Non-Canonical Hamiltonian systems and Implementations

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Introduction

- Non-Canonical Hamiltonian Systems
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Constrained Mechanical Systems

Consider a mechanical system described by position coordinates $q_1, \ldots, q_d$ and suppose that the motion is constrained to satisfy $g(q) = 0$. Let $U(q)$ be the potential energy and $T(q, \dot{q}) = \frac{1}{2}\dot{q}^T M(q)\dot{q}$ the kinetic energy and put:

$$L(q, \dot{q}) = T(q, \dot{q}) - U(q) - q(q)^T \lambda \qquad (1.1)$$

where λ are a vector of Lagrangian multipliers.
The Euler-Lagrange of the variational problem for $\int_0^t L(q, \dot{q})dt$ is then given by:

$$\frac{d}{dt}\left(\frac{\partial L}{\partial \dot{q}}\right) - \frac{\partial L}{\partial q} = 0 \qquad (1.2)$$

Constrained Mechanical Systems

Written as first order differential equations:

$$\begin{aligned} \dot{q} &= v \\ M(q)\dot{v} &= f(q,v) - G(q)^T\lambda \\ 0 &= g(q) \end{aligned} \tag{1.3}$$

where $f(q,v) = -\frac{\partial}{\partial q}(M(q)v) + \nabla_q T(q,v) - \nabla_q U(q)$ and $G(q) = \frac{\partial g}{\partial q}(q)$
Which is a differential algebraic equation.

Constrained Mechanical Systems

We solve this system by differentiating until an ODE is obtained (2 times), which gives:

$$0 = G(q)v, \quad 0 = g''(q)(v, v) + G(q)\dot{v} \tag{1.4}$$

This together with the second relation in Equation (1.3) gives the following system:

$$\begin{pmatrix} M(q) & G(q)^T \\ G(q) & 0 \end{pmatrix} \begin{pmatrix} \dot{v} \\ \lambda \end{pmatrix} = \begin{pmatrix} f(q, v) \\ -g''(q)(v, v) \end{pmatrix} \tag{1.5}$$

furthermore the solution have to fulfil:

$$\dot{q} = v, \quad \dot{v} = \dot{v}(q, v) \tag{1.6}$$

which we from the ODE course know has a locally unique solution.

Index reduction

Consider the *configuration manifold*:

$$\mathcal{Q} = \{q; g(q) = 0\}. \tag{1.7}$$

Then Equation 1.6 thus define a differential equation on the manifold.

Solving Equation 1.6 in stead of Equation 1.3 is called index reduction, further we can use methods on manifolds, to further induce the system to stay on the manifold.

Linear growth in the Hamiltonian $\implies$ Not compatible with symplectic methods as it is no longer a Hamiltonian system.

Using Hamiltonian Formulation

$$\begin{aligned} \dot{q} &= H_p(p,q) \\ \dot{p} &= -H_q(p,q) - G(q)^T\lambda \\ 0 &= g(q) \end{aligned} \tag{1.8}$$

where $H(p,q) = \frac{1}{2}p^T M(q)^{-1} p + U(q)$

Differentiating the constraint two times yields:

$$\lambda = \frac{\frac{\partial}{\partial q}\left(G(q)H_p(p,q)\right)H_p(p,q) - G(q)H_{pp}(p,q)H_q(p,q)}{G(q)H_{pp}(p,q)G(q)^T} \tag{1.9}$$

and the manifold:

$$\mathcal{M} = \{(p,q); g(q) = 0, G(q)H_p(p,q) = 0\} \tag{1.10}$$

Symplectic first order method

Algorithm

We extend the symplectic Euler to Hamiltonian systems with constraints:

$$\begin{aligned} \hat{p}_{n+1} &= p_n - h(H_q(\hat{p}_{n+1} q_n) + G(q_n)^T \lambda_{n+1}) \\ q_{n+1} &= q_n + hH_p(\hat{p}_{n+1}, q_n) \\ 0 &= g(q_{n+1}) \end{aligned} \tag{1.11}$$

