

Geometric integration and discrete variational calculus: some new developments

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Geometry, Dynamics and Mechanics Seminar

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① Motivation

② Retraction maps and symplectic integration

③ Parallel iterative methods for variational
integration

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Adams—Bashforth method

AN ATTEMPT
TO TEST
THE THEORIES OF CAPILLARY ACTION
BY COMPARING
THE THEORETICAL AND MEASURED FORMS
OF DROPS OF FLUID,

BY
FRANCIS BASHFORTH, B.D.
LATE PROFESSOR OF APPLIED MATHEMATICS TO THE ADVANCED CLAM
OF ROYAL ARTILLERY OFFICERS, WOOLWICH,
AND FORMERLY FELLOW OF ST JOHN'S COLLEGE, CAMBRIDGE.

WITH
AN EXPLANATION OF THE METHOD OF INTEGRATION
EMPLOYED IN CONSTRUCTING THE TABLES WHICH GIVE THE THEORETICAL
FORMS OF SUCH DROPS,

BY
J. C. ADAMS, M.A., F.R.S.
FELLOW OF PEMROKE COLLEGE, AND LOWNDEN PROFESSOR OF ASTRONOMY AND GEOMETRY
IN THE UNIVERSITY OF CAMBRIDGE.

Cambridge:
AT THE UNIVERSITY PRESS.
1883

$$y' = f(t, y)$$

$$y_{n+1} = y_n + hf(t_n, y_n), \quad \text{Euler method}$$

$$y_{n+2} = y_{n+1} + h \left(\frac{3}{2}f(t_{n+1}, y_{n+1}) - \frac{1}{2}f(t_n, y_n) \right),$$

$$y_{n+3} = y_{n+2} + h \left(\frac{23}{12}f(t_{n+2}, y_{n+2}) - \frac{4}{3}f(t_{n+1}, y_{n+1}) + \frac{5}{12}f(t_n, y_n) \right),$$

$$y_{n+4} = y_{n+3} + h \left(\frac{55}{24}f(t_{n+3}, y_{n+3}) - \frac{59}{24}f(t_{n+2}, y_{n+2}) \right. \\ \left. + \frac{37}{24}f(t_{n+1}, y_{n+1}) - \frac{3}{8}f(t_n, y_n) \right),$$

$$y_{n+5} = y_{n+4} + h \left(\frac{1901}{720}f(t_{n+4}, y_{n+4}) - \frac{1387}{360}f(t_{n+3}, y_{n+3}) \right. \\ \left. + \frac{109}{30}f(t_{n+2}, y_{n+2}) - \frac{637}{360}f(t_{n+1}, y_{n+1}) + \frac{251}{720}f(t_n, y_n) \right).$$

Runge-Kutta method

Eine ähnliche Ueberlegung führt nun auch für die Differentialgleichungen zu einer wesentlichen Verbesserung des Euler'schen Verfahrens. Ich will mich zunächst auf Differentialgleichungen erster Ordnung beschränken.

Statt

$$(1) \quad \Delta y = f(x_0 y_0) \Delta x \text{ u. s. w.}$$

ist es schon viel besser wenn man

$$(2) \quad \Delta y = f\left(x_0 + \frac{1}{2} \Delta x, y_0 + \frac{1}{2} f(x_0 y_0) \Delta x\right) \Delta x$$

u. s. w.

setzt. Diese Art der Berechnung entspricht dem aus der Summe der Tangententrapeze gebildeten Näherungswerthe eines Integrals und deckt sich völlig damit, wenn $f(xy)$ von y unabhängig vorausgesetzt wird.

Oder man kann der Summe der Sehnentrapeze entsprechend setzen:

$$(3) \quad \Delta y = \frac{f(x_0 y_0) + f\left(x_0 + \Delta x, y_0 + f(x_0 y_0) \Delta x\right)}{2} \Delta x$$

u. s. w.

Second-order methods with two stages: Midpoint

$$y_{n+1} = y_n + hf \left(t_n + \frac{1}{2}h, y_n + \frac{1}{2}hf(t_n, y_n) \right)$$

Second-order methods with two stages: Euler-Heun method

$$y_{n+1} = y_n + h \left(\left(1 - \frac{1}{2}\right)f(t_n, y_n) + \frac{1}{2}f\left(t_n + h, y_n + hf(t_n, y_n)\right) \right)$$

Runge–Kutta method RK4

$$y_{n+1} = y_n + \frac{1}{6}h(k_1 + 2k_2 + 2k_3 + k_4),$$

$$t_{n+1} = t_n + h$$

$$k_1 = f(t_n, y_n), \quad k_2 = f\left(t_n + \frac{h}{2}, y_n + h\frac{k_1}{2}\right),$$

$$k_3 = f\left(t_n + \frac{h}{2}, y_n + h\frac{k_2}{2}\right), \quad k_4 = f(t_n + h, y_n + hk_3).$$

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Iserles A., Munthe-Kaas H.Z., Nørsett S.P., Zanna A. [Lie-group methods](#) Acta Numer., 9 (2000), pp. 215-365

Celledoni E., Marthinsen H., Owren B. [An introduction to Lie group integrators—basics, new developments and applications](#), J. Comput. Phys., 257 (2014), pp. 1040-1061

....

and many books about the topic: Iserles; Sanz-Serna, Calvo; Hairer, Ernst; Lubich, Christian; Wanner, Gerhard, Leimkuhler, Benedict; Reich, Sebastian; Blanes, Sergio; Casas, Fernando....

Geometric Integration

Motion is described by differential equations derived from laws of physics

Geometric Integration

Motion is described by differential equations derived from laws of physics

$$\frac{d^2q}{dt^2} = F\left(t, q, \frac{dq}{dt}\right)$$

The equations contains not just a statement of acceleration but *all the physical laws relevant* (phase space, symmetries, invariance properties...)

Geometric Integration

- **Conservation laws.** Functions that stay constant along the solution trajectories. For example, the energy $H(q(t), p(t))$ of a Hamiltonian system

$$\frac{dq}{dt} = \frac{\partial H}{\partial p}(q, p), \quad \frac{dp}{dt} = -\frac{\partial H}{\partial q}(q, p)$$

remains constant along a solution trajectory.

$$p, q \in \mathbb{R}^n \quad \mathcal{M} = \{(x, y) \in \mathbb{R}^n \times \mathbb{R}^n \mid H(x, y) = H(q(0), p(0))\}$$

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Differentiable manifolds

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Differentiable manifolds

- **Symmetries.** Transformations which, when applied to dependent or independent variables, gives another solution to the same system of differential equations.

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Differentiable manifolds

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Lie groups

Geometric Integration

- **Symplectic structure** in Hamiltonian systems. Symplecticity:

$$\frac{\partial(p(t), q(t))}{\partial(p(0), q(0))}^\top \begin{pmatrix} 0 & I \\ -I & 0 \end{pmatrix} \frac{\partial(p(t), q(t))}{\partial(p(0), q(0))} = \begin{pmatrix} 0 & I \\ -I & 0 \end{pmatrix}, t \geq 0$$

Geometric Integration

Geometric mechanics

- Reducing the degrees of freedom
- Detecting the relevant geometric structures
- Identifying the symmetries and invariants of different physical systems, such as conservation of energy, conservation of linear or angular momentum
- Describing variational principles
- ...

