A nonholonomic Newmark method

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Classical Newmark method

Consider a second order differential equation

$$\frac{d^2q}{dt^2} = \Gamma(q, \dot{q}) \qquad \text{(Here } q \in Q = \mathbb{R}^n.\text{)}$$

The (classical) Newmark method is given by

$$q_{k+1} = q_k + h\dot{q}_k + h^2\left(\frac{1}{2} - \beta\right)\Gamma(q_k, \dot{q}_k) + h^2\beta\Gamma(q_{k+1}, \dot{q}_{k+1})$$
$$\dot{q}_{k+1} = \dot{q}_k + h(1-\gamma)\Gamma(q_k, \dot{q}_k) + h\gamma\Gamma(q_{k+1}, \dot{q}_{k+1})$$

where $0 \leq \gamma \leq 1$ and $0 \leq \beta \leq 1/2$.
Important case: $\gamma = 1/2$ (second-order method)

The exponential map for a SODE

- SODE: $\dfrac{d^2q}{dt^2} = \Gamma(q, \dot{q})$
- $q \in Q$, $h > 0$ sufficiently small

Exponential map:

$$\exp_{q,h} : U \subseteq T_qQ \to Q$$

Take $v \in U \subseteq T_qQ$, consider the unique trajectory $\gamma(t)$ with this initial condition, and define

$$\exp_{q,h}(v) = \gamma(h)$$

A natural idea to derive a numerical method is to consider a discretization of the exponential map $\exp^d_{q,h} : U \subseteq T_qQ \to Q$ that is, an approximation of the continuous exponential map. If Q is a vector space, a common example of a discretization is the second order Taylor expansion of $\gamma(h)$

$$\exp^T_{q,h}(v) = q + hv + \frac{h^2}{2}\Gamma(q,v)\ .$$

Definition

A discretization of the exponential map of a second order differential equation is a family of maps $\exp^d_{q,h} : T_qQ \to Q$ depending on a parameter $h \in (-h_0, h_0)$ with $h_0 > 0$ such that $\exp^d_{q,0}(v_q) = q$ and the first and second derivatives with respect to h satisfy

$$\left.\frac{d}{dh}\right|_{h=0} \exp^d_{q,h}(v) = v, \quad \left.\frac{d^2}{dh^2}\right|_{h=0} \exp^d_{q,h}(v) = \Gamma(q,v), \quad \forall v \in T_qQ.$$

Given a discretization $\exp^d_{q,h} : T_q Q \to Q$ we now want to approximate the velocity $\dot{\gamma}(h)$.

Write

$$\begin{cases} q_{k+1} = \exp^d_{q_k,h}(v_k) \\ q_k = \exp^d_{q_{k+1},-h}(v_{k+1}) \end{cases}$$

This defines, under suitable regularity conditions, a map $\Phi^h_d : TQ \to TQ$, $\Phi^h_d(q_k, v_k) = (q_{k+1}, v_{k+1})$ (discrete flow).

Any discretization $\exp^d_{q,h}$, along with the resulting discrete flow Φ^h_d, induces a family of maps depending on a parameter $\beta \in [0, 1/2]$:

$$\exp^\beta_{q_k,h}(v_k) = q_k + hv_k + \frac{h^2}{2}\Big((1-2\beta)\Gamma(q_k, v_k) + 2\beta\Gamma(\Phi^h_d(q_k, v_k))\Big)$$

For $\beta = 0$, this is $\exp^T_{q,h}$.

Writing $\Phi^h_d(q_k, v_k) = (q_{k+1}, v_{k+1})$ we get the alternative expression

$$\exp^\beta_{q_k,h}(v_k) = q_k + hv_k + \frac{h^2}{2}\big((1-2\beta)\Gamma(q_k, v_k) + 2\beta\Gamma(q_{k+1}, v_{k+1})\big)$$

Newmark method in terms of exp

It turns out that the Newmark method can be written as

$$\begin{cases} q_{k+1} = \exp^{\beta}_{q_k,h}(v_k) \\ q_k = \exp^{\beta'}_{q_{k+1},-h}(v_{k+1}) \end{cases}$$

with parameters $0 \leq \beta, \beta' \leq 1/2$. That is

$$q_{k+1} = q_k + hv_k + \frac{h^2}{2}(1-2\beta)\Gamma(q_k, v_k) + h^2\beta\Gamma(q_{k+1}, v_{k+1})$$

$$q_k = q_{k+1} - hv_{k+1} + \frac{h^2}{2}(1-2\beta')\Gamma(q_{k+1}, v_{k+1}) + h^2\beta'\Gamma(q_k, v_k)$$

Newmark's parameter γ is $\gamma = \frac{1}{2}(1-2\beta'+2\beta)$.
Note $\gamma = 1/2 \iff \beta = \beta'$.

