N-1$$

Degenerate Variational Integrators

- for sake of clarity introduce a velocity

$$v_n^1 = \frac{q_{n+1}^1 - q_n^1}{h},$$

$\rightarrow$ assuming appropriate invertibility conditions, v can be solved for by

$$v_n^1 = \big(D_2 \vartheta_1(q_n^1, q_n^2) \big)^{-1} D_2 H(q_n^1, q_n^2)$$

$\rightarrow$ the discrete Euler–Lagrange equations become

$$\begin{aligned} \vartheta_1(q_n^1, q_n^2) &= \vartheta_1(q_{n-1}^1, q_{n-1}^2) + h\, D_1 \vartheta_1(q_n^1, q_n^2)\, v_n^1 - h\, D_1 H(q_n^1, q_n^2) && \text{for } n = 1, \dots, N-1 \\ v_n^1 &= \big(D_2 \vartheta_1(q_n^1, q_n^2) \big)^{-1} D_2 H(q_n^1, q_n^2) && \text{for } n = 0, \dots, N-1 \\ q_{n+1}^1 &= q_n^1 + h v_n^1 && \text{for } n = 0, \dots, N-1 \end{aligned}$$

$\rightarrow$ underdetermined system of equations: no functional dependence on q_N^2

Degenerate Variational Integrators

- close the discrete Euler–Lagrange equations by

$$\begin{aligned} \vartheta_1(q_N^1, q_N^2) &= \vartheta_1(q_{N-1}^1, q_{N-1}^2) + h D_1 \vartheta_1(q_N^1, q_N^2) \cdot v_N^1 - h D_1 H(q_N^1, q_N^2), \\ v_N^1 &= \big(D_2 \vartheta_1(q_N^1, q_N^2) \big)^{-1} D_2 H(q_N^1, q_N^2) \end{aligned}$$

→ motivated by the discrete symplecticity condition following from the boundary values in the action principle

$$\delta \mathcal{A}_d[q_{DEL}] = -\big[\vartheta_1(q_0) - D_1 \vartheta_1(q_0) \cdot v_0^1 + D_1 H(q_0) \big] \, \delta q_0^1 + \big[\vartheta_1(q_{N-1}) \big] \, \delta q_N^1$$

→ conservation of the discrete symplectic structure $\omega_d = \mathrm{d}\vartheta_d$ with

$$\vartheta_d(q_n) = \big[\vartheta_1(q_n^1, q_n^2) - \nabla_1 \vartheta_1(q_n^1, q_n^2) \cdot v_n^1 + \nabla_1 H(q_n^1, q_n^2) \big] \mathrm{d} q_n^1$$

Degenerate Variational Integrators

- allows to obtain one-step methods for degenerate Lagrangians directly from a discrete action principle
- alternative derivation from discrete Hamilton–Pontryagin principle that includes the velocities in the formulation of the action principle
- first order accurate
- not composable: adjoint methods preserve a different symplectic structure
- preservation of a discrete symplectic structure

Degenerate Variational Integrators

2nd-Order Leapfrog DVIs

Leapfrog Degenerate Variational Integrators

- centred, staggered discretisations of the Lagrangian
- midpoint discretisation (MDVI)

$$L_d(q_n^1, q_{n+1/2}^2, q_{n+1}^1) = h\left[\vartheta_1\left(\frac{q_n^1 + q_{n+1}^1}{2},\, q_{n+1/2}^2\right)\frac{q_{n+1}^1 - q_n^1}{h} - H\left(\frac{q_n^1 + q_{n+1}^1}{2},\, q_{n+1/2}^2\right)\right]$$

- trapezoidal discretisation (TDVI)

$$\begin{aligned} L_d(q_n^1, q_{n+1/2}^2, q_{n+1}^1) = \frac{h}{2}\Bigg[\left(\vartheta_1(q_n^1,\, q_{n+1/2}^2) + \vartheta_1(q_{n+1}^1,\, q_{n+1/2}^2)\right)\frac{q_{n+1}^1 - q_n^1}{h} \\ - H(q_n^1,\, q_{n+1/2}^2) - H(q_{n+1}^1,\, q_{n+1/2}^2)\Bigg] \end{aligned}$$