Geometric Integration

- Standard methods for simulating motion called numerical integrators completely ignore all of the previous hidden physical laws.
- Since about 1990 new methods have been developed called [geometric integrators](#) which obey some of these extra laws.

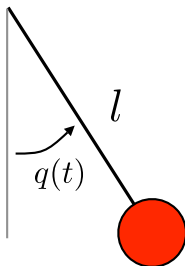
Geometric Integration

It is natural to look forward to those discrete systems which preserve as much as possible the intrinsic properties of the continuous system.

Feng Kang 1985



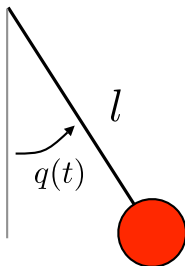
Example: the pendulum



Motion is described by the second-order differential equation

$$\ddot{\theta} = -\frac{g}{l} \sin \theta$$

Example: the pendulum



Motion is described by the second-order differential equation

$$\ddot{\theta} = -\frac{g}{l} \sin \theta$$

or equivalently, with $H = \frac{1}{2ml^2} p^2 + mgl(1 - \cos \theta)$

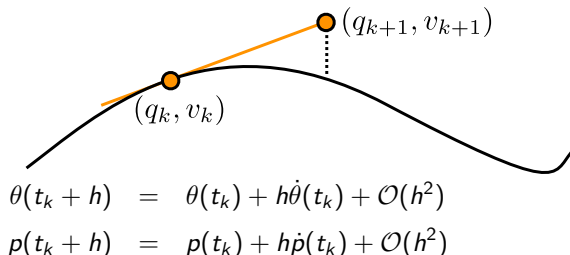
$$\dot{\theta} = \frac{p}{ml^2}$$

$$\dot{p} = -mgl \sin \theta$$

Explicit Euler method

Standard numerical methods:

- Replace $\theta(t)$ and $p(t)$ by θ_k and p_k
- Approximate the differential equations, e.g. by first-order Taylor approximation (Euler methods)



We obtain the **Explicit Euler method**

$$\begin{aligned}\theta_{k+1} &= \theta_k + h \frac{1}{ml^2} p_k \\ p_{k+1} &= p_k - hmg \sin \theta_k\end{aligned}$$

Implicit Euler method

$$\begin{aligned}\theta_{k+1} &= \theta_k + h \frac{1}{ml^2} p_{k+1} \\ p_{k+1} &= p_k - hmg \sin \theta_{k+1}\end{aligned}$$

Symplectic Euler method

$$\begin{aligned}\theta_{k+1} &= \theta_k + h \frac{1}{ml^2} p_{k+1} \\ p_{k+1} &= p_k - hmg \sin \theta_k\end{aligned}$$

Symplectic Euler method

$$\begin{aligned}\theta_{k+1} &= \theta_k + h \frac{1}{ml^2} p_{k+1} \\ p_{k+1} &= p_k - hmg \sin \theta_k\end{aligned}$$

Symplecticity

$$d\theta_{k+1} \wedge dp_{k+1} = d\theta_k \wedge dp_k$$

(Loading...)

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Thanks Ari!!!!

Symplectic integration

Poincaré H. 1893. [Les méthodes nouvelles de la mécanique céleste III](#).
Gauthier–Villars, Paris.

$$\begin{aligned}q_1 - q_0 &= h \frac{\partial H}{\partial p} \left(\frac{q_0 + q_1}{2}, \frac{p_0 + p_1}{2} \right) \\p_1 - p_0 &= -h \frac{\partial H}{\partial q} \left(\frac{q_0 + q_1}{2}, \frac{p_0 + p_1}{2} \right)\end{aligned}$$

A key development of modern [geometric mechanics](#) has been to study dynamical systems on general manifolds such as spheres, tori, and Lie groups, etc not only on vector spaces.

Hamiltonian mechanics and differential geometric methods

The cotangent bundle T^*Q of a **differentiable manifold** Q is equipped with a canonical exact symplectic structure $\omega_Q = d\theta_Q$, where θ_Q is the canonical 1-form on T^*Q . In canonical bundle coordinates (q^i, p_i) on T^*Q the projection reads as $\pi_Q(q^i, p_i) = (q^i)$, and

$$\theta_Q = p_i dq^i, \quad \omega_Q = dq^i \wedge dp_i.$$

Given a Hamiltonian function $H : T^*Q \rightarrow \mathbb{R}$ we define the Hamiltonian vector field

$$\iota_{X_H}\omega_Q = dH$$

Its integral curves are determined by **Hamilton's equations**:

$$\begin{aligned}\frac{dq^i}{dt} &= \frac{\partial H}{\partial p_i}, \\ \frac{dp_i}{dt} &= -\frac{\partial H}{\partial q^i}.\end{aligned}$$

- **Preservation of energy.**

$$0 = \omega_Q(X_H, X_H) = dH(X_H) = X_H(H)$$

we have the $H : T^*Q \rightarrow \mathbb{R}$ is preserved.

- **Preservation of the symplectic form.** $L_{X_H}\omega_Q = 0$. That is, if $\{\phi_{X_H}^t\}$ is the flow of X_H then

$$(\phi_{X_H}^t)^*\omega_Q = \omega_Q .$$

- **Symmetries** and **constants of the motion**

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$$(\phi_{X_H}^t)^*\omega_Q = \omega_Q .$$

- **Symmetries** and **constants of the motion**

Goal: To design numerical methods for X_H preserving the configuration manifold and preserving the canonical symplectic form (or the Hamiltonian).

① Motivation

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③ Parallel iterative methods for variational
integration

Symplectic integration

$$\begin{aligned}\theta_{k+1} &= \theta_k + h \frac{1}{ml^2} p_{k+1} \\ p_{k+1} &= p_k - hmg l \sin \theta_k\end{aligned}$$

$$\begin{aligned}q_1 - q_0 &= h \frac{\partial H}{\partial p} \left(\frac{q_0 + q_1}{2}, \frac{p_0 + p_1}{2} \right) \\ p_1 - p_0 &= -h \frac{\partial H}{\partial q} \left(\frac{q_0 + q_1}{2}, \frac{p_0 + p_1}{2} \right)\end{aligned}$$

A **retraction map on a manifold** M is a smooth map $R: U \subseteq TM \rightarrow M$ such that the restriction map $R_x = R|_{T_x M}$ satisfies

❶ $R_x(0_x) = x$,

❷ identifying $T_{0_x} T_x M \simeq T_x M$

$$DR_x(0_x) = T_{0_x} R_x = \text{Id}_{T_x M}.$$

Example: (M, g) Riemannian manifold. The exponential map $\exp^g: U \subset TM \rightarrow M$ is a typical example

$$\exp_x^g(v_x) = \gamma_{v_x}(1),$$

where γ_{v_x} is the unique Riemannian geodesic satisfying $\gamma_{v_x}(0) = x$ and $\gamma'_{v_x}(0) = v_x$.