This satisfies the constraint $g(q) = 0$ *but not* $G(q)H_p(p, q) = 0$*, we append the projection:*

$$\begin{aligned} p_{n+1} &= p_{n+1} + hG(q_{n+1}^T \mu_{n+1}) \\ 0 &= G(q_{n+1})H_p(p_{n+1}, q_{n+1}) \end{aligned} \tag{1.12}$$

RATTLE (for General Hamiltonians)

Algorithm (Jay and Reich 1993-94)

For consistent values $(p_n, q_n) \in \mathcal{M}$ *define:*

$$\begin{aligned}
p_{n+\frac{1}{2}} &= p_n - \frac{h}{2}(H_q(p_{n+\frac{1}{2}}, q_n) + G(q_n)^T \lambda_n) \\
q_{n+1} &= q_n + \frac{h}{2}(H_q(p_{n+\frac{1}{2}}, q_n) + H_q(p_{n+\frac{1}{2}}, q_{n+1}) \\
0 &= g(q_{n+1}) \\
p_{n+1} &= p_{n+\frac{1}{2}} - \frac{h}{2}(H_q(p_{n+\frac{1}{2}}, q_{n+1}) + G(q_{n+1})^T \mu_n) \\
0 &= G(q_{n+1}) H_p(p_{n+1}, q_{n+1})
\end{aligned} \tag{1.13}$$

This algorithm makes sure that the approximation stays exactly on the solution manifold. Further it is symmetric, symplectic and converges of second order.

Splitting

Lemma

Consider a Hamiltonian, a function $g(q)$ with $G(q) = g'(q)$ and let the manifold $\mathcal{M}$ be as before. if:

$$G(q)H_p^{[i]}(p,q) = 0, \quad \forall (p,q) \in \mathcal{M} \tag{1.14}$$

then the system

$$\begin{aligned} \dot{q} &= H_p^{[i]}(p,q) \\ \dot{p} &= -H_q(p,q)^{[i]} - G(q)^T\lambda \\ 0 &= G(q)H_p(p,q) \end{aligned} \tag{1.15}$$

defines a differential equation on the manifold $\mathcal{M}$ and its flow is a symplectic transformation on the manifold.

A special case of this lemma is where the Hamiltonian is the total energy, then we (can) use the splitting:

$$H(p,q) = T(p,q) + U(q) \tag{1.16}$$

Poisson Systems

Definition (Lie derivative)

For a differential equation

$$\dot{y} = f^{[1]}(y) + f^{[2]}(y) \tag{2.1}$$

we define the Lie derivative

$$D_i = \sum_j f_j^{[i]}(y) \frac{\partial}{\partial y_j} \tag{2.2}$$

The derivative of a function $F(p, q)$ along the flow of a Hamiltonian system is given by its Lie derivative:

$$\frac{d}{dt}(F(p(t), q(t))) = \sum_{i=1}^{d} \left(\frac{\partial F}{\partial q_i} \frac{\partial H}{\partial p_i} - \frac{\partial F}{\partial p_i} \frac{\partial H}{\partial q_i} \right) \tag{2.3}$$

Poisson Systems

Definition (Canonical Poisson Bracket)

The (canonical) Poisson bracket of two smooth functions $F(p,q)$ and $G(p,q)$ is the function:

$$\{F,G\}(y) = \sum_{i=1}^{d} \left(\frac{\partial F}{\partial q_i}\frac{\partial G}{\partial p_i} - \frac{\partial F}{\partial p_i}\frac{\partial G}{\partial q_i} \right) \qquad (2.4)$$

or in vector notation $\{F,G\}(y) = \nabla F(y)^T J^{-1} \nabla G(y)$,
where $J = \begin{pmatrix} 0 & I \\ -I & 0 \end{pmatrix}$

Properties:

- Bilinear
- Skew-Symmetric
- $\{\{F,G\},H\} + \{\{G,H\},F\} + \{\{H,F\},G\} = 0$ (Jacobi)
- $\{F \cdot G, H\} = F\{G,H\} + G\{F,H\}$ (Leibniz)

Poisson Systems

In this notation the Lie derivative changes to

$$\frac{d}{dt}F(y(t)) = \{F, H\}(y(t)) \tag{2.5}$$

Further an invariant is a function that satisfies:

$$\{I, H\} = 0 \tag{2.6}$$

Note that the Hamiltonian is an invariant.