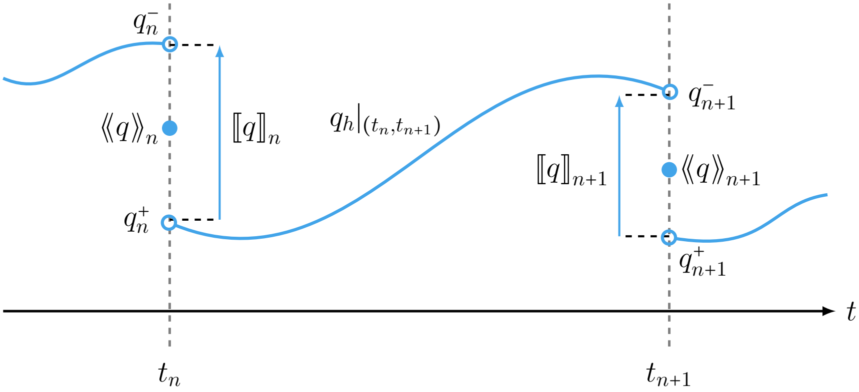
- the discrete Hessian is degenerate (rank $d = 1$)

Leapfrog Degenerate Variational Integrators

- allows to obtain one-step methods for degenerate Lagrangians directly from a discrete action principle
- second order accurate
- composable: symmetric and self-adjoint
- requires processing for initialisation of half steps
- obtaining the genuine one-step form of the integrator not always straightforward
- preservation of a discrete symplectic structure

Discontinuous Galerkin DVIs

Discontinuous Galerkin Approximation



- piecewise-continuous polynomial basis $q_h\big|_{\mathcal{I}_n} \in \mathbb{P}^r(\mathcal{I}_n)$ with $\mathcal{I}_n = (t_n, t_{n+1})$
- allow for discontinuities at t_n and t_{n+1}

Discontinuous Galerkin Degenerate Variational Integrators

- consider a Galerkin discretisation of the Lagrangian, formally written as

$$L_h(q_n^+, q_{n+1}^-) = h \sum_{i=1}^{s} b_i \, L\Big(q_h(t_n + c_i h), \, \dot{q}_h(t_n + c_i h)\Big),$$

  where q_h is a piecewise polynomial approximation of the trajectory q with

$$q_n^+ = \lim_{t \downarrow t_n} q_h(t), \qquad\qquad q_{n+1}^- = \lim_{t \uparrow t_{n+1}} q_h(t)$$

- the following construction works in a similar way also for Runge–Kutta discretisations

Discontinuous Galerkin Degenerate Variational Integrators

- the discontinuous approximation of the Lagrangian needs to be connected by appropriate jump terms

$$L_d(q_n, q_{n+1}) = L_h(q_n^+, q_{n+1}^-) + \vartheta(\langle\!\langle q \rangle\!\rangle_n^+) \cdot [\![q]\!]_n^+ + \vartheta(\langle\!\langle q \rangle\!\rangle_{n+1}^-) \cdot [\![q]\!]_{n+1}^- ,$$

with averages and jumps defined as

$$\langle\!\langle q^\mu \rangle\!\rangle_n^+ = \begin{cases} q_n^{+,\mu} & \text{for} \quad \mu = 1, \dots, d, \\ q_n^\mu & \text{for} \quad \mu = d+1, \dots, 2d, \end{cases} \qquad [\![q]\!]_n^+ = q_n^+ - q_n,$$

$$\langle\!\langle q^\mu \rangle\!\rangle_n^- = \begin{cases} q_n^{-,\mu} & \text{for} \quad \mu = 1, \dots, d, \\ q_n^\mu & \text{for} \quad \mu = d+1, \dots, 2d, \end{cases} \qquad [\![q]\!]_n^- = q_n - q_n^-$$

- the q_n are varied as independent variables

Discontinuous Galerkin Degenerate Variational Integrators

- the discontinuous Galerkin Lagrangian

$$L_d(q_n, q_{n+1}) = L_h(q_n^+, q_{n+1}^-) + \vartheta(\langle\!\langle q \rangle\!\rangle_n^+) \cdot (q_n^+ - q_n) + \vartheta(\langle\!\langle q \rangle\!\rangle_{n+1}^-) \cdot (q_{n+1} - q_{n+1}^-)$$

  is guaranteed to be degenerate as the discrete Hessian is degenerate (rank 0)

- discrete Euler–Lagrange equations

$$\begin{aligned} \delta q_n^1 : \quad & 0 = \vartheta_1(\langle\!\langle q \rangle\!\rangle_n^+) - \vartheta_1(\langle\!\langle q \rangle\!\rangle_n^-), \\ \delta q_n^2 : \quad & 0 = D_2\vartheta_1(\langle\!\langle q \rangle\!\rangle_n^{+,1}) \cdot (q_n^{+,1} - q_n^1) + D_2\vartheta_1(\langle\!\langle q \rangle\!\rangle_n^{-,1}) \cdot (q_n^1 - q_n^{-,1}) \end{aligned}$$

  plus discrete Euler–Lagrange equations resulting from variations w.r.t. internal variables of $L_h(q_n^+, q_{n+1}^-)$