²P.-A. Absil, R. Mahony, and R. Sepulchre. Optimization algorithms on matrix manifolds. Princeton University Press, Princeton, NJ, 2008.

Let U be an open neighbourhood of the zero section of TM ,

$$\begin{aligned} R_d: U \subset TM &\longrightarrow M \times M \\ v_x &\longmapsto (R^1(v_x), R^2(v_x)) \end{aligned}$$

such that

- $R_d(0_x) = (x, x)$,
- $T_{0_x} R_x^2 - T_{0_x} R_x^1 = \text{Id}_{T_x M}: T_{0_x} T_x M \simeq T_x M \rightarrow T_x M$ is equal to the identity map on $T_x M$ for any x in M .

Consequence: The extended retraction map R_d is a local diffeomorphism.

Examples of extended retraction maps

On **Euclidean vector spaces**:

- Explicit Euler method: $R_d(x, v) = (x, x + v)$.
- Midpoint rule: $R_d(x, v) = \left(x - \frac{v}{2}, x + \frac{v}{2}\right)$.
- θ -methods with $\theta \in [0, 1]$: $R_d(x, v) = (x - \theta v, x + (1 - \theta) v)$.

More general: Let $R: TM \rightarrow M$ be a retraction map,

$$R_d(x, v) = (R(x, -\theta v), R(x, (1 - \theta) v))$$

is an extended retraction map for $\theta \in [0, 1]$.

Examples of extended retraction maps

- **Riemannian manifold** (M, g) and associated exponential map $\exp_x : T_x M \rightarrow M$:

$$R_d(v_x) = (\exp_x^g(-v_x/2), \exp_x^g(v_x/2)) .$$

- On the sphere S^2 :

$$R_d(x, \xi) = \left(\frac{x - \xi/2}{\|x - \xi/2\|}, \frac{x + \xi/2}{\|x + \xi/2\|} \right) .$$

- Lie groups....

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- Lie groups....

Goal: How to obtain retraction on tangent and cotangent bundles for mechanical systems and optimal control theory

Tangent lift of extended retraction maps

- Canonical tangent bundle projection: $\tau_{TQ} : TTQ \rightarrow TQ$.
- Canonical involution $\kappa_Q : TTQ \rightarrow TTQ$ such that $\kappa_Q^2 = id_{TTQ}$.
Locally,

$$\kappa_Q(q^i, v^i, \dot{q}^i, \dot{v}^i) = (q^i, \dot{q}^i, v^i, \dot{v}^i).$$

Objective

To define an extended retraction map on TQ :

$$R_d^{TTQ} : U \subset TTQ \rightarrow TQ \times TQ.$$

Tangent lift of extended retraction maps

$$\begin{array}{ccc}
 TTQ & \xrightarrow{R_d^T} & TQ \times TQ \\
 \uparrow \kappa_Q \downarrow \kappa_Q & & \uparrow \\
 TTQ & \xrightarrow{TR_d} & T(Q \times Q) \\
 \downarrow \tau_{TQ} & & \downarrow \tau_{Q \times Q} \\
 TQ & \xrightarrow{R_d} & Q \times Q
 \end{array}$$

Proposition (tangent lift)

If $R_d: TQ \rightarrow Q \times Q$ is an extended retraction map on Q , then

$$R_d^T = TR_d \circ \kappa_Q$$

is an extended retraction map on TQ .

Cotangent lift of extended retraction maps

Three ingredients:

- Cotangent lift of a diffeomorphism $F : M_1 \rightarrow M_2$:

$$\hat{F} : T^*M_1 \longrightarrow T^*M_2 \text{ such that } \hat{F} = (TF^{-1})^*.$$

- Canonical symplectomorphism:

$$\alpha_Q : T^*TQ \longrightarrow TT^*Q \text{ such that } \alpha_Q(q, v, p_q, p_v) = (q, p_v, v, p_q).$$

Cotangent lift of extended retraction maps

- The symplectomorphism between $(T^*(Q \times Q), \omega_{Q \times Q})$ and $(T^*Q \times T^*Q, \Omega_{12} = pr_2^* \omega_Q - pr_1^* \omega_Q)$:

$$\Phi : T^*Q \times T^*Q \longrightarrow T^*(Q \times Q), \quad \Phi(q_0, p_0; q_1, p_1) = (q_0, q_1, -p_0, p_1).$$

Objective

To define an extended retraction map on T^*Q :

$$R_d^{TT^*Q} : U \subset TT^*Q \rightarrow T^*Q \times T^*Q.$$

Cotangent lift of extended retraction maps

$$\begin{array}{ccc}
 TT^*Q & \xrightarrow{R_d^{T^*}} & T^*Q \times T^*Q \\
 \alpha_Q \downarrow & & \uparrow \Phi^{-1} \\
 T^*TQ & \xrightarrow{\widehat{R}_d} & T^*(Q \times Q) \\
 \pi_{TQ} \downarrow & & \downarrow \pi_{Q \times Q} \\
 TQ & \xrightarrow{R_d} & Q \times Q
 \end{array}$$

Proposition (cotangent lift)

Let $R_d: TQ \rightarrow Q \times Q$ be an extended retraction map on Q . Then

$$R_d^{T^*} = \Phi^{-1} \circ \widehat{R}_d \circ \alpha_Q: TT^*Q \rightarrow T^*Q \times T^*Q$$

is an extended retraction map on T^*Q .

Corollary

$R_d^{T*} = \Phi^{-1} \circ (TR_d^{-1})^* \circ \alpha_Q: T(T^*Q) \rightarrow T^*Q \times T^*Q$ is a **symplectomorphism** between $(T(T^*Q), d_T\omega_Q)$ and $(T^*Q \times T^*Q, \Omega_{12})$.

Duality between both lifts

$$\langle \Phi(\alpha_{q_0}, \alpha_{q_1}), R_d^T(w) \rangle = \langle (R_d^{T*})^{-1}(\alpha_{q_0}, \alpha_{q_1}), w \rangle^T$$

where $w \in TTQ$ and $(R_d)^{-1}(q_0, q_1) = T\tau_Q(w)$.