Nonholonomic mechanics

Configuration space Q
Lagrangian function $L : TQ \to \mathbb{R}$
Nonholonomic constraints given by a (nonintegrable) distribution $\mathcal{D}$.
In coordinates,

$$\mu_i^a(q)\,\dot{q}^i = 0, \quad m+1 \leq a \leq n\,,$$

where $\operatorname{rank}(\mathcal{D}) = m \leq n$. The annihilator $\mathcal{D}^\circ$ is locally given by

$$\mathcal{D}^\circ = \operatorname{span}\left\{\mu^a = \mu_i^a(q)\,dq^i;\ m+1 \leq a \leq n\right\}\,,$$

where the 1-forms μ^a are linearly independent at every point.

The equations of motion are given by the Lagrange-d'Alembert principle. A curve $q : [0, T] \to Q$ is an admissible motion of the system if

$$\delta \mathcal{J} = \delta \int_0^T L\big(q(t), \dot{q}(t)\big)\, dt = 0\,,$$

for all variations satisfying $\delta q(t) \in \mathcal{D}_{q(t)}$, $0 \le t \le T$, $\delta q(0) = \delta q(T) = 0$. The velocity of the curve itself must also satisfy the constraints, that is, $\mu_i^a(q(t))\, \dot{q}^i(t) = 0$.

Nonholonomic equations of motion:

$$\frac{d}{dt}\left(\frac{\partial L}{\partial \dot{q}^i}\right) - \frac{\partial L}{\partial q^i} = \lambda_a \mu_i^a\,,$$
$$\mu_i^a(q)\, \dot{q}^i = 0\,,$$

where λ_a, $m+1 \le a \le n$, are Lagrange multipliers to be determined.

If we assume that the nonholonomic system is regular, which is guaranteed if the Hessian matrix

$$(W_{ij}) = \left(\frac{\partial^2 L}{\partial \dot{q}^i \partial \dot{q}^j} \right)$$

is positive (or negative) definite, then the nonholonomic equations can be represented as a second order differential equation Γ_{nh} restricted to the constraint space determined by $\mathcal{D}$. We can rewrite the equations of motion as a vector field on the tangent bundle $\Gamma_{nh} = \Gamma_L + \lambda_a Z^a$ where

$$\Gamma_L = \dot{q}^i \frac{\partial}{\partial q^i} + W^{ij} \left(\frac{\partial L}{\partial q^j} - \frac{\partial^2 L}{\partial \dot{q}^j \partial q^k} \dot{q}^k \right) \frac{\partial}{\partial \dot{q}^i}$$

$$Z^a = W^{ij} \mu_j^a \frac{\partial}{\partial \dot{q}^i}$$

where (W^{ij}) is the inverse matrix of (W_{ij}).

Moreover, the Lagrange multipliers are completely determined and are given by the expression

$$\lambda_a = -\mathcal{C}_{ab} \Gamma_L(\mu_i^b \dot{q}^i),$$

where $(\mathcal{C}_{ab})$ is the inverse matrix of $(\mathcal{C}^{ab}) = (\mu_j^a W^{ij} \mu_i^b)$. This matrix is invertible if and only if the nonholonomic system $(L, \mathcal{D})$ is regular.

Remark: For the case of linear constraints, the energy is preserved by the motion.

The exponential map for nonholonomic systems

We can define an exponential map analogous to the one we had before:

$$\begin{aligned} \exp^{nh}_{q,h} : \mathcal{U}_q \subseteq \mathcal{D}_q &\longrightarrow Q \\ v_q &\mapsto \gamma(h) \end{aligned}$$

where γ is the solution curve starting from q, and with initial velocity v_q.

Define the exact discrete constraint space at q:

$$\mathcal{M}^{nh}_{q,h} := \exp^{nh}_{q,h}(\mathcal{U}_q)$$

which is a submanifold of Q of dimension $\mathrm{rank}(\mathcal{D})$.