Discontinuous Galerkin Degenerate Variational Integrators

- discrete Euler–Lagrange equations from jump terms

$$
\begin{aligned}
\delta q_n^1 : \quad & 0 = \vartheta_1(q_n^{+,1}, q_n^2) - \vartheta_1(q_n^{-,1}, q_n^2), \\
\delta q_n^2 : \quad & 0 = D_2\vartheta_1(q_n^{+,1}, q_n^2) \cdot (q_n^{+,1} - q_n^1) + D_2\vartheta_1(q_n^{-,1}, q_n^2) \cdot (q_n^1 - q_n^{-,1})
\end{aligned}
$$

- for sufficiently small time steps and some mild assumptions on ϑ the first equation implies $\langle\!\langle q \rangle\!\rangle_n^+ = \langle\!\langle q \rangle\!\rangle_n^-$ and thus $q_n^{+,1} = q_n^{-,1}$

- this this, the second equation trivialises, leaving us with a system that is under-determined by Nd equations

→ allows us to add the continuity condition $q_n^1 = q_n^{+,1} = q_n^{-,1}$

Discontinuous Galerkin Degenerate Variational Integrators

- the boundary terms of the discrete action principle read

$$\mathrm{d}\mathcal{A}_d[q_{DEL}] = -\vartheta(\langle\!\langle q \rangle\!\rangle_0^+) \cdot \mathrm{d}q_0 + \vartheta(\langle\!\langle q \rangle\!\rangle_N^-) \cdot \mathrm{d}q_N$$

- identifying q_n^1 with $q_n^{+,1} = q_n^{-,1}$, this becomes

$$\mathrm{d}\mathcal{A}_d[q_{DEL}] = -\vartheta(q_0) \cdot \mathrm{d}q_0 + \vartheta(q_N) \cdot \mathrm{d}q_N$$

→ DG-DVIs preserve the continuous symplectic structure

Discontinuous Galerkin Degenerate Variational Integrators

- no closed-form expression for degenerate discrete Lagrangians: obtaining one-step methods requires implicit arguments (but is otherwise straightforward)
- arbitrary order accurate
- composable: includes symmetric and self-adjoint methods
- no processing for initialisation required
- preservation of the continuous symplectic structure

Discontinuous Galerkin DVIs

Some Examples

Hamilton–Pontryagin Principle

- Hamilton–Pontryagin principle: action principle on $\mathrm{T}\mathcal{M} \oplus \mathrm{T}^*\mathcal{M}$

$$\delta \int_0^T \Big[L(q, v) + \langle p, \dot{q} - v \rangle \Big] \, dt = 0$$

- variations of v are left free, a kinematic constraint ensures the second-order condition $v = \dot{q}$ with the momentum p as a Lagrange multiplier
(Hamilton's action principle: variations $\delta\dot{q}$ are induced by variations δq)

- requiring stationarity of the Hamilton–Pontryagin action, leads to the implicit Euler–Lagrange equations

$$\dot{q} = v, \qquad\qquad p = \frac{\partial L}{\partial v}, \qquad\qquad \dot{p} = \frac{\partial L}{\partial q}$$

(second-order condition, fibre derivative, Euler-Lagrange equations)

First-Order DVIs (Variant A)

- piecewise linear polynomial approximation of q

$$q_h(t)\big|_{(t_n,t_{n+1})} = \frac{t_{n+1}-t}{t_{n+1}-t_n}\, q_n^+ + \frac{t-t_n}{t_{n+1}-t_n}\, q_{n+1}^-$$

- continuous linear polynomial approximation of v

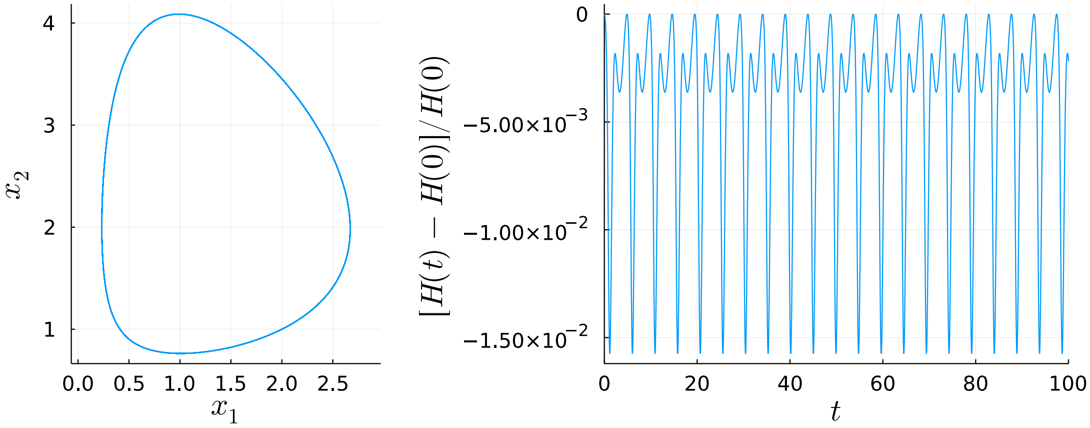
$$v_h(t)\big|_{[t_n,t_{n+1}]} = \frac{t_{n+1}-t}{t_{n+1}-t_n}\, v_n + \frac{t-t_n}{t_{n+1}-t_n}\, v_{n+1}$$