Locally,

$$\begin{aligned} R_d^T(q, \dot{q}, v, \dot{v}) &= (R_d^1(q, v), DR_d^1(q, v)(\dot{q}, \dot{v})^T; \\ &\quad R_d^2(q, v), DR_d^2(q, v)(\dot{q}, \dot{v})^T), \\ R_d^{T*}(q, p, \dot{q}, \dot{p}) &= (R_d^1(q, \dot{q}), -(\dot{p}, p)DR_d^{-1}(R_d(q, \dot{q}))_{*1}; \\ &\quad R_d^2(q, \dot{q}), (\dot{p}, p)DR_d^{-1}(R_d(q, \dot{q}))_{*2}) \end{aligned}$$

- Extended retraction map on Q :

$$R_d(q, v) = \left(q - \frac{1}{2}v, q + \frac{1}{2}v \right).$$

- **Tangent lift** of R_d :

$$R_d^T(q, \dot{q}, v, \dot{v}) = \left(q - \frac{1}{2}v, \dot{q} - \frac{1}{2}\dot{v}; q + \frac{1}{2}v, \dot{q} + \frac{1}{2}\dot{v}, \right).$$

- **Cotangent lift** of R_d :

$$R_d^{T*}(q, p, \dot{q}, \dot{p}) = \left(q - \frac{1}{2}\dot{q}, p - \frac{\dot{p}}{2}; q + \frac{1}{2}\dot{q}, p + \frac{\dot{p}}{2} \right).$$

Construction of geometric integrators using retraction maps

For a Hamiltonian function $H: T^*Q \rightarrow \mathbb{R}$, the solutions to Hamilton's equations

$$i_{X_H}\omega = dH$$

are the integral curves to the Hamiltonian vector field given locally by

$$X_H = \frac{\partial H}{\partial p_i} \frac{\partial}{\partial q^i} - \frac{\partial H}{\partial q^i} \frac{\partial}{\partial p_i}.$$

Discretization of such a vector field using an extended retraction map on T^*Q , $R_d^{TT^*Q}: TT^*Q \rightarrow T^*Q \times T^*Q$.

Numerical Method

$$h X_H \left(\tau_{TQ} \left(\left(R_d^{TT^*Q} \right)^{-1} (q_k, p_k; q_{k+1}, p_{k+1}) \right) \right) = \left(R_d^{TT^*Q} \right)^{-1} (q_k, p_k; q_{k+1}, p_{k+1}).$$

The solution $\gamma: I \rightarrow T^*Q$ of Hamilton's equations must satisfy

$$i_{\dot{\gamma}(t)}\omega_Q(\gamma(t)) = dH(\gamma(t)), \text{ equivalently } \dot{\gamma}(t) = \sharp_{\omega_Q}(dH(\gamma(t))).$$

Let $R_d^{TT^*Q}: T(T^*Q) \rightarrow T^*Q \times T^*Q$ be an extended retraction map on T^*Q .

Numerical integrator

$$\left(R_d^{TT^*Q}\right)^{-1}(q_0, p_0; q_1, p_1) = \sharp_{\omega_Q}(h dH((\tau_{T^*Q} \circ \left(R_d^{TT^*Q}\right)^{-1})(q_0, p_0; q_1, p_1))).$$

Proposition [María Barbero-Liñán, DMdD, 2021]

If $R_d^{TT^*Q}: T(T^*Q) \rightarrow T^*Q \times T^*Q$ is the cotangent lift of an extended retraction map on TQ , then

$$\left(R_d^{T^*}\right)^{-1}(q_0, p_0; q_1, p_1) = \sharp_{\omega_Q}(h dH((\tau_{T^*Q} \circ \left(R_d^{T^*}\right)^{-1})(q_0, p_0; q_1, p_1)))$$

defines a **symplectic numerical integrator**.

- Extended retraction map on Q : $R_d(q, v) = (q - v, q)$.
- Cotangent lift of R_d : $R_d^{T*}(q, p, \dot{q}, \dot{p}) = (q - \dot{q}, p, q, p + \dot{p})$.
- Inverse of the cotangent lift:
 $(R_d^{T*})^{-1}(q_0, p_0, q_1, p_1) = (q_1, p_0, q_1 - q_0, p_1 - p_0)$.

Explicit symplectic method for $H(p, q) = \frac{p^2}{2} + V(q)$:

$$\begin{aligned} \frac{q_1 - q_0}{h} &= \frac{\partial H}{\partial p}(q_1, p_0) \\ \frac{p_1 - p_0}{h} &= -\frac{\partial H}{\partial q}(q_1, p_0) \end{aligned}$$

Schematic representation

A schematic representation of a commutative diagram in symplectic geometry. The diagram consists of four nodes and four arrows:

- Top-left node:** $T^*Q \times T^*Q$ (written in red).
- Top-middle node:** TT^*Q .
- Top-right node:** T^*T^*Q .
- Bottom node:** T^*Q .

The arrows and their labels are:

- A horizontal arrow from TT^*Q to $T^*Q \times T^*Q$ labeled $R_d^{T^*}$ (in red).
- A horizontal arrow from T^*T^*Q to TT^*Q labeled \sharp_{ω_Q} .
- A diagonal arrow from T^*Q to TT^*Q labeled X_H .
- A diagonal arrow from T^*Q to T^*T^*Q labeled dH .

The diagram illustrates the relationship between the cotangent bundle T^*Q , its double cotangent bundle TT^*Q , and the product of two cotangent bundles $T^*Q \times T^*Q$.

$$H : T^*S^2 \rightarrow \mathbb{R}$$

$$T^*S^2 \equiv \{(x, p) \in \mathbb{R}^3 \times \mathbb{R}^3 \mid \|x\| = 1, x \cdot p = 0\}.$$

$$\text{Retraction map } R_d : TS^2 \rightarrow S^2 \times S^2 \text{ given by } R_d(x, \xi) = \left(x, \frac{x+\xi}{\|x+\xi\|}\right),$$

$$R_d^{-1}(x_0, x_1) = \left(x_0, \frac{x_1}{x_0 \cdot x_1} - x_0\right),$$

Consider C the matrix with entries

$$c_{ij} = \begin{cases} (x \cdot y) [1 + (x \cdot y)y_i x_i - y_i^2] & \text{if } i = j, \\ (x \cdot y) [(x \cdot y)y_i x_j - y_i y_j] & \text{if } i \neq j. \end{cases}$$

$$\left(R_d^{T^*}\right)^{-1}(x_0, p_0; x_1, p_1) = \left(x_0, p_1 C; \frac{1}{x_0 \cdot x_1} x_1 - x_0, -p_0 + (x_0 \cdot x_1) p_1\right)$$

Symplectic integrator for Hamilton's equations:

$$\begin{aligned} \frac{1}{x_k \cdot x_{k+1}} x_{k+1} - x_k &= h \frac{\partial H}{\partial p}(x_k, p_{k+1} C), \\ -p_k + (x_k \cdot x_{k+1}) p_{k+1} &= -h \frac{\partial H}{\partial q}(x_k, p_{k+1} C). \end{aligned}$$

Optimal control problem (OCP)

$$\min \int_{t_0}^{t_f} F(q(t), u(t)) dt,$$
$$\dot{q} = X(q, u).$$

Pontryagin's Hamiltonian function:

$$H: T^*Q \times U \rightarrow \mathbb{R},$$
$$H(q, p, u) = \langle p, X(q, u) \rangle - F(q, u).$$

If the OCP is regular, controls can be solved from the maximization condition in Pontryagin's Maximum Principle

$$\frac{\partial H}{\partial u} = 0.$$

Use a cotangent lift of a retraction map to define a symplectic integrator for optimal control problems.

$$\begin{array}{ccccc}
 T^*Q \times T^*Q & \xleftarrow{R_d^{T^*}} & TT^*Q & \xleftarrow{\sharp\omega_Q} & T^*T^*Q \xleftarrow{\quad} \mathcal{L}_H \\
 & & \searrow \pi_{T^*Q} & & \swarrow \tau_{T^*Q} \\
 & & T^*Q & &
 \end{array}$$

$$\mathcal{L}_H = \{(q, p, P_q, P_p) \mid P_q = \frac{\partial H}{\partial q}(q, p, u), P_p = \frac{\partial H}{\partial p}(q, p, u), \frac{\partial H}{\partial u}(q, p, u) = 0\}$$

is a Lagrangian submanifold of T^*T^*Q .