Roughly speaking, these are the points that are reachable from q.

Nonholonomic dynamics given by

$$\Gamma_{nh}(q, v, \lambda) = \Gamma_L(q, v) + \lambda Z(q, v)$$

where the Lagrange multipliers are derived from the nonholonomic constraints $\dot{c}(t) \in \mathcal{D}_{c(t)}$.
Given q, v_q, write $\tilde{q} = \gamma(h) = \exp^{nh}_{q,h}(v_q)$, and $\tilde{v}_{\tilde{q}} = \dot{\gamma}(h)$.
From the properties of the flow of the (second order) vector field Γ_{nh}, we have

$$\tilde{q} = \exp^{nh}_{q,h}(v_q)$$
$$q = \exp^{nh}_{\tilde{q},-h}(\tilde{v}_{\tilde{q}})$$

Observe that the final position and velocity satisfy the constraints $\tilde{q} \in \mathcal{M}^{nh}_{q,h}$ and $\tilde{v}_{\tilde{q}} \in \mathcal{D}_{\tilde{q}}$.

The nonholonomic Newmark method

For the holonomic case, we had $\Gamma(q, v)$, defined the exponential map $\exp_{q,h}$, and wrote

$$\exp^{\beta}_{q_k,h}(v_k) = q_k + hv_k + \frac{h^2}{2}\big((1-2\beta)\Gamma(q_k, v_k) + 2\beta\Gamma(q_{k+1}, v_{k+1})\big)$$

Now we have $\Gamma_{nh}(q, v, \lambda)$, the (exact) exponential map $\exp^{nh}_{q,h}$, and we define

$$\exp^{d,\beta,\lambda,\lambda'}_{q,h} : \mathcal{D}_q \to Q$$

$$\exp^{d,\beta,\lambda,\lambda'}_{q_k,h}(v_k) = q_k + hv_k + \frac{h^2}{2}\Big((1-2\beta)\Gamma_{nh}(q_k, v_k, \lambda_k) + 2\beta\Gamma_{nh}(q_{k+1}, v_{k+1}, \lambda'_{k+1})\Big)$$

where $\beta \in [0, 1/2]$ and the Lagrange multipliers λ and λ' force the final (for this step) conditions $q_{k+1} \in \mathcal{M}^d_{q_k,h}$ and $v_{k+1} \in \mathcal{D}_{q_{k+1}}$.

Nonholonomic Newmark method

The **nonholonomic Newmark method** with parameters (β, β'), $0 \leq \beta, \beta' \leq 1/2$ is the integrator $F_h^{\beta,\beta'} : \mathcal{D} \to \mathcal{D}$ implicitly given by

$$\begin{aligned} q_{k+1} &= \exp^{d,\beta,\lambda,\lambda'}_{q_k,h}(v_k) \\ q_k &= \exp^{d,\beta',\lambda',\lambda}_{q_{k+1},-h}(v_{k+1}) \\ q_{k+1} &\in \mathcal{M}^d_{q_k,h} \\ v_{k+1} &\in \mathcal{D}_{q_{k+1}} \end{aligned}$$

or

$$\begin{cases} q_{k+1} = q_k + h v_k + \frac{h^2}{2}\left((1-2\beta)\Gamma_{nh}(q_k, v_k, \lambda_k) + 2\beta\Gamma_{nh}(q_{k+1}, v_{k+1}, \lambda'_{k+1})\right) \\ q_k = q_{k+1} - h v_{k+1} + \frac{h^2}{2}\left(2\beta'\Gamma_{nh}(q_k, v_k, \lambda_k) + (1-2\beta')\Gamma_{nh}(q_{k+1}, v_{k+1}, \lambda'_{k+1})\right) \\ q_{k+1} \in \mathcal{M}^d_{q_k,h} \\ v_{k+1} \in \mathcal{D}_{q_{k+1}} \end{cases}$$

Discretization of the constraints

Nonholonomic constraint distribution $\mathcal{D}$ defined by the equations

$$\phi^a(q,v) = \langle \mu^a(q), v \rangle$$

Possible discretizations of the constraints:

$$\Phi^a(q_k, q_{k+1}) = \left\langle \mu^a\left((1-\alpha)q_k + \alpha q_{k+1}\right), \frac{q_{k+1}-q_k}{h} \right\rangle, \quad \alpha \in [0,1].$$

or

$$\tilde{\Phi}^a(q_k, q_{k+1}) = \left\langle (1-\alpha)\mu^a\left(q_k\right) + \alpha\mu^a\left(q_{k+1}\right), \frac{q_{k+1}-q_k}{h} \right\rangle, \ \alpha \in [0,1].$$

Whenever it is clear which of the constraint discretizations we are using, we will simply denote the associated nonholonomic Newmark flow by $F_h^{\beta,\beta',\alpha} : \mathcal{D} \to \mathcal{D}$.

