Sensitivity Analysis for Multibody Dynamics Using Spatial Operators

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Plan

* Illustrate use of spatial operators as mathematical tools to make the inherently complex multibody dynamics tractable for
  - analysis
  - numerical computations

* touch upon selected topics to illustrate scope + use of spatial operators.

Such analytical & computational tools are directly relevant for the numerical integration of multibody dynamics.

Why Sensitivities?

- Sensitivities are needed for
  - implicit integration schemes
  - Newton iterations
  - linearized dynamics
  - stiff system
  - constrained dynamics

- Challenges
  - equations of motion are complex + nonlinear
  - numeric linearization / differentiation schemes are computationally expensive and offer limited accuracy

Key Quantities in Multibody Dynamics

n-dimensional (n degrees of freedom)

Equations of Motion

$$\mathcal{M}(\theta)\ddot{\theta} + \mathcal{C}(\theta, \dot{\theta}) = T$$

"tree" topology systems

$\theta \in \mathbb{R}^n$ = generalized hinge coordinates

T = generalized forces

configuration dependent $\left\{ \begin{array}{l} \mathcal{M}(\theta) = \text{mass matrix} \in \mathbb{R}^{n \times n} \\ \mathcal{C}(\theta, \dot{\theta}) = \text{velocity–dependent Coriolis/centrifugal forces} \end{array} \right.$

- "internal" coordinates formulation
- minimal dimension & ODE form

non-seperable Hamiltonians

Kinetic Energy $= \frac{1}{2}\dot{\theta}^* \mathcal{M}(\theta)\dot{\theta}$

There is little structural information about $\mathcal{M}$ or $\mathcal{C}$ available from this form of the equations of motion.

ODE form

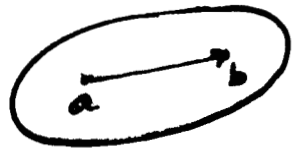
$$\ddot{\theta} = \underbrace{\mathcal{M}^{-1}(\theta)\left[\tau - \mathcal{C}(\theta,\dot{\theta})\right]}_{\text{potentially } O(N^3) \text{ computation}}$$

expensive as $N \uparrow$

Can we do better?

Yes — in $\underline{\underline{O(N)}}$!

6-dimensional "spatial" quantities for a rigid body



rigid body

spatial velocity: $V = \begin{pmatrix} \omega \\ v \end{pmatrix} \in R^6$

spatial force: $f = \begin{pmatrix} N \\ F \end{pmatrix} \in R^6$

spatial inertia: $M = \begin{pmatrix} \mathcal{J} & m\tilde{p} \\ -m\tilde{p} & mI \end{pmatrix} \in R^{6\times 6}$

spatial transformation matrix: $\phi(a,b) = \begin{pmatrix} I & \tilde{l}(a,b) \\ 0 & I \end{pmatrix} \in R^{6\times 6}$

velocity transformation: $V(b) = \phi^*(a,b)V(a)$

force transformation: $f(a) = \phi(a,b)f(b)$

Parallel theorem: $M(a) = \phi(a,b)M(b)\phi^*(a,b)$

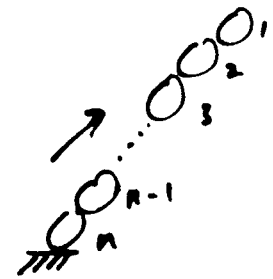
rate of work: $V(a)^* f(a)$

6-dimensional cross product

6-dimensional equations of motion: $M\dot{V} + V \times MV = f$

3-dim. at CM: $I\dot{\omega} + \omega \times I\omega = N$

Duality Between Operators and Computational Algorithms



$$V = \mathrm{col}\left\{V(k)\right\} = \phi^* H^* \dot{\theta} \iff \begin{cases} V(n+1) = 0 \\ \textbf{for } k = n \cdots 1 \\ \quad V(k) = \phi^*(k+1,k)V(k+1) + H^*(k)\dot{\theta}(k) \\ \textbf{end loop} \end{cases}$$

(base-to-tip)

hinge vector

Operator Expression

explicit computation of ϕ & H is never needed!

$$\phi = \begin{pmatrix} I & 0 & \dots & 0 \\ \phi(2,1) & I & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ \phi(n,1) & \phi(n,2) & \dots & I \end{pmatrix} \in \mathbb{R}^{6n \times 6n}, \qquad H = \begin{pmatrix} H(1) & 0 & \dots & 0 \\ 0 & H(2) & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \dots & H(n) \end{pmatrix} \in \mathbb{R}^{n \times 6n}$$