- Extension to more complex mechanical systems such as forced systems, constrained systems, control systems, reduced systems, etc.
- Define higher-order retraction maps and study higher-order Lagrangian systems.
- Establish relations with the discrete gradient methods [McLahlan, Quispel, Robioux, 1999; Celledoni et al. 2017].
- Describe geometric integration of Dirac systems.
- Describe symplectic methods using Lagrangian submanifolds defined by Morse families.

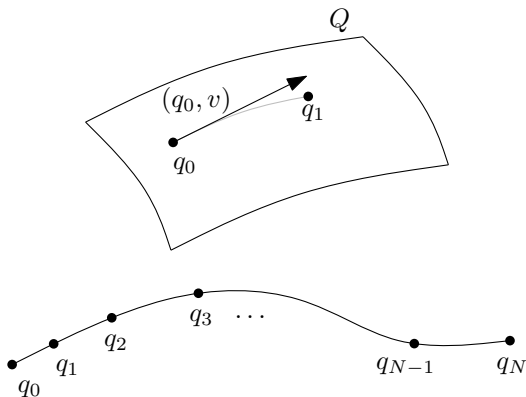
① Motivation

② Retraction maps and symplectic integration

③ Parallel iterative methods for variational
integration

Discrete variational principle

Replace TQ by $Q \times Q$ (velocities by nearby points) and curves by finite sequences of points.



Discrete Euler-Lagrange equations

Given a *discrete Lagrangian*, which is a function $L_d : Q \times Q \rightarrow \mathbb{R}$, a number of steps N and two points $q_0, q_N \in Q$, consider the space \mathcal{C}_d of sequences (q_0, q_1, \dots, q_N) (fixed endpoints). A *trajectory* of the system described by L_d is a critical point of the action sum $\mathcal{S}_d : \mathcal{C}_d \rightarrow \mathbb{R}$,

$$\begin{aligned}\mathcal{S}_d(q_0, q_1, \dots, q_N) &= \sum_{i=1}^N L_d(q_{i-1}, q_i) \\ &= L_d(q_0, q_1) + L_d(q_1, q_2) + \dots + L_d(q_{N-1}, q_N)\end{aligned}$$

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discrete Euler-Lagrange equations (DEL equations)

$$D_1 L_d(q_k, q_{k+1}) + D_2 L_d(q_{k-1}, q_k) = 0, \quad k = 1, \dots, N-1.$$

The boundary conditions are the given values for q_0 and q_N .

Geometric preservation properties

$$D_1 L_d(q_k, q_{k+1}) + D_2 L_d(q_{k-1}, q_k) = 0, \quad k = 1, \dots, N-1.$$

For each k , we can locally solve for q_{k+1} if $D_{12} L_d(q_k, q_{k+1})$ is regular, which in coordinates reads

$$\det \left(\frac{\partial^2 L_d}{\partial q_k^i \partial q_{k+1}^j} \right) \neq 0.$$

The method is symplectic and momentum-preserving.

From continuous to discrete

Let $L : TQ \rightarrow \mathbb{R}$ and $[0, T]$ be given.

Divide $[0, T]$ into N pieces of size $h = T/N$ (time step).

From continuous to discrete

Let $L : TQ \rightarrow \mathbb{R}$ and $[0, T]$ be given.

Divide $[0, T]$ into N pieces of size $h = T/N$ (time step).

For arbitrary (nearby) $q_0, q_1 \in Q$, define $L_d(q_0, q_1) \approx \int_0^h L(q(t), \dot{q}(t)) dt$, where $q(t)$ is a trajectory of the continuous system joining q_0 to q_1 for time h . Since this trajectory is not known in general, we must resort to an approximation such as

$$q(t) \approx \frac{q_0 + q_1}{2}, \quad \dot{q}(t) \approx \frac{q_1 - q_0}{h},$$

so we can define

$$L_d(q_0, q_1) = \int_0^h L\left(\frac{q_0 + q_1}{2}, \frac{q_1 - q_0}{h}\right) dt = hL\left(\frac{q_0 + q_1}{2}, \frac{q_1 - q_0}{h}\right).$$

Momentum preservation. Discrete Noether theorem

L_d is G -invariant

Momentum preservation. Discrete Noether theorem

L_d is G -invariant

$$J_d : Q \times Q \longrightarrow \mathfrak{g}^*$$

$$\langle J_d(x, y), \xi \rangle = \langle D_2 L_d(x, y), \xi_Q(y) \rangle$$

$$\langle D_2 L_d(q_{k-1}, q_k), \xi_Q(q_k) \rangle = \langle D_2 L_d(q_k, q_{k+1}), \xi_Q(q_{k+1}) \rangle$$

Discrete Hamiltonian mechanics

- The discrete Legendre transformations

$$\mathbb{F}^- L_d : Q \times Q \rightarrow T^*Q$$

$$\mathbb{F}^- L_d(q_0, q_1)(X_{q_0}) = -(D_1 L_d)(q_0, q_1)(X_{q_0}), \quad \text{for } X_{q_0} \in T_{q_0}Q$$

$$\mathbb{F}^+ L_d : Q \times Q \rightarrow T^*Q$$

$$\mathbb{F}^+ L_d(q_0, q_1)(X_{q_1}) = (D_2 L_d)(q_1, q_2)(X_{q_1}), \quad \text{for } X_{q_1} \in T_{q_1}Q$$

- The discrete Hamiltonian flow

$F_{L_d} = \mathbb{F}^+ L_d \circ (\mathbb{F}^- L_d)^{-1} : T^*Q \rightarrow T^*Q$ is a symplectomorphism:

$$F_{L_d}^* \omega_Q = \omega_Q$$

Exact discrete Lagrangian

$$\mathbb{L}_h^e(q_0, q_1) = \int_0^h L(q(t), \dot{q}(t)) dt,$$

where $q(t)$ is a trajectory of the continuous system joining q_0 to q_1 for time h . If L is regular, then \mathbb{L}_h^e regular.

Exact discrete Lagrangian

If $q(t)$ is a solution of the continuous system, then the evolution of the discrete system for \mathbb{L}_h^e yields the sequence $q(0)$, $q(h)$, $q(2h)$, $q(3h)$, \dots

Exact discrete Lagrangian

If $q(t)$ is a solution of the continuous system, then the evolution of the discrete system for \mathbb{L}_h^e yields the sequence $q(0)$, $q(h)$, $q(2h)$, $q(3h)$, \dots

In order to write \mathbb{L}_h^e explicitly we need to solve the E-L equations...?