Some special cases

- If the discrete constraints are symmetric (which is true if $\alpha = 1/2$), and $\beta = \beta'$, then the nonholonomic Newmark method is at least of order 2.
- If $\beta = \beta' = 0$ we recover the DLA algorithm.
- $(F_h^{0,0,0})^* = F_h^{0,0,1}$ (adjoint of a method Φ_h is $\Phi_h^* = (\Phi_{-h})^{-1}$)
- $(F_h^{\beta,\beta',\alpha})^* = F_h^{\beta',\beta,1-\alpha}$
- $\Psi_h = F_{h/2}^{0,0,1} \circ F_{h/2}^{0,0,0}$ is a second order method.
- The case $\beta + \beta' = 1/2$ should be avoided, because the system of equations for the method becomes ill-conditioned.

Example: Chaotic nonholonomic particle

[McLachlan and Perlmutter, 2006].

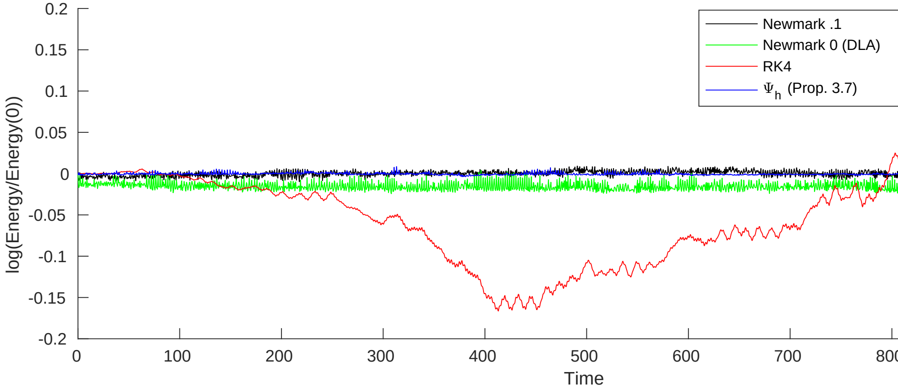
$Q = \mathbb{R}^5$ with coordinates $q = (x, y_1, y_2, z_1, z_2)$

$$L(q, \dot{q}) = \frac{1}{2}\|\dot{q}\|^2 - \frac{1}{2}(\|q\|^2 + z_1^2 z_2^2 + y_1^2 z_1^2 + y_2^2 z_2^2),$$

Constraint $\dot{x} + y_1\dot{z}_1 + y_2\dot{z}_2 = 0$.

The motion of the chaotic particle is given by the system of differential equations

$$\begin{cases} \ddot{x} = -x + \lambda \\ \ddot{y}_1 = -y_1 - y_1 z_1^2 \\ \ddot{y}_2 = -y_2 - y_2 z_2^2 \\ \ddot{z}_1 = -z_1 - z_1 z_2^2 - y_1^2 z_1 + \lambda y_1 \\ \ddot{z}_2 = -z_2 - z_1^2 z_2 - y_2^2 z_2 + \lambda y_2 \\ \dot{x} + y_1\dot{z}_1 + y_2\dot{z}_2 = 0. \end{cases}$$



Energy drift: $\log(\text{Energy}/\text{Energy}_0)$

Black: Newmark with $\beta = \beta' = .1$, $\alpha = 1/2$
Green: Newmark with $\beta = \beta' = 0$, $\alpha = 1/2$ (DLA)
Red: 4th-order Runge-Kutta for the continuous equations (with λ computed from constraints)
Blue: Composite method $\Psi_h = F_{h/2}^{0,0,1} \circ F_{h/2}^{0,0,0}$.