- use left Riemann quadrature on L_h and right Riemann quadrature on the Pontryagin constraint

$$L_d(q_n, q_{n+1}) = h\Big[\vartheta_1(q_n^{+,1}, q_n^{+,2}) \cdot v_n^1 - H(q_n^{+,1}, q_n^{+,2})\Big] + h\, p_{n+1}^1 \cdot \left[\frac{q_{n+1}^{-,1} - q_n^{+,1}}{h} - v_{n+1}^1\right]$$

$$+ \vartheta_1(q_n^{+,1}, q_n^2) \cdot (q_n^{+,1} - q_n^1) + \vartheta_1(q_{n+1}^{-,1}, q_{n+1}^2) \cdot (q_{n+1}^1 - q_{n+1}^{-,1})$$

Lotka–Volterra System with DVI1A



First-Order DVIs (Variant B)

- piecewise linear polynomial approximation of q

$$q_h(t)\big|_{(t_n,t_{n+1})} = \frac{t_{n+1}-t}{t_{n+1}-t_n}\, q_n^+ + \frac{t-t_n}{t_{n+1}-t_n}\, q_{n+1}^-$$

- continuous linear polynomial approximation of v

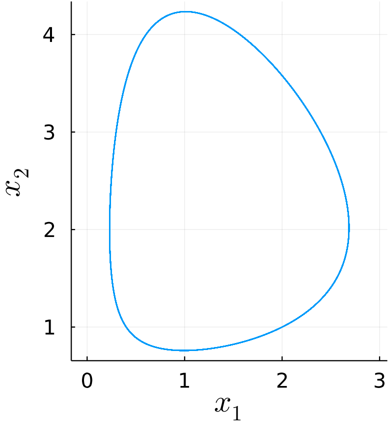
$$v_h(t)\big|_{[t_n,t_{n+1}]} = \frac{t_{n+1}-t}{t_{n+1}-t_n}\, v_n + \frac{t-t_n}{t_{n+1}-t_n}\, v_{n+1}$$

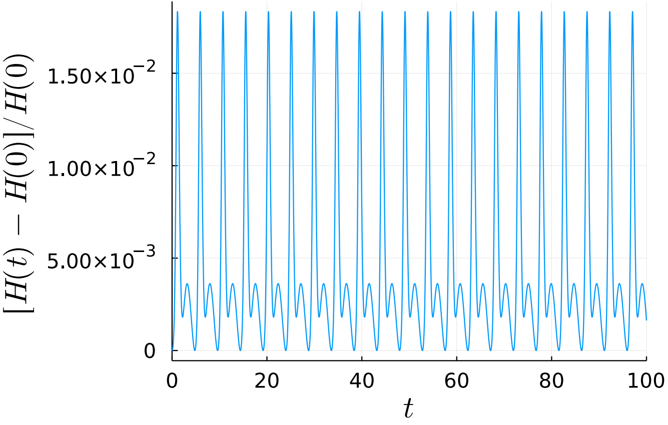
- use right Riemann quadrature on L_h and left Riemann quadrature on the Pontryagin constraint

$$L_d(q_n, q_{n+1}) = h\left[\vartheta_1(q_{n+1}^{-,1}, q_{n+1}^{-,2}) \cdot v_{n+1}^1 - H(q_{n+1}^{-,1}, q_{n+1}^{-,2})\right] + h\, p_n^1 \cdot \left[\frac{q_{n+1}^{-,1} - q_n^{+,1}}{h} - v_n^1\right]$$

$$+ \vartheta_1(q_n^{+,1}, q_n^2) \cdot (q_n^{+,1} - q_n^1) + \vartheta_1(q_{n+1}^{-,1}, q_{n+1}^2) \cdot (q_{n+1}^1 - q_{n+1}^{-,1})$$