We can write Taylor expansions of \mathbb{L}_h^e in h . The discrete Lagrangians that we will consider must approximate \mathbb{L}_h^e , and the order of approximation will be the order of convergence of the corresponding algorithm.

Variational error analysis

Theorem

Let $L : TQ \rightarrow \mathbb{R}$ be a regular Lagrangian function. Suppose that $L_h^d : Q \times Q \rightarrow \mathbb{R}$ is a regular discrete Lagrangian function and that \mathbb{L}_h^e is the exact discrete Lagrangian function on $Q \times Q$ associated with L . If L_h^d is an order r discretization then

$$F_{L_h^d} = F_{\mathbb{L}_h^e} + O(h^{r+1}),$$

where $F_{L_h^d}$ is the discrete Hamiltonian flow for L_h^d and $F_{\mathbb{L}_h^e}$ is the exact Hamiltonian flow.

Marsden-West 2001, Patrick and Cuell 2009

CONSTRUCTION OF VARIATIONAL INTEGRATORS

We explicitly evaluate the first few terms of the expansion of the exact discrete Lagrangian to give

$$\mathbb{L}_h^e(q(0), q(h), h) = hL(q, \dot{q}) + \frac{h^2}{2} \left(\frac{\partial L}{\partial q} \cdot \dot{q} + \frac{\partial L}{\partial \dot{q}} \cdot \ddot{q} \right) + \mathcal{O}(h^3)$$

where $q = q(0)$, $\dot{q} = \dot{q}(0)$ and so forth. Higher derivatives of $q(t)$ are determined by the Euler-Lagrange equations.

A class of discrete Lagrangian is given by

$$L_d^\alpha(q_0, q_1; h) = hL((1 - \alpha)q_0 + \alpha q_1, \frac{q_1 - q_0}{h})$$

for some parameter $\alpha \in [0, 1]$. Calculating the expansion in h gives

$$L_d^\alpha(q_0, q_1; h) = hL(q, \dot{q}) + \frac{h^2}{2} \left(2\alpha \frac{\partial L}{\partial q} \cdot \dot{q} + \frac{\partial L}{\partial \dot{q}} \cdot \ddot{q} \right) + \mathcal{O}(h^3)$$

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Comparing the expansions of L_d^α and for the exact discrete Lagrangian shows that the method is second-order if and only if $\alpha = 1/2$; otherwise it is only consistent.

$$L(q, \dot{q}) = \dot{q}^T M \dot{q} - V(q)$$

$$\frac{q_1 - q_0}{h} = h M^{-1}(\alpha p_0 + (1 - \alpha)p_1)$$

$$\frac{p_1 - p_0}{h} = -\nabla V(\alpha q_0 + (1 - \alpha)q_1)$$

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Many other Examples: Newmark algorithms, symplectic partitioned Runge-Kutta algorithms, Verlet, etc.

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Many other Examples: Newmark algorithms, symplectic partitioned Runge-Kutta algorithms, Verlet, etc.

BUT other interesting extensions.

Composition of Lagrangian submanifolds [Sniatycki, Tulczyjew, 1972]²

- 1 Let R_d^1 and $R_d^2: TQ \rightarrow Q \times Q$ be 2 different extended retraction maps on Q .
- 2 For $L_d^i = L \circ (R_d^i)^{-1}: Q \times Q \rightarrow \mathbb{R}$, a discrete dynamical system is defined:

$$S_i = \left\{ (q_0, p_0, q_1, p_1) \in T^*Q \times T^*Q \left| \begin{array}{l} p_0 = -D_1 L_d^i(q_0, q_1) \\ p_1 = D_2 L_d^i(q_0, q_1) \end{array} \right. \right\}.$$

- 3 Composition of Lagrangian submanifolds:

$$S_{12} = \left\{ (\alpha_1, \alpha_2) \left| \exists \alpha_{1/2} \in T^*Q \text{ such that } \begin{array}{l} (\alpha_1, \alpha_{1/2}) \in S_1 \\ (\alpha_{1/2}, \alpha_2) \in S_2 \end{array} \right. \right\}.$$

Composition of geometric integrators and Lagrangian submanifolds

Discrete Lagrangian: $L_d^3(q_0, q_2) = L_d^1(q_0, q_1) + L_d^2(q_1, q_2)$.

The discrete equations are

$$\begin{aligned} p_0 &= -D_1 L_d^1(q_0, q_1), \\ 0 &= D_2 L_d^1(q_0, q_1) + D_1 L_d^2(q_1, q_2), \\ p_2 &= D_2 L_d^2(q_1, q_2). \end{aligned}$$

Störmer–Verlet method as composition of geometric integrators

$$R_{d,1}^{-1}(q_0, q_1) = \left(q_0, \frac{q_1 - q_0}{h/2} \right) \quad L_d^1(q_0, q_1) = \frac{h}{2} L \left(q_0, \frac{q_1 - q_0}{h/2} \right)$$

$$R_{d,2}^{-1}(q_1, q_2) = \left(q_2, \frac{q_2 - q_1}{h/2} \right) \quad L_d^2(q_1, q_2) = \frac{h}{2} L \left(q_2, \frac{q_2 - q_1}{h/2} \right).$$

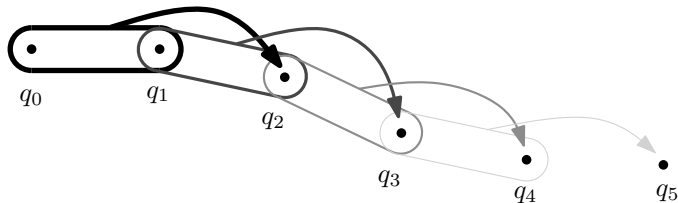
The composition gives the following set of equations:

$$\begin{aligned} p_0 &= p_1 - \frac{h}{2} D_1 L \left(q_0, \frac{q_1 - q_0}{h/2} \right), \\ D_2 L \left(q_0, \frac{q_1 - q_0}{h/2} \right) &= D_2 L \left(q_2, \frac{q_2 - q_1}{h/2} \right), \\ p_2 &= p_1 + \frac{h}{2} D_1 L \left(q_2, \frac{q_2 - q_1}{h/2} \right). \end{aligned}$$

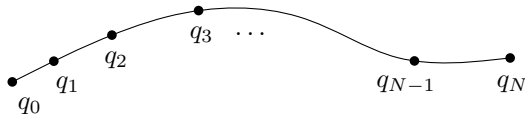
For $L(q, \dot{q}) = \dot{q} M \dot{q} - V(q)$, **Störmer–Verlet method** is recovered.

Boundary conditions

For any regular discrete Lagrangian system, the discrete Euler-Lagrange equations allow us to obtain a new point in the sequence from the last two.