Theorem (Poisson 1809)

If I_1 and I_2 are invariants, then their Poisson bracket $\{I_1, I_2\}$ is a again an invariant.

Further we have that the Hamiltonian system can be written as:

$$\dot{y}_i = \{y_i, H\}, \quad i = 1, \ldots, 2d \tag{2.7}$$

General Poisson Structures

The idea is now to generalize the Canonical Poisson bracket such that we have a general smooth-valued matrix in stead of the the constant matrix J.

Definition (Generalized Poisson Bracket)

The (Generalized) Poisson bracket of two smooth functions $F(p,q)$ *and* $G(p,q)$ *is the function:*

$$\{F,G\}(y) = \sum_{i,j=1}^{n} \left(\frac{\partial F(y)}{\partial y_i} b_{ij}(y) \frac{\partial G(y)}{\partial y_j} \right) \qquad (2.8)$$

or in vector notation $\{F,G\}(y) = \nabla F(y)^T B(y) \nabla G(y)$*,*
where $B(y) = (b_{ij}(y))$

General Poisson Structures

Lemma

The generalized Poisson bracket is bilinear, skew-symmetric and satisfies Leibniz' rule as well as the Jacobi identity if and only if:

$$b_{ij}(y) = -b_{ji}, \quad \forall i, j \tag{2.9}$$

and for all i, j, k

$$\sum_{l=1}^{n} \left(\frac{\partial b_{ij}(y)}{\partial y_l} b_{lk}(y) + \frac{\partial b_{jk}(y)}{\partial y_l} b_{li}(y) + \frac{\partial b_{ki}(y)}{\partial y_l} b_{lj}(y) \right) = 0 \tag{2.10}$$

Definition (General Poisson System)

If the matrix $B(y)$ satisfies the properties above, then $\dot{y}_i = \{y_i, H\}$ for $i = 1, \ldots, 2d$ defines a Poisson system. It can also be written as: $\dot{y} = B(y)\nabla H(y)$

Note: The Hamiltonian is still an invariant

General Poisson Structures

Consider the following constrained Hamiltonian system:

$$\dot{x} = J^{-1}\left(\nabla H(x) + \sum_{i=1}^{m} \lambda_i(x)\nabla g_i(x)\right), \quad x = (p,q)^T \tag{2.11}$$

on the manifold:

$$\mathcal{M} = \{x | \, (g(q), G(q)H(p,q))^T = 0\} \tag{2.12}$$

We use y as local coordinates on the manifold via the transformation:

$$x = \mathcal{X}(y) \tag{2.13}$$

The equation now changes to $(X(y) = \mathcal{X}'(y))$:

$$X(y)\dot{y} = J^{-1}\left(\nabla H(\mathcal{X}(y)) + \sum_{i=1}^{m} \lambda_i(\mathcal{X}(y))\nabla g_i(\mathcal{X}(y))\right) \tag{2.14}$$

General Poisson Structures

Multiplying from the left with $X(y)^T J$ and note that the columns of $X(y)$ are orthogonal to the gradients ∇g_i. This yields

$$X(y)^T J X(y)\dot{y} = X(y)^T \nabla H(\mathcal{X}(y)) \tag{2.15}$$

From a previous assumption we know that $X(y)^T J X(y)$ is invertible, so we set $B(y) = \left(X(y)^T J X(y)\right)^{-1}$ and $K(y) = H(\mathcal{X}(y))$ we thus get:

$$\dot{y} = B(y)\nabla K(y) \tag{2.16}$$

General Poisson Structures

The following theorem sums it up:

Theorem

For a Hamiltonian system on a symplectic submanifold $\mathcal{M}$, the equivalent differential equation in local coordinates (the above equations) is a Poisson system.

