CS 101

Numerical Geometric Integration

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The Plan

Projection Methods & Constraints
- Classical Methods
- Symmetric Methods
- Symplectic Methods
- Variational Approach

Pendulum Revisited

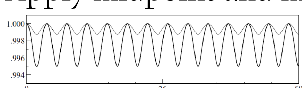
Pendulum in 2D (m=g=L=1):

$$\begin{pmatrix}\dot{q}_x\\ \dot{q}_y\end{pmatrix} = \begin{pmatrix}p_x\\ p_y\end{pmatrix} \qquad \begin{pmatrix}\dot{p}_x\\ \dot{p}_y\end{pmatrix} = \begin{pmatrix}-q_x\lambda\\ -1-q_y\lambda\end{pmatrix}$$

$$\lambda = \frac{||p||^2 - q_y}{||q||^2}$$

Start with $||q||^2=1$ and differentiate

Apply midpoint and measure $||q||^2$



What happened to preserving quadratic invariants?

Weak Invariants

Suppose we have:

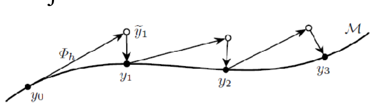
$$\dot{y} = f(y)$$
$$M = \{y : g(y) = 0\}$$
$$y_0 \in M \;\Rightarrow\; y(t) \in M \;\; \forall t$$

Then: $g'(y)f(y) = 0 \;\; \forall y \in M$ ∀ y would be strong

Midpoint won't preserve this
- Measures f off of M

Standard Projection

Idea
- Take a normal time step
- Project onto M

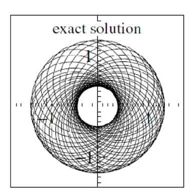


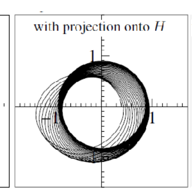
$$\tilde{y}_{n+1} = \Phi_h(y_n) \qquad y_{n+1} = P(\tilde{y}_{n+1})$$

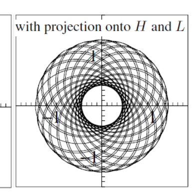
Constrained Minimization

Example: Energy Preservation

Why not use this to preserve energy
- "Force" explicit Euler?



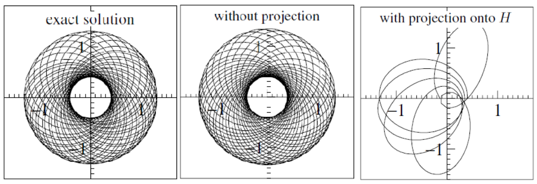




Example: Energy Preservation

Why not use this to preserve energy

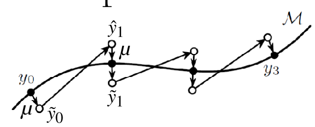
- “Force” symplectic Euler



Projection won’t preserve your integrator’s properties!

Symmetric Projection

Can we keep some structure?



$$\tilde{y}_n = y_n + (\nabla g(y_n))^T \mu$$
$$\tilde{y}_{n+1} = \Phi_h(\tilde{y}_n)$$
$$y_{n+1} = \tilde{y}_{n+1} + (\nabla g(y_{n+1})^T \mu)$$

Find μ s.t.

$$g(y_{n+1}) = 0$$

Check this is symmetric!

Reminder: Holonomic Constraints

Have some standard Lagrangian

$$L(q,\dot{q}) = K(\dot{q}) - W(q)$$

Want to enforce $g(q) = 0$

- “Holonomic” since g depends only on q

Augmented Lagrangian

$$L(q,\dot{q},\lambda,\dot{\lambda}) = K(\dot{q}) - W(q) - g(q)^T \lambda$$

- Do variations w.r.t q & λ

Reminder: Holonomic Constraints

$$L(q,\dot{q},\lambda,\dot{\lambda}) = K(\dot{q}) - W(q) - g(q)^T \lambda$$
$$m\ddot{q} = -\nabla W(q) - (\nabla g)^T \lambda$$
$$g(q) = 0$$