Boundary conditions: Initial and final conditions



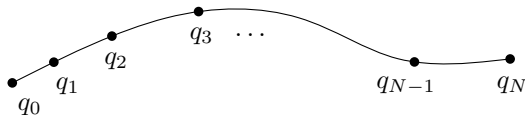
$$D_1 L_d(\textcolor{red}{q}_0, q_1) + D_2 L_d(q_1, q_2) = 0,$$

$$D_1 L_d(q_1, q_2) + D_2 L_d(q_2, q_3) = 0,$$

$$\dots = \dots$$

$$D_1 L_d(q_{N-2}, q_{N-1}) + D_2 L_d(q_{N-1}, \textcolor{red}{q}_N) = 0$$

Boundary conditions: Initial and final conditions



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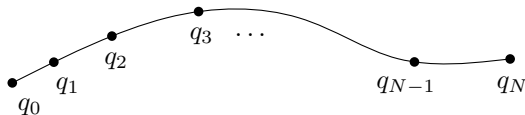
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A standard method of solving a boundary-value problem is to reduce it to the solution of an initial-value problem using the method of **shooting**.

Boundary conditions: Initial and final conditions



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A standard method of solving a boundary-value problem is to reduce it to the solution of an initial-value problem using the method of **shooting**.

For example, if $q_0, q_N \in Q$ and N are given, one can try assigning some value to q_1 , run the sequential algorithm and compare the resulting q_N with the final condition; then adjust the value of q_1 and repeat the process, until the final condition is met within a certain tolerance.

Boundary conditions: Initial and final conditions

However, this approach can often fail to converge in practice, because of a high sensitivity of q_N with respect to the starting guess q_1 . This issue is even more prevalent in optimal control problems.

Parallel iterative methods for variational integration

Sebastián J. Ferraro, DMdD, Rodrigo T. Sato Martín de Almagro.

Parallel iterative methods for variational integration applied to navigation problems, 7th IFAC Workshop on Lagrangian and Hamiltonian Methods for Nonlinear Control

We propose a relaxation strategy for solving boundary value problems for the discrete equations given above. The algorithm can be implemented using a **parallel computing approach**, which can significantly improve its performance and simplify the way to find approximate solutions.

Parallel iterative methods for variational integration

Our method starts with a sequence $\{q_k\}$ chosen as initial guess, solely required to satisfy the boundary conditions.

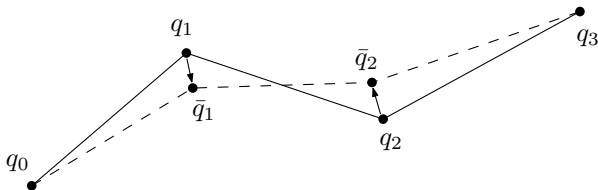
Parallel iterative methods for variational integration

Our method starts with a sequence $\{q_k\}$ chosen as initial guess, solely required to satisfy the boundary conditions.

Produce a **new sequence** $\{\bar{q}_k\}$ with $\bar{q}_0 = q_0$ and $\bar{q}_N = q_N$. For each $k = 1, \dots, N - 1$, we find \bar{q}_k by solving a modified (“parallelized”) version of the discrete Euler-Lagrange equations:

$$D_2 L_d(q_{k-1}, \bar{q}_k) + D_1 L_d(\bar{q}_k, q_{k+1}) = 0. \quad (1)$$

At the endpoints, we simply take $\bar{q}_0 = q_0$ and $\bar{q}_N = q_N$. Computing \bar{q}_k for all k completes one iteration, and the following one will use $\{\bar{q}_k\}$ in place of $\{q_k\}$.



Parallel iterative methods for variational integration

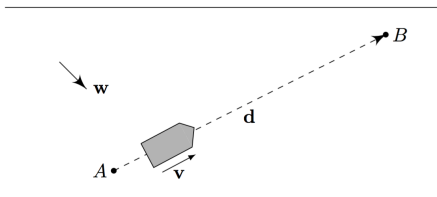
In general, neither $\{q_k\}$ nor $\{\bar{q}_k\}$ will be a solution of DEL equations but by iterating this procedure we can approach a solution $\{q_k^*\}$ of the DEL equations with fixed boundary conditions, under certain reasonable assumptions.

Parallel iterative methods for variational integration

In general, neither $\{q_k\}$ nor $\{\bar{q}_k\}$ will be a solution of DEL equations but by iterating this procedure we can approach a solution $\{q_k^*\}$ of the DEL equations with fixed boundary conditions, under certain reasonable assumptions.

$$D_2 L_d(q_{k-1}, q_k) + D_1 L_d(q_k, q_{k+1}) + \\ (D_{22} L_d(q_{k-1}, q_k) + D_{11} L_d(q_k, q_{k+1})) \cdot (\bar{q}_k - q_k) = 0,$$

Zermelo's navigation problem



The minimum time trajectories are precisely the geodesics for a particular type of **Finsler metric**, a Randers metric defined by

$$F(q, v_q) = \sqrt{a(v_q, v_q)} + \langle b(q), v_q \rangle$$

$$a(v_q, v_q) = \frac{1}{\alpha(q)} g(v_q, v_q) + \frac{1}{\alpha(q)^2} g(W(q), v_q)^2$$

$$\langle b(q), v_q \rangle = -\frac{1}{\alpha(q)} g(W(q), v_q) = -\left\langle \frac{b_g(W(q))}{\alpha(q)}, v_q \right\rangle$$

$$\alpha(q) = 1 - g(W(q), W(q)) = 1 - |W(q)|^2 > 0.$$

Zermelo's navigation problem

The time it takes the ship to move along a curve $\gamma: [t_0, t_N] \rightarrow Q$ is

$$\int_{t_0}^{t_N} F(\gamma(s), \dot{\gamma}(s)) ds. \quad (2)$$

Zermelo's navigation problem

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$$\int_{t_0}^{t_N} F(\gamma(s), \dot{\gamma}(s)) ds. \quad (2)$$

Note that this integral is invariant under orientation-preserving reparametrizations of γ , since Finsler metrics are positively 1-homogeneous, that is, $F(q, \lambda v_q) = \lambda F(q, v_q)$ for any $\lambda > 0$. Therefore, the solution curves are not unique. In fact, F is not regular as a Lagrangian function. Similar to the case of Riemannian metrics and the problem of minimizing length or energy, this can be circumvented by considering instead the functional

$$\int_{t_0}^{t_N} (F(\gamma(s), \dot{\gamma}(s)))^2 ds. \quad (3)$$

Any extremal of this functional will be an extremal of (2), and any extremal of (2) admits an orientation-preserving reparametrization that makes it an extremal of (3).

Zermelo's navigation problem

As a particular case, consider $Q = \mathbb{R}^2$ with the Euclidean metric, where we are to find critical curves $(x, y) = (x(s), y(s))$ for the functional

$$\int_{t_0}^{t_N} \left[\sqrt{\frac{1}{\alpha}(\dot{x}^2 + \dot{y}^2) + \frac{1}{\alpha^2}(W_1(x, y)\dot{x} + W_2(x, y)\dot{y})^2} - \frac{1}{\alpha}(W_1(x, y)\dot{x} + W_2(x, y)\dot{y}) \right]^2 ds$$

with $\alpha = 1 - (W_1^2 + W_2^2)$.