Computational Algorithm

$$\phi = (I - \mathcal{E}_\phi)^{-1}$$

nilpotent

where we have the semi-group property

$$\phi(k,j) \triangleq \phi(k,k-1)\cdots\phi(j+1,j) \text{ for } k > j,$$

Operator Expression for the Mass Matrix

$$\begin{cases} V = \phi^* H^* \dot{\theta} & \text{spatial velocities} \\ \alpha = \phi^*[H^* \underline{\ddot{\theta}} + a] & \text{spatial accelerations} \\ f = \phi[M\alpha + b] & \text{inter-body spatial forces} \\ \underline{T} = Hf & \text{generalized forces} \end{cases}$$

$$T = \underbrace{H\phi M\phi^* H^*}_{\substack{\mathcal{M}(\theta) \\ \text{mass matrix} \\ \text{(symm., pos. definite)}}} \ddot{\theta} + \underbrace{H\phi[M\phi^* a + b]}_{\substack{C(\theta,\dot{\theta}) \\ \text{Coriolis, gyroscopic} \\ \text{terms}}} = \mathcal{M}(\theta)\ddot{\theta} + \mathcal{C}(\theta,\dot{\theta})$$

This factorization of $\mathcal{M}$ is called the <u>*Newton–Euler Factorization of the Mass Matrix.*</u>

Operator Factorization and Inversion of the Mass Matrix ('88)

parallels with Kalman filtering techniques from optimal estimation theory

Newton–Euler Factorization of $\mathcal{M}$

$$\mathcal{M} = \underset{\text{non-square}}{H}\phi M \phi^* H^*$$

Innovations Factorization of $\mathcal{M}$

$$\mathcal{M} = \underbrace{[I + H\phi K]}_{\text{square + lower triang.}} \overset{\text{diagonal}}{D} [I + H\phi K]^* \quad \sim \; LDL^* \text{ decomposition}$$

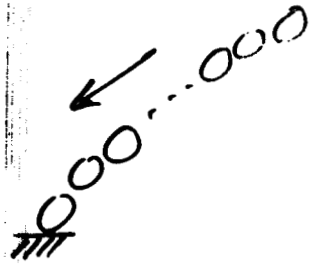
$$[I + H\phi K]^{-1} = [I - H\psi K]$$

Operator Factorization of $\mathcal{M}^{-1}$

$$\mathcal{M}^{-1} = [I - H\psi K]^* D^{-1} [I - H\psi K] \quad \sim \; L^* DL \text{ decomposition}$$

Riccati Equation for Articulated Inertias

A Riccati equation for the <u>*articulated body inertias*</u> *needs to be solved to obtain the innovations representation*



discrete Riccati equation for $P(\cdot)$

$$
\begin{cases}
P^+(0) = 0 \\
\textbf{for } k = 1 \cdots N \\
\quad P(k) = \phi(k,k-1)P^+(k-1)\phi^*(k,k-1) + M(k) \\
\quad D(k) = H(k)P(k)H^*(k) \\
\quad G(k) = P(k)H^*(k)D^{-1}(k) \\
\quad \overline{\tau}(k) = I - G(k)H(k) \\
\quad P^+(k) = \overline{\tau}(k)P(k) \\
\quad \psi(k+1.k) = \phi(k+1,k)\overline{\tau}(k) \\
\textbf{end loop}
\end{cases}
$$

articulated body inertia

kalman gain

$$
\psi = \begin{bmatrix} I & 0 & & \\ \psi(2,1) & I & & 0 \\ \vdots & & \ddots & \\ \psi(N,1) & \cdots & \cdots & I \end{bmatrix}
$$

same structure as ϕ

Examples of Spatial Operator Identities

$$HG = I \qquad GH = \boldsymbol{\tau}, \text{a projection}$$

$$\begin{aligned}
\boldsymbol{\tau} P \boldsymbol{\tau}^* &= \boldsymbol{\tau} P \\
\boldsymbol{\psi}^{-1} - \boldsymbol{\phi}^{-1} &= KH \\
[I - H\boldsymbol{\psi}K]H\boldsymbol{\phi} &= H\boldsymbol{\psi} \\
\boldsymbol{\phi}K[I - H\boldsymbol{\psi}K] &= \boldsymbol{\psi}K \\
\boldsymbol{\phi}M\boldsymbol{\phi}^* &= R + \tilde{\boldsymbol{\phi}}R + R\tilde{\boldsymbol{\phi}}^* \\
\boldsymbol{\psi}M\boldsymbol{\psi}^* &= P + \tilde{\boldsymbol{\psi}}P + P\tilde{\boldsymbol{\psi}}^* \\
H\boldsymbol{\psi}M\boldsymbol{\psi}^*H^* &= D \\
\boldsymbol{\psi}^*H^*D^{-1}H\boldsymbol{\psi} &= \Upsilon + \tilde{\boldsymbol{\psi}}^*\Upsilon + \Upsilon\boldsymbol{\psi}
\end{aligned}$$