Lemma

A Hamiltonian system without constraints becomes a Poisson system in non-canonical coordinates

General Poisson Structures

Theorem (Darboux 1882, Lie 1888)

Suppose that the matrix $B(y)$ defines a Poisson bracket and is of constant rank $n - q = 2m$ in a neighbourhood of $y_0 \in \mathbb{R}^n$. Then, there exist functions $P_1(y), \dots, P_m(y)$, $Q_1(y), \dots, Q_m(y)$, and $C_1(y), \dots, C_q(y)$ satisfying

$$\begin{array}{lll} \{P_i, P_j\} = 0 & \{P_i, Q_j\} = -\delta_{ij} & \{P_i, C_l\} = 0 \\ \{Q_i, P_j\} = \delta_{ij} & \{Q_i, Q_j\} = 0 & \{Q_i, C_l\} = 0 \\ \{C_K, P_j\} = 0 & \{C_K, Q_j\} = 0 & \{C_k, C_l\} = 0 \end{array} \tag{2.17}$$

on a neighbourhood of y_0. The gradients of P_i, Q_i, C_k are linearly independent, so that $y \mapsto (P_i(y), Q_i(y), C_k(y))$ constitutes local change of coordinates to canonical form

General Poisson Structures

Lemma (Transformation to Canonical Form)

Denote the transformation of the previous theorem by $z = (P_i(y), Q_i(y), C_k(y))$*. With this change of coordinates, the Poisson system* $\dot{y} = B(y)\nabla H(y)$ *becomes:*

$$\dot{p} = -K_q(p,q,c), \quad \dot{q} = -K_p(p,q,c), \quad \dot{c} = 0 \qquad (2.18)$$

Poisson Integrators

Consider the differential equation:

$$\dot{y} = B(y)\nabla H(y) \tag{2.19}$$

Definition

A transformation $\phi : U \to \mathbb{R}^n$ (U is an open set in $\mathbb{R}^n$) is called a Poisson map with respect to the Poisson bracket if its Jacobian matrix satisfies:

$$\phi'(y)B(y)\phi'(y)^T = B(\phi(y)) \tag{2.20}$$

Note that for canonical Hamiltonian system this is equivalent to a symplectic map.

Definition

A map $\psi : \mathcal{M} \to \mathcal{M}$ on a symplectic manifold $\mathcal{M}$ is called symplectic if for every $x \in \mathcal{M}$

$$\omega_{\psi(x)}(\psi'(x)\xi_1, \psi'(x)\xi_2) = \omega_x(\xi_1, \xi_2), \quad \forall \xi_1, \xi_2 \in T_x\mathcal{M} \tag{2.21}$$

Poisson Integrators

Theorem

If $B(y)$ is the structure matrix of a Poisson bracket, then the exact solution of the Poisson system is a Poisson map.

Theorem

The exact solution of a Constrained Hamiltonian system on a symplectic submanifold is symplectic

This shows us how we are able to use symplectic solver again.

Definition (Casimirs)

A function $C(y)$ is called a Casimir function of the Poisson system if:

$$\nabla C(y)^T B(y) = 0, \quad \forall y \tag{2.22}$$

A Casimir function is an invariant of all Poisson systems with structure matrix $B(y)$ whatever the Hamiltonian is.

Poisson Integrators

Theorem

Let $f(y)$ and $B(y)$ be smooth on an open set $U \subset \mathbb{R}^m$, and assume that $B(y)$ represents the Poisson bracket. Then $\dot{y} = f(y)$ is locally of the Poisson form if and only if:

- *The exact solution respects the Casimirs of $B(y)$ i.e. $C_i(\phi_t(y)) =$const.*
- *The exact solution is a Poisson map for all $y \in U$ and for all sufficiently small t*

in other words: Being a Poisson map and respecting the Casimirs is characteristic for the exact solution of a Poisson system.