Lotka–Volterra System with DVI1B





Trapezoidal DVI

- the approximation of q is given by

$$q_h^1(t)|_{(t_n,t_{n+1})} = \frac{t_{n+1} - t}{t_{n+1} - t_n}\, q_n^{+,1} + \frac{t - t_n}{t_{n+1} - t_n}\, q_{n+1}^{-,1},$$
$$q_h^2(t)|_{(t_n,t_{n+1})} = q_{n+1/2}^2$$

- use trapezoidal quadrature on the Lagrangian

$$L_d(q_n, q_{n+1}) = \frac{h}{2}\Big[\big(\vartheta_1(q_n^{+,1}, q_{n+1/2}^2) + \vartheta_1(q_{n+1}^{-,1}, q_{n+1/2}^2)\big)\cdot v_{n+1/2}^1 - H(q_n^{+,1}, q_{n+1/2}^2) - H(q_{n+1}^{-,1}, q_{n+1/2}^2)\Big]$$
$$+ h\, p_{n+1/2}^1 \cdot \left[\frac{q_{n+1}^{-,1} - q_n^{+,1}}{h} - v_{n+1/2}^1\right] + \vartheta_1(q_n^{+,1}, q_n^2)\cdot(q_n^{+,1} - q_n^1) + \vartheta_1(q_{n+1}^{-,1}, q_{n+1}^2)\cdot(q_{n+1}^1 - q_{n+1}^{-,1})$$

Trapezoidal DVI

$$p^1_{n+1/2} = \vartheta_1(q^1_n, q^2_n) + \frac{h}{2} D_1\vartheta_1(q^1_n, q^2_{n+1/2}) \cdot v^1_{n+1/2} - \frac{h}{2} D_1 H(q^1_n, q^2_{n+1/2}),$$

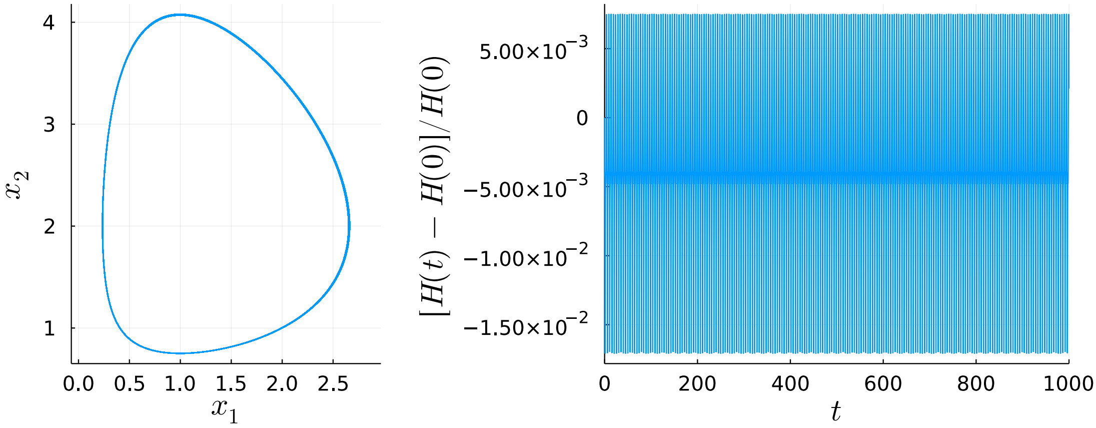
$$\begin{aligned}\vartheta_1(q^1_{n+1}, q^2_{n+1}) = \vartheta_1(q^1_n, q^2_n) &+ \frac{h}{2}\Big(D_1\vartheta_1(q^1_n, q^2_{n+1/2}) + D_1\vartheta_1(q^1_{n+1}, q^2_{n+1/2})\Big) \cdot v^1_{n+1/2} \\ &- \frac{h}{2}\Big(D_1 H(q^1_n, q^2_{n+1/2}) + D_1 H(q^1_{n+1}, q^2_{n+1/2})\Big),\end{aligned}$$

$$p^1_{n+1/2} = \frac{1}{2}\Big(\vartheta_1(q^1_n, q^2_{n+1/2}) + \vartheta_1(q^1_{n+1}, q^2_{n+1/2})\Big),$$

$$\begin{aligned}v^1_{n+1/2} = \Big(D_2\vartheta_1(q^1_n, q^2_{n+1/2}) + D_2\vartheta_1(q^1_{n+1}, q^2_{n+1/2})\Big)^{-1} \Big(&D_2 H(q^1_n, q^2_{n+1/2}) \\ &+ D_2 H(q^1_{n+1}, q^2_{n+1/2})\Big),\end{aligned}$$

$$q^1_{n+1} = q^1_n + h\, v^1_{n+1/2}$$

Lotka–Volterra System with DG-TDVI



Midpoint DVI

- the approximation of q is given by

$$q_h^1(t)\big|_{(t_n,t_{n+1})} = \frac{t_{n+1}-t}{t_{n+1}-t_n}\, q_n^{+,1} + \frac{t-t_n}{t_{n+1}-t_n}\, q_{n+1}^{-,1},$$
$$q_h^2(t)\big|_{(t_n,t_{n+1})} = q_{n+1/2}^2$$