There is a large class of operator identities to work with – *do not need to rely on estimation theory!*

Other work & applications

closed-chain topology
flexible bodies
flexible/geared hinges
under-actuated systems
prescribed motion

Generalizations

internal coord. models
Nose-Hoover dynamics
compensating potentials

Molec. Dynamics

linearized models
op. sensitivities
diagonalized dyn.
parallel algorithms.

"Miscellaneous"

Analytical Expressions for Mass Matrix Sensitivities

Spatial operators can also be used to derive analytical expressions for the sensitivities of mass matrix and other quantities:

$$\frac{\partial \mathcal{M}(\boldsymbol{\theta})}{\partial \boldsymbol{\theta}(i)} = \boldsymbol{H}\boldsymbol{\phi}\left[\mathbb{H}_\delta^i \boldsymbol{\phi} \boldsymbol{M} - \boldsymbol{M}\boldsymbol{\phi}^* \mathbb{H}_\delta^i\right]\boldsymbol{\phi}^* \boldsymbol{H}^*$$

Such gradients are often useful for higher order mechanical integration schemes.

$$\frac{\partial KE}{\partial \theta(i)} = \frac{1}{2}\dot{\theta}^* \frac{\partial \mathcal{M}(\theta)}{\partial \theta(i)} \dot{\theta} = \frac{1}{2}\dot{\theta}^* H \phi \left[\mathbb{H}_\delta^i \phi M - M \phi \mathbb{H}_\delta^i\right] \phi^* H^* \dot{\theta}$$

$$= \underline{V^* \mathbb{H}_\delta^i \phi M V}$$

Linearized Dynamics

$$\ddot{\theta} = M^{-1}(\theta)\left[-\ell(\theta,\dot{\theta}) + \tau\right]$$

<u>Need</u> : $\underbrace{\nabla_\theta M(\theta)}_{\text{already seen}}$, $\nabla_\theta \ell(\theta,\dot{\theta})$, $\nabla_{\dot{\theta}} \ell(\theta,\dot{\theta})$

Spatial operator expression for $\nabla_{\dot{\theta}} \ell(\theta,\dot{\theta})$

$$\nabla_{\dot{\theta}} \ell(\theta,\dot{\theta}) = 2 H_{II} \Pi \left[\hat{M}_{II} \Pi^* - M_{II} \Pi^* \Omega_{II}^* \right] H_{II}^*$$

Can derive a similar expression for $\nabla_\theta \ell(\theta,\dot{\theta})$

Diagonalization

$$M(\theta)\,\ddot{\theta} + \ell(\theta, \dot{\theta}) = T$$

<u>Question:</u> Can we find smooth coordinate transformations to <u>diagonalize</u> (& simplify) equations of motion?

* diagonalizing $\theta \mapsto g(\theta)$ <u>rarely</u> exists.

* however, $\underline{\dot{\theta} \longmapsto v \triangleq M^{1/2}\,\dot{\theta}}$ results in "almost" diagonalization

  Always exists!

Diagonalized Dynamics

$$\underbrace{\mathcal{M}(\theta)\ddot{\theta} + \mathcal{C}(\theta,\dot{\theta}) = T}_{\text{highly coupled}} \quad \rightarrow \quad \underbrace{\dot{\nu} + \mathcal{C}(\theta,\nu) = \epsilon}_{\text{largely decoupled}}$$

$(\dot{\nu} = \epsilon)$

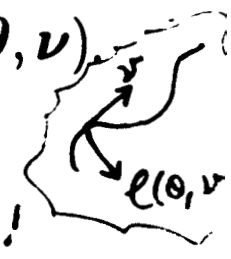
Global diagonalizing transformations require that the curvature tensor associated with the mass matrix vanish. This is rarely the case.

Use new diagonalizing coordinates (θ, ν)

$$\dot{\theta}\nu = \underbrace{D^{-\frac{1}{2}}[I - H\psi K]^*}_{\mathcal{M}^{-1/2}}\dot{\theta}\nu \quad \text{and} \quad \epsilon = [I - H\psi K]D^{-\frac{1}{2}}T$$

- These smooth diagonalizing transformations always exist.
- The ν's are non–integrable time derivatives of quasi–coordinates.
- Have closed–form operator expression and computational algorithm for $\mathcal{C}(\theta,\nu)$.
- $\mathcal{C}(\theta,\nu)$ does no work, i.e., $\nu^*\mathcal{C}(\theta,\nu) = 0$. $\rightarrow$ like for a rigid body!
- This formulation leads to some simple control laws.