Pendulum-driven CVT (continuous variable transmission)

[Modin and Verdier, 2020]
$Q = \mathbb{R}^3$ with coordinates (x, y, ξ). We denote $q = (x, y)$.
Nonholonomic continuous variable transmission (CVT) system determined by an independent Hamiltonian subsystem called the driver system.

$$L(x, y, \xi, \dot{x}, \dot{y}, \dot{\xi}) = \frac{1}{2}\left(\sum_{i=1}^{2} \dot{q}_i^2 + \kappa_i q_i^2\right) + l(\xi, \dot{\xi}),$$

where $l(\xi, \dot{\xi}) = \frac{1}{2}\dot{\xi}^2 - V(\xi)$. The nonholonomic constraint is of the form

$$\dot{y} + f(\xi)\dot{x} = 0.$$

The motion of this family of systems is given by the equations

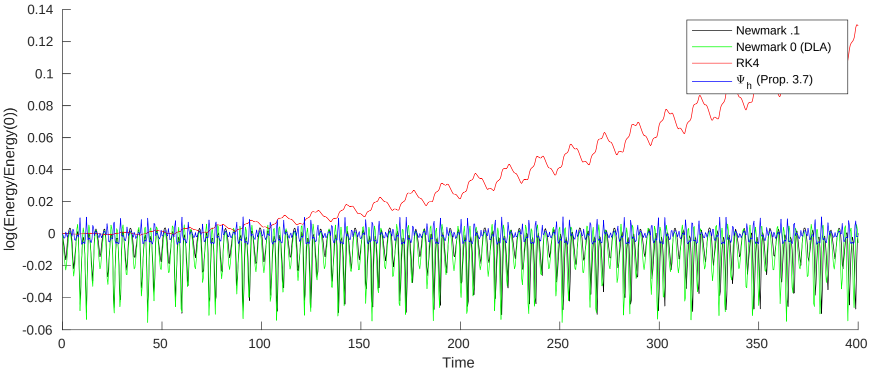
$$\begin{cases} \ddot{x} = \kappa_1 x + \lambda f(\xi) \\ \ddot{y} = \kappa_2 y + \lambda \\ \ddot{\xi} = -V'(\xi) \\ \dot{y} + f(\xi)\dot{x} = 0 \end{cases}$$

From now on, we take

$$V(\xi) = \cos(\xi) - \frac{\epsilon \sin(2\xi)}{2}, \quad f(\xi) = \sin(\xi), \quad \kappa_1 = \kappa_2 = -1.$$

This example has the property that for $\epsilon \neq 0$, the system is no longer integrable reversible and so, good long time behaviour observed in most nonholonomic integrators is lost in this case [Modin and Verdier 2020].

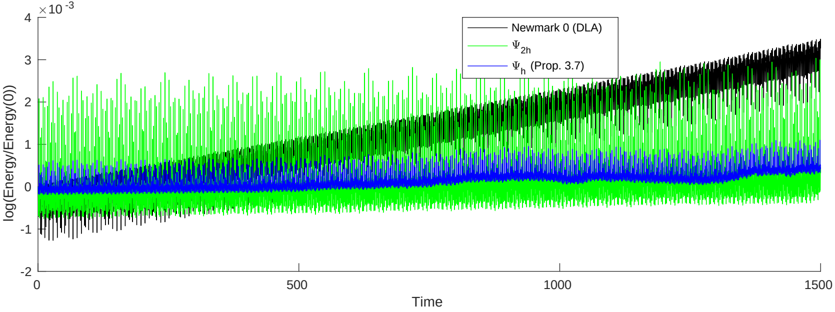
The case $\epsilon = 0$



Energy drift

Black: Newmark with $\beta = \beta' = .1$, $\alpha = 1/2$
Green: Newmark with $\beta = \beta' = 0$, $\alpha = 1/2$ (DLA)
Red: 4th-order Runge-Kutta for the continuous equations (with λ computed from constraints)
Blue: Composite method $\Psi_h = F_{h/2}^{0,0,1} \circ F_{h/2}^{0,0,0}$.

The case $\epsilon = .1$



High energy value (6.0), localized in the driver subsystem

Black: Newmark with $\beta = \beta' = 0$, $\alpha = 1/2$ (DLA)
Blue: Composite method $\Psi_h = F_{h/2}^{0,0,1} \circ F_{h/2}^{0,0,0}$
Green: "Fair" Composite method Ψ_{2h}

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¡Muchas gracias!