- use midpoint quadrature on the Lagrangian

$$L_d(q_n, q_{n+1}) = h\left[\vartheta_1(\bar{q}_{n+1/2}^1, q_{n+1/2}^2)\cdot v_{n+1/2}^1 - H(\bar{q}_{n+1/2}^1, q_{n+1/2}^2)\right] + h\, p_{n+1/2}^1 \cdot \left[\frac{q_{n+1}^{-,1} - q_n^{+,1}}{h} - v_{n+1/2}^1\right]$$
$$+ \vartheta_1(q_n^{+,1}, q_n^2)\cdot(q_n^{+,1} - q_n^1) + \vartheta_1(q_{n+1}^{-,1}, q_{n+1}^2)\cdot(q_{n+1}^1 - q_{n+1}^{-,1})$$

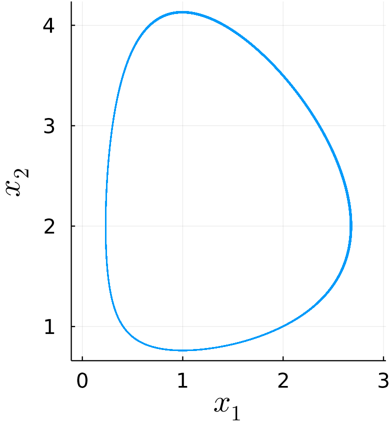
with

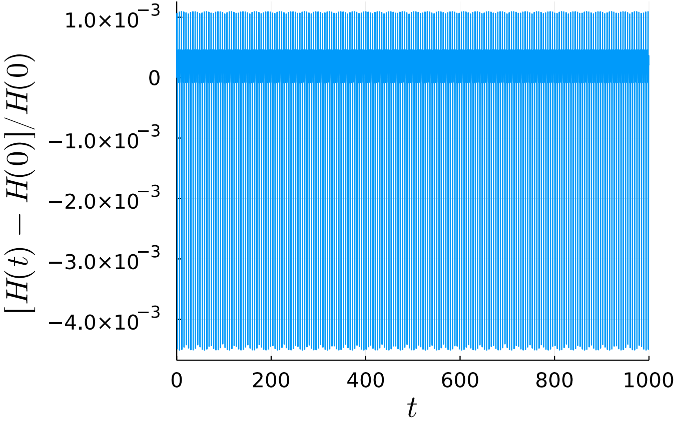
$$\bar{q}_{n+1/2}^1 = \frac{q_n^{+,1} + q_{n+1}^{-,1}}{2}$$

Midpoint DVI

$$\begin{aligned}
\vartheta_1(\bar{q}^1_{n+1/2}, q^2_{n+1/2}) &= \vartheta_1(q^1_n, q^2_n) + \frac{h}{2}\, D_1\vartheta_1(\bar{q}_{n+1/2}, q^2_{n+1/2}) \cdot v^1_{n+1/2} - \frac{h}{2}\, D_1 H(\bar{q}_{n+1/2}, q^2_{n+1/2}), \\
\vartheta_1(q^1_{n+1}, q^2_{n+1}) &= \vartheta_1(q^1_n, q^2_n) + h\, D_1\vartheta_1(\bar{q}_{n+1/2}, q^2_{n+1/2}) \cdot v^1_{n+1/2} - h\, D_1 H(\bar{q}_{n+1/2}, q^2_{n+1/2}), \\
v^1_{n+1/2} &= \Big(D_2\vartheta_1(\bar{q}^1_{n+1/2}, q^2_{n+1/2})\Big)^{-1} D_2 H(\bar{q}^1_{n+1/2}, q^2_{n+1/2})\Big), \\
q^1_{n+1} &= q^1_n + h\, v^1_{n+1/2}, \\
\bar{q}^1_{n+1/2} &= \frac{q^1_n + q^1_{n+1}}{2}
\end{aligned}$$