$\Rightarrow$ If $\epsilon = 0 \Rightarrow \|\nu\|$ constant!



Special Case: Manipulator with 1 dof rotational hinges

$$\boldsymbol{\mathcal{C}}(\boldsymbol{\theta},\boldsymbol{\nu}) = \boldsymbol{\ell}[\dot{\boldsymbol{m}}\boldsymbol{\nu} - \frac{1}{2}\nabla_{\boldsymbol{\theta}}(\dot{\boldsymbol{\theta}}^*\boldsymbol{\mathcal{M}}\dot{\boldsymbol{\theta}})]$$

It can be shown that

$$\begin{aligned}
\boldsymbol{\mathcal{C}}(\boldsymbol{\theta},\boldsymbol{\nu}) &= \frac{1}{2}\boldsymbol{D}^{-\frac{1}{2}}\boldsymbol{H}\boldsymbol{\psi}\left[\boldsymbol{\mathcal{E}}_{\boldsymbol{\psi}}\dot{\boldsymbol{\lambda}} - \dot{\boldsymbol{\lambda}}\boldsymbol{\mathcal{E}}_{\boldsymbol{\psi}}^* - \tilde{\boldsymbol{\Omega}}_{\delta}\boldsymbol{P} - \boldsymbol{P}\tilde{\boldsymbol{\Omega}}_{\delta} - 2\tilde{V}^*\boldsymbol{M}\right]\boldsymbol{\psi}^*\boldsymbol{H}^*\boldsymbol{D}^{-\frac{1}{2}}\boldsymbol{\nu} \\
&= \frac{1}{2}\boldsymbol{D}^{-\frac{1}{2}}\boldsymbol{H}\boldsymbol{\psi}\left[\boldsymbol{\mathcal{E}}_{\boldsymbol{\psi}}\dot{\boldsymbol{\lambda}} - \dot{\boldsymbol{\lambda}}\boldsymbol{\mathcal{E}}_{\boldsymbol{\psi}}^* - \tilde{\boldsymbol{\Omega}}_{\delta}\boldsymbol{P} - \boldsymbol{P}\tilde{\boldsymbol{\Omega}}_{\delta} - 2\tilde{V}^*\boldsymbol{M}\right]V
\end{aligned}$$

This provides an explicit <u>analytical expression</u> for the Coriolis and gyroscopic forces vector $\boldsymbol{\mathcal{C}}(\boldsymbol{\theta},\boldsymbol{\nu})$.

Compensating Potential for Constrained Molecular Systems

The introduction of hard constraints introduces systematic errors in computed thermodynamic quantities. Need to use a compensating potential (Fixman)

$$P(\boldsymbol{\theta}) = \ln\{\det[\mathcal{M}(\boldsymbol{\theta})]\}$$

— has been difficult to compute

This is straightforward because

$(\mathcal{M} = [I + H\phi K] D [I + H\phi K]^T)$

$$\ln\{\det[\mathcal{M}(\boldsymbol{\theta})]\} = \ln\left\{\prod_i D(i)\right\} = \sum_i \ln\{D(i)\}$$

The forces arising from this potential are computed using the closed form expressions for the sensitivity of $D(i)$.

Compensating Potential Gradient for Constrained Systems

During simulations we actually need the *gradient* of the *compensating potential*

$$T_c(k) = \frac{\partial \mathcal{V}_c(\boldsymbol{\theta})}{\partial \boldsymbol{\theta}(k)} = \frac{1}{2}\frac{\partial \ln \det \{\boldsymbol{\mathcal{M}}(\boldsymbol{\theta})\}}{\partial \boldsymbol{\theta}(k)}$$

Using operators, we can derive the analytical and computable expression

$$T_c(k) = \mathrm{Trace}\,\{\boldsymbol{P}(k)\Upsilon(k)_{\mathbf{H}}(k)\}$$

Conclusion

spatial operators

⇓

analysis

computational algorithms.

multibody systems.

References: http://dshell.jpl.nasa.gov CL97-1001

DARTS, NEIMO s/w packages

Future work:

* integration methods — w/ deterministic cost (for real-time); catering to multibody systems; with conservation properties; non-conservative applications.
* molecular dynamics — which dofs to freeze? hierarchy of models; "close encounters" problem with large time steps; statistical properties