Rewrite with (augmented) Hamiltonian:

$$\dot{q} = H_p(p,q)$$
$$\dot{p} = -H_q(p,q) - (\nabla g)^T \lambda$$
$$0 = g(q)$$
$$0 = (\nabla g) H_p(p,q)$$

} configuration manifold (p,q) ∈ M

Symplectic Euler?

p implicit, q explicit

$$\tilde{p}_{n+1} = p_n - h(H_q(\tilde{p}_{n+1}) + (\nabla g)^T \lambda_{n+1})$$
$$q_{n+1} = q_n + h H_p(\tilde{p}_{n+1})$$
$$0 = g(q_{n+1})$$

p not in cotangent space!

$$p_{n+1} = \tilde{p}_{n+1} + (\nabla g)^T \mu_{n+1}$$
$$0 = \nabla g(q_{n+1}) H_p(p_{n+1}, q_{n+1})$$

This is still symplectic

A Note on Symplecticity

Test it as before and get:

$$\left(\frac{\partial(\tilde{p}_{n+1}, q_{n+1})}{\partial(p_n, q_n)}\right)^T J \left(\frac{\partial(\tilde{p}_{n+1}, q_{n+1})}{\partial(p_n, q_n)}\right) = \begin{pmatrix} 0 & I - h\lambda_p^T(\nabla g) \\ -I + h(\nabla g)^T \lambda_p & h((\nabla g)^T \lambda_q - \lambda_q^T(\nabla g)) \end{pmatrix}$$

~~This is not J!~~

Remember it’s a 2 form

$$J(\omega_1, \omega_2) = \omega_1^T J \omega_2$$

Take ω_1, $\omega_2 \in$ M

- Then remember $(\nabla g)\omega = 0 \quad \forall \omega \in M$

SHAKE

2^{nd} order, symmetric, symplectic

- Assuming H separable, M constant
- Störmer-Verlet

$$q_{n+1} - 2q_n + q_{n-1} = -h^2 M^{-1}(\nabla W(q_n) + (\nabla g(q_n))^T \lambda_n)$$

$$g(q_{n+1}) = 0$$

What happened to p?

- Approximate via finite differences
- Or rewrite as before...

RATTLE

$$p_{n+\frac{1}{2}} = p_n - \frac{h}{2}(\nabla W(q_n) + (\nabla g)^T \lambda_n)$$

$$q_{n+1} = q_n + hM^{-1} p_{n+\frac{1}{2}}$$

$$g(q_{n+1}) = 0$$

Solved together

$$p_{n+1} = p_{n+\frac{1}{2}} - \frac{h}{2}(\nabla W(q_{n+1}) + (\nabla g(q_{n+1}))^T \lambda_{n+1})$$

μ

What's wrong? Don't have this value

Rattle: project p onto cotangent space instead

$$\nabla g(q_{n+1}) M^{-1} p_{n+1} = 0$$

Variational Integrators

Augmented discrete Lagrangian

$$L_d(q_k, q_{k+1}, \lambda_k) =$$
$$h[K_d(q_k, q_{k+1}) - W(q_k, q_{k+1}) - g(q_k)^T \lambda_k]$$

Vary q_{k+1} and λ_{k+2}:

$$D_1 L_d(q_{k+1}, q_{k+2}, \lambda_{k+1}) + D_2 L_d(q_k, q_{k+1}, \lambda_k) = 0$$

$$g(q_{k+1}) = 0$$

Pendulum Re-revisited (m=g=L=1)

$$L_d(q_k, q_{k+1}, \lambda_k) =$$
$$h\left[\frac{1}{2}\left|\left|\frac{q_{k+1} - q_k}{h}\right|\right|^2 - \frac{q_k^y + q_{k+1}^y}{2} - \lambda_k(||q_k||^2 - 1)\right]$$

To the board!

$$\frac{q_k - 2q_{k+1} + q_{k+2}}{h^2} = -\begin{pmatrix} 0 \\ 1 \end{pmatrix} - 2\lambda_{k+1} q_{k+1}$$

$$||q_{k+1}|| - 1 = 0$$

First Slide: $\begin{pmatrix} \dot{p}_x \\ \dot{p}_y \end{pmatrix} = \begin{pmatrix} -q_x \lambda \\ -1 - q_y \lambda \end{pmatrix}$