As the discrete Lagrangian, we used

$$L_d(q_0, q_1) = \frac{h}{2} \left(F^2 \left(q_0, \frac{q_1 - q_0}{h} \right) + F^2 \left(q_1, \frac{q_1 - q_0}{h} \right) \right).$$

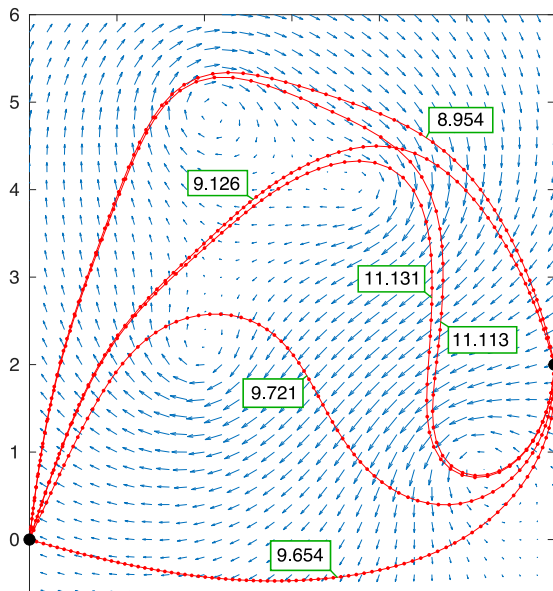
Zermelo's navigation problem

(Zermelo)

Zermelo's navigation problem

(Zermelo)

Zermelo's navigation problem



A minimal fuel trajectory

We also consider a non-equivalent variant of Zermelo's problem. If $T > 0$ is a fixed time, we seek trajectories minimizing the cost function

$$\int_0^T \frac{1}{2}(u_1^2 + u_2^2) dt ,$$

which can be interpreted as a measure of fuel expenditure.

$$\dot{x} = u_1 + W_1(x, y) ,$$

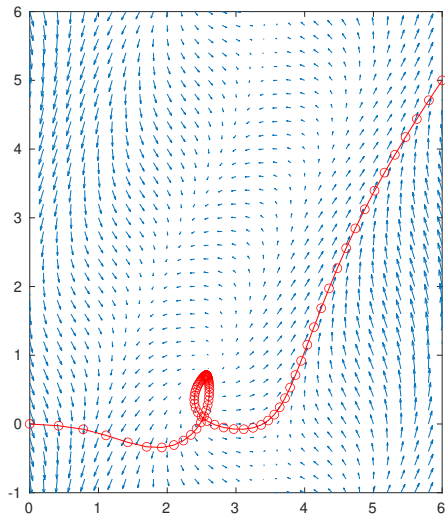
$$\dot{y} = u_2 + W_2(x, y) .$$

The goal is to arrive at a given destination at time T , extremizing fuel expenditure with no a priori bounds on the engine's power. This problem is equivalent to solving the Euler-Lagrange equations for the Lagrangian

$$L(x, y, \dot{x}, \dot{y}) = \frac{1}{2} [(\dot{x} - W_1(x, y))^2 + (\dot{y} - W_2(x, y))^2] ,$$

with fixed $(x(0), y(0))$ and $(x(T), y(T))$ as boundary conditions.

A minimal fuel trajectory for a fixed total duration $T = 30$, joining $(0,0)$ to $(6,5)$, with $N = 200$.



Interpolation problems

Fuel-optimal control problem with a weight minimizing the total variation in the control variables. Minimize the cost functional

$$\int_0^T \frac{1}{2}(u_1^2 + u_2^2 + cv_1^2 + cv_2^2) dt$$

subject to the control equations

$$\begin{aligned} \dot{x} &= u_1 + W_1(x, y), & \dot{y} &= u_2 + W_2(x, y), \\ \dot{u}_1 &= v_1, & \dot{u}_2 &= v_2. \end{aligned}$$

Interpolation problems

The continuous problem is equivalent to solving the fourth-order Euler-Lagrange equations for the second-order Lagrangian

$$\begin{aligned} L(x, y, \dot{x}, \dot{y}, \ddot{x}, \ddot{y}) = & \frac{1}{2} [(\dot{x} - W_1(x, y))^2 + (\dot{y} - W_2(x, y))^2 \\ & + c(\ddot{x} - D_1 W_1(x(t), y(t))\dot{x} - D_2 W_1(x(t), y(t))\dot{y})^2 \\ & + c(\ddot{y} - D_1 W_2(x(t), y(t))\dot{x} - D_2 W_2(x(t), y(t))\dot{y})^2] \end{aligned}$$

As boundary conditions, we consider $(q(0), \dot{q}(0))$ and $(q(T), \dot{q}(T))$ fixed. In addition, the system is subject to the interpolation constraints

$$q(\hat{t}_a) = \hat{q}_a, \quad \text{for all } a = 1, \dots, l-1 \quad (4)$$

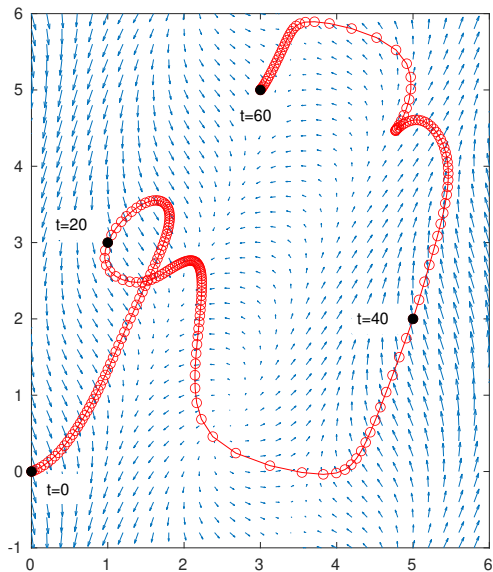
with $0 < \hat{t}_a < \hat{t}_b < T$ for all $a, b \in \{1, \dots, l-1\}$ and $a < b$.

Interpolation problems

As a discretization of the cost function we propose, for instance, a 2-stage Lobatto discretization:

$$\begin{aligned} L_d(q_k, v_k, q_{k+1}, v_{k+1}) = \\ \frac{h}{2} \left[L \left(q_k, v_k, \frac{2}{h^2} (3(q_{k+1} - q_k) - h(v_{k+1} + 2v_k)) \right) \right. \\ \left. + L \left(q_{k+1}, v_{k+1}, -\frac{2}{h^2} (3(q_{k+1} - q_k) - h(2v_{k+1} + v_k)) \right) \right] \end{aligned}$$

An optimal trajectory for the second-order problem with interpolation nodes



Conclusions

Ferraro, S., DMdD., and Sato Martín de Almagro, R.T. (2021). [A parallel iterative method for variational integration](#). Work in progress.

- We prove rigorous conditions for the convergence of the parallel DEL equations
- Extensions to second-order Lagrangians.
- time-dependent water currents can be added to the proposed navigation problems.
- We adapt our parallel iterative method for the case of invariant first and second order Lagrangian systems where the configuration space is a Lie group.
- Problems involving sharp univariate constraints such as state space or control space exclusion zones have not yet been studied using this approach (penalty potentials).

Thank you!!!