Poisson Integrators

Lemma

An integrator for a Hamiltonian system on a manifold is symplectic if and only if the integrator written in local coordinates corresponding to a coordinate map $x = \mathcal{X}(y)$*, is a Poisson integrator for the structure matrix* $B(y)$*.*

Lemma (Symplectic Euler)

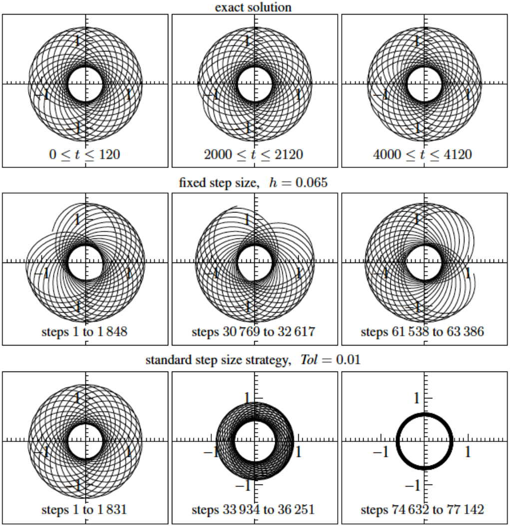
The symplectic euler is a Poisson integrator for all separable Hamiltonians

Lemma (Splitting)

Suppose that the Hamiltonian permits a decomposition as $H(y) = H^{[1]}(y) + \ldots + H^{[m]}(y)$ *such that the individual problem can be solved explicitly. Then the composition is a Poisson solver.*

Structure preserving Implementations

Consider the Kepler problem solved with the Störmer Verlet scheme (and symplectic euler).



Time Transformation

Now consider a non-equidistant discretization chosen in advance. If such transformation is given as the solution of a differential equation, it follows from the chain rule $\frac{dy}{d\tau} = \frac{dy}{dt}\frac{dt}{d\tau}$ that the transformed system is

$$y' = \sigma(y) f(y), \quad t' = \sigma(y) \tag{3.1}$$

here prime indicates derivative with respect to τ, and the letter y is used for both differential equations.

If $\sigma(y) > 0$ the correspondence $t \leftrightarrow \tau$ is bijective.

Applying a numerical method with constant stepsize ε to equation (3.1) yields identical approximations of $y(t_n) = y(\tau_n)$, where $\tau_n = n\varepsilon$ and $t_{n+1} - t_n \approx \varepsilon\sigma(y_n)$.

Disadvantage: An explicit splitting will typically not be possible

Time Transformation (Symplecticity)

Theorem

For $\dot{y} = f(y) = J^{-1}\nabla H(y)$ being a Hamiltonian system, then $y' = \sigma(y)f(y)$ is a Hamiltonian system if and only if $\sigma(y) = constant$

Theorem

The function

$$K(y) = \sigma(y)\left(H(y) - H_0\right) \tag{3.2}$$

is a Hamiltonian function, which means that the corresponding Hamiltonian system is:

$$y' = \sigma(y)J^{-1}\nabla H(y) + \left(H(y) - H_0\right)J^{-1}\sigma(y) \tag{3.3}$$

Compared to the real Hamiltonian we have introduced a perturbation, which vanished along the solution which passes through y_0

Time Transformation (Symplecticity)

Algorithm

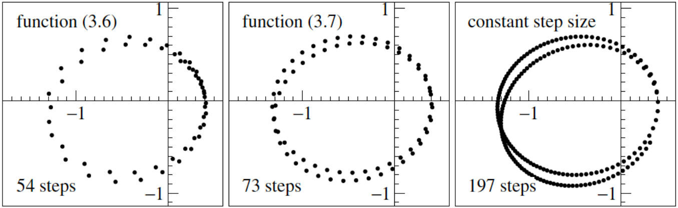
Apply an arbitrary symplectic one-step method with constant step-size ε to the Hamiltonian system (3.3), augmented by $t' = \sigma(y)$. This yields numerical approximations (y_n, t_n) with $y_n \approx y(t_n)$.