Lotka–Volterra System with DG-MDVI





Discontinuous Galerkin DVIs

Symplectic Runge–Kutta Methods

Symplectic Runge–Kutta Methods for Phasespace Lagrangians

$$Q_{n,i} = q_n + h \sum_{j=1}^{s} a_{ij} V_{n,j}, \qquad P_{n,i} = \frac{\partial L}{\partial \dot{q}}(Q_{n,i}, V_{n,i}),$$

$$P_{n,i} = p_n + h \sum_{j=1}^{s} a_{ij} F_{n,j}, \qquad F_{n,i} = \frac{\partial L}{\partial q}(Q_{n,i}, V_{n,i}),$$

$$q_{n+1}^{\mu} = q_n^{\mu} + h \sum_{i=1}^{s} b_i V_{n,i}^{\mu}, \qquad \mu = 1, \ldots, d,$$

$$p_{n+1}^{\mu} = p_n^{\mu} + h \sum_{i=1}^{s} b_i F_{n,i}^{\mu}, \qquad \mu = 1, \ldots, d,$$

$$p_{n+1}^{\mu} = \vartheta^{\mu}(q_{n+1}), \qquad \mu = 1, \ldots, 2d$$

Remarks on Projection Methods

Position–Momentum Form

- use discrete fibre derivative to obtain position-momentum form

$$\begin{aligned} p_n &= -D_1 L_d(q_n, q_{n+1}), \\ p_{n+1} &= D_2 L_d(q_n, q_{n+1}) \end{aligned}$$

- can be solved as the discrete Lagrangian L_d is not degenerate

→ provides an update rule of the form

$$\tilde{\Psi}_{L_d} : (q_n, p_n) \mapsto (q_{n+1}, p_{n+1})$$

- use continuous fibre derivative to obtain an exact second initial condition p_0

$$p_0 = \frac{\partial L}{\partial \dot{q}}(q_0) = \vartheta(q_0)$$

Position–Momentum Form

- position-momentum form: rewrite the equations of motion as an index-2 DAE

$$\begin{aligned} \dot{z} &= \Omega^{-1}\big(\nabla H(z) + \nabla\phi^T(z)\,\lambda\big), \\ 0 &= \phi(z), \end{aligned}$$

with

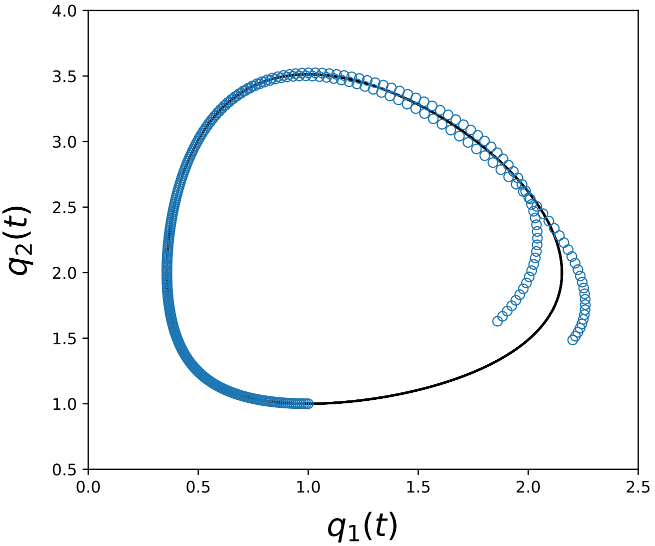
$$z = (q, p), \qquad \phi(q, p) = p - \vartheta(q), \qquad \Omega = \begin{pmatrix} \mathbb{0} & -\mathbb{1} \\ \mathbb{1} & \mathbb{0} \end{pmatrix}$$

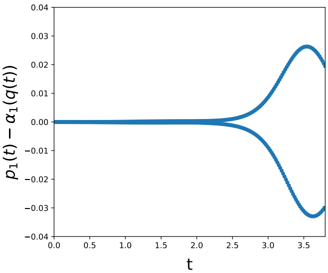
- the variational integrator does not preserve the constraint $\phi(q, p) = 0$

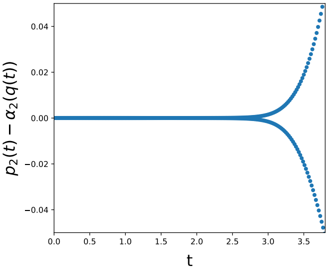
→ the numerical solution drifts away from the constraint submanifold

$$p_n \neq \vartheta(q_n) \quad \text{for } n \geq 1, \text{ even though} \quad p_0 = \vartheta(q_0)$$