Choices of $\sigma(y)$

1. In general $\sigma(y) = \|f(y)\|^{-1}$ (McLeod and Sanz-Serna 1982, and Huang and Leimkuhler 1997)
2. Two body problem $\sigma(p, q) = \|q\|^{\alpha}$ (Budd and Piggott 2003)
3. General Hamiltonian Systems $\sigma(q) = \left((H_0 - U(q)) + \nabla U(q)^T M^{-1} \nabla U(q)\right)^{-1/2}$
4. Equidistant steps in the $q-$space $\sigma(q) = (H_0 - U(q))^{-1/2}$

Time Transformation (Symplecticity)

Choices 3 and 4, and constant step-size applied to the Kepler problem:



Time Transformation (Reversibility)

Theorem

For ρ-reversible differential equations $\dot{y} = f(y)$the transformed problem, remains ρ-reversible if

$$\sigma(\rho y) = \sigma(y) \tag{3.4}$$

Reversible Controllers

Similar to the previous approach we consider:

$$y' = \frac{1}{z} f(y), \quad z\sigma(y) = 1. \tag{3.5}$$

Here we would like discretize the relation $z\sigma(y) = 1$, and then solve the differential equation using this information.

So consider the derivative of $z\sigma(y) = 1$ (using Leibniz' rule):

$$z'\sigma(y) + z\nabla\sigma(y)^T y' = 0 \tag{3.6}$$

which leads to the system of equations

$$\begin{aligned} y' &= \tfrac{1}{z} f(y) \\ z' &= -\tfrac{1}{\sigma(y)} z\nabla\sigma(y)^T f(y) =: G(y) \end{aligned} \tag{3.7}$$

Note: $I(y, z) = z\sigma(y)$ is an invariant

Reversible Controllers

Algorithm

Let $\Phi_h(y)$ be a one step method for the initial value problem. With $G(y)$ be as above, $z_0 = 1/\sigma(y_0)$ and constant ε, we let:

$$\begin{aligned} z_{n+1/2} &= z_n + \varepsilon G(y_n)/2 \\ y_{n+1} &= \Phi_{\varepsilon/z_{n+1/2}}(y) \\ z_{n+1} &= z_{n+1/2} + \varepsilon G(y_n)/2 \end{aligned} \tag{3.8}$$

The values y_n approximates $y(t_n)$ where $t_{n+1} = t_n + \varepsilon/z_{n+1/2}$

Notice the relation to the Strang splitting.

With the notation:

$$\hat{\Phi}_\varepsilon : \begin{pmatrix} y_n \\ z_n \end{pmatrix} \to \begin{pmatrix} y_{n+1} \\ z_{n+1} \end{pmatrix}, \quad \hat{\rho} = \begin{pmatrix} \rho & 0 \\ 0 & 1 \end{pmatrix}$$

then the algorithm has the following properties:

- Symmetric whenever the Φ_h is symmetric
- ρ-reversible whenever Φ_h is ρ-reversible and $G(\rho y) = -G(y)$

Reversible Controllers

Algorithm (Störmer Verlet)

Using the Störmer Verlet method as basic method on a separable Hamiltonian system, then the above algorithm writes:

$$\begin{aligned} z_{n+1/2} &= z_n + \varepsilon G(y_n)/2 \\ p_{n+1/2} &= p_n - \varepsilon \nabla U(q_n)/(2z_{n+1/2}) \\ q_{n+1} &= q_n + \varepsilon \nabla T(p_{n+1/2})/z_{n+1/2} \\ z_{n+1} &= z_{n+1/2} + \varepsilon G(y_n)/2 \end{aligned} \tag{3.9}$$

Multiple Time stepping

Used in situations where:

- Many solution components of the differential equation vary slowly and only a few components have fast dynamics
- Computationally expensive parts of the right-hand side do not contribute much to the dynamics of the solution.

Fast-Slow splitting

Consider the differential equation

$$\dot{y} = f(y), \quad f(y) = f^{[\text{fast}]} + f^{[\text{slow}]} \tag{3.10}$$

where $f^{[\text{slow}]}$ is more expensive to evaluate than $f^{[\text{fast}]}$ then we have the following algorithm

Algorithm

For a given $N \geq 1$ and for the differential equation above a multiple time stepping method is obtained from:

$$(\Phi_{h/2}^{[slow]})^* \circ (\Phi_{h/N}^{[fast]})^N \circ (\Phi_{h/2}^{[slow]}) \tag{3.11}$$