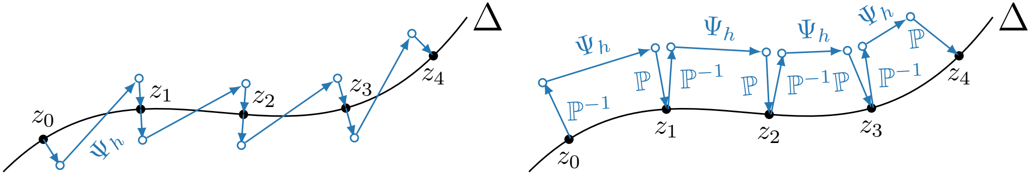
Lotka–Volterra System with Variational Integrator







Symmetric Projection on Primary Constraint



$$\tilde{z}_n = z_n + h\,\Omega^{-1}\nabla\phi^T(z_n)\,\lambda_{n+1}$$ perturb

$$\tilde{z}_{n+1} = \Psi_h(\tilde{z}_n)$$ apply arbitrary one-step method

$$z_{n+1} = \tilde{z}_{n+1} + h\,R(\infty)\,\Omega^{-1}\nabla\phi^T(z_{n+1})\lambda_{n+1}$$ project on constraint submanifold

$$0 = \phi(z_{n+1})$$ constraint

($R(\infty) = \pm 1$ is the stability function of Ψ_h)

Symmetric Projection and Symplecticity

- symplecticity condition

$$\mathrm{d}q_n^\mu \wedge \mathrm{d}p_n^\mu - \mathrm{d}\Big(\lambda_{n+1}^T \phi_{q^\mu}(p_n, q_n)\Big) \wedge \mathrm{d}\Big(\lambda_{n+1}^T \phi_{p^\mu}(p_n, q_n)\Big) =$$
$$= \mathrm{d}q_{n+1}^\mu \wedge \mathrm{d}p_{n+1}^\mu - \big|R(\infty)\big|^2 \mathrm{d}\Big(\lambda_{n+1}^T \phi_{q^\mu}(p_{n+1}, q_{n+1})\Big) \wedge \mathrm{d}\Big(\lambda_{n+1}^T \phi_{p^\mu}(p_{n+1}, q_{n+1})\Big)$$

- for $|R(\infty)| = 1$ a variational integrator with symmetric projection is symplectic iff

$$\lambda_{n+1}^T \phi_{p^\mu}(p_n, q_n) = \lambda_{n+1}^T \phi_{p^\mu}(p_{n+1}, q_{n+1}) \qquad \text{for all } \mu,$$
$$\lambda_{n+1}^T \phi_{q^\mu}(p_n, q_n) = \lambda_{n+1}^T \phi_{q^\mu}(p_{n+1}, q_{n+1}) \qquad \text{for all } \mu$$

- the first condition is always satisfied
- for special phasespace Lagrangians, λ_{n+1}^1 vanishes to machine precision while ϑ^2 is zero by assumption so that also the second condition is satisfied

Summary and Outlook

Summary and Outlook

- Degenerate Variational Integrators (DVIs)
  - one-step methods for degenerate Lagrangians obtained directly from a discrete action
  - original work (C. L. Ellison): 1st order, not composable
  - leapfrog methods (J. W. Burby): 2nd order, composable, require processing for initialisation
  - preservation of a discrete symplectic structure
- Discontinuous Galerkin Degenerate Variational Integrators (DG-DVIs)
  - Galerkin- and Runge–Kutta methods with arbitrary order
  - recover 1st-order DVIs, symplectic Runge–Kutta methods, and some projection methods
  - preservation of the continuous symplectic structure
- Open Problems
  - generalisation to arbitrary degenerate Lagrangians
  - closed-form expression for degenerate discrete Lagrangians

References

- References

  - C. L. Ellison et al. Degenerate variational integrators for magnetic field line flow and guiding center trajectories, Physics of Plasmas 25, 052502, 2018
  - C. L. Ellison. Development of Multistep and Degenerate Variational Integrators for Applications in Plasma Physics, Doctoral Thesis, Princeton University, 2016
  - J. W. Burby et al. Improved accuracy in degenerate variational integrators for guiding center and magnetic field line flow, 2021
  - MK. Projected Variational Integrators for Degenerate Lagrangian Systems, arXiv:1708.07356
  - MK. Symplectic Runge–Kutta Methods for Degenerate Lagrangian Systems, in preparation
  - MK. Discontinuous Galerkin Variational Integrators for Degenerate Lagrangians, in preparation
  - MK. On Action Principles and Degenerate Lagrangians: Continuous and Discrete, in preparation

- Implementation
  - https://github.com/JuliaGNI/GeometricIntegrators.jl
  - https://github.com/JuliaGNI/GeometricProblems.jl
  - https://github.com/JuliaPlasma/ChargedParticleDynamics.jl
  - https://github.com/JuliaPlasma/ElectroMagneticFields.jl