Abstract—Optimization-based control methods for robots often rely on first-order dynamics approximation methods like in iLQR. Using second-order approximations of the dynamics is expensive due to the costly second-order partial derivatives of dynamics with respect to the state and control. Current approaches for calculating these derivatives typically use automatic differentiation (AD) and chain-rule accumulation or finite-difference. In this paper, for the first time, we present closed-form analytical second-order partial derivatives of inverse dynamics for rigid-body systems with floating base and multi-DoF joints. A new extension of spatial vector algebra is proposed that enables the analysis. A recursive $O(Nd^2)$ algorithm is also provided where $N$ is the number of bodies and $d$ is the depth of the kinematic tree. A comparison with AD in CasADi shows speedups of 1.5–3×.

In recent years, optimization-based methods have become popular for robot motion generation and control. Although full second-order (SO) optimization methods offer superior convergence properties, most work has focused on using only the first-order (FO) dynamics approximation, such as in iLQR [1], [2]. Differential Dynamic Programming (DDP) [3] is a use-case for full SO optimization that has gained wide interest for robotics applications [4]–[7]. Variants of DDP using multiple first-order (FO) dynamics approximation, such as in iLQR [1], [2], and the RNEA [12], [17]. Analytical expressions for partial derivatives of ID. The resulting expressions and chain-rule accumulation or finite-difference. In this paper, for the first time, we present closed-form analytical second-order partial derivatives of inverse dynamics for rigid-body systems with floating base and multi-DoF joints. A new extension of spatial vector algebra tools is presented for the first time, we contribute an extension of Featherstone’s spatial vector algebra tools [12] for tensor use.

II. DERIVATIVES OF RIGID-BODY DYNAMICS

Rigid-Body Dynamics: For a rigid-body system, the state variables are the configuration $q$ and the generalized velocity vector $\dot{q}$, while the control variable is the generalized torque vector $\tau$. The Inverse Dynamics (ID), is given by

$$\tau = M(q)\dot{q} + C(q, \dot{q})\dot{q} \dot{\dot{q}}$$

(1)

where $M \in \mathbb{R}^{n \times n}$ is the mass matrix, $C \in \mathbb{R}^{n \times n}$ is the Coriolis matrix, $g \in \mathbb{R}^{n}$ is the vector of generalized gravitational forces, and $n$ is the DoF of the system. An efficient $O(N)$ algorithm for ID is the RNEA [12], [17]. Analytical expressions for partial derivatives of ID w.r.t $q$, $\dot{q}$ were presented in Ref. [13], among other similar formulations [14], [15]. From Eq. (1) the first order partial derivative w.r.t $\dot{q}$ is simply $\partial \tau / \partial \dot{q} = M(q)$. Therefore, this relation results in $\partial^2 \tau / \partial q \partial \dot{q}$ being zero, and the SO cross-derivative w.r.t $\dot{q}$ and $\dot{q}$, $\partial^2 \tau / \partial \dot{q} \partial \ddot{q}$ being zero as well. However, the cross-derivative w.r.t $\ddot{q}$ is non-trivial and equals $\partial M(q) / \partial q$. Garofalo et al. [18] presents a recursive algorithm for the partial derivative of $M(q)$ w.r.t $\ddot{q}$ for multi-DoF Lie group joints. In this work we re-derive that result using newly developed spatial matrix operators and contribute new closed-form SO partial derivatives of ID w.r.t $\dot{q}$ and $\ddot{q}$.

In the following sections, Spatial Vector Algebra (SVA) is reviewed for dynamics analysis, followed by an extension of SVA for matrices. Then, the algorithm is developed for the SO partial derivatives of ID. The resulting expressions and algorithm are very complicated, but are provided in the form of open-source algorithm with full derivation in Ref. [19] while keeping the current paper self-contained. The performance of this new SO algorithm is compared to AD using CasADi [20] in MATLAB.

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III. SPATIAL VECTOR ALGEBRA (SVA)

Notation: Spatial vectors are 6D vectors that combine the linear and angular aspects of a rigid-body motion or net force [12]. Cartesian vectors are denoted with lower-case letters with a bar (\(\bar{v}\)), spatial vectors with lower-case bold letters (e.g., \(\mathbf{v}\)), matrices with capitalized bold letters (e.g., \(\mathbf{A}\)), and tensors with capitalized calligraphic letters (e.g., \(\Omega\)). Motion vectors, such as velocity and acceleration, belong to a 6D vector space denoted \(M^6\). Force-like vectors, such as force and momentum, belong to another 6D vector space \(F^6\). Spatial vectors are usually expressed in either the ground coordinate frame or a body coordinate (local coordinate) frame. For example, the spatial velocity \(\bar{v}_k \in M^6\) of a body \(k\) expressed in the body frame is \(\bar{v}_k = [\bar{\omega}_k \ 0]^{T}\) where \(\bar{\omega}_k \in \mathbb{R}^3\) is the angular velocity expressed in a coordinate frame fixed to the body, while \(\bar{\omega}_k \in \mathbb{R}^3\) is the linear velocity of the origin of the body frame. When the frame used to express a spatial vector is omitted, the ground frame is assumed.

A spatial cross product between motion vectors (\(v, u\), written as \((v \times u)\), is given by Eq. [3]. This operation gives the time rate of change of \(u\), when \(u\) is moving with a spatial velocity \(v\). For a Cartesian vector, \(\bar{\omega} \times\) is the 3D cross-product matrix.

A spatial cross product between a motion and a force vector is written as \((v \times f)\), as defined by Eq. [4].

\[
v \times = \begin{bmatrix} \bar{\omega} \times & 0 \\ \bar{v} \times & \bar{\omega} \times \end{bmatrix} \quad (3) \quad v \times f = \begin{bmatrix} \bar{\omega} \times & \bar{v} \times \\ 0 & \bar{\omega} \times \end{bmatrix} \quad (4)
\]

An operator \(\overline{\times}\) is defined by swapping the order of the cross product, such that \((f \overline{\times})v = (v \times)f\) [21]. Further introduction to SVA is provided in Ref. [22, Appendix A].

Connectivity: An open-chain kinematic tree with serial or branched connectivity (Fig. 1) is considered with \(N\) links connected by joints, each with up to 6 DoF. Body \(i\)'s parent toward the root of the tree is denoted as \(\lambda(i)\). The set \(\nu(i)\) denotes the set of bodies in the subtree rooted at body \(i\), while \(\nu(i)\) denotes the set of bodies in \(\nu(i)\) excluding the body \(i\). We define \(i \preceq j\) if body \(i\) is in the path from body \(j\) to the base. With this numbering, \(j\) precedes body \(i\).

We consider joints whose configurations form a sub-group of the Lie group \(SE(3)\). For a prismatic or revolute joint, the configuration and rate are represented by \(q_i, \dot{q}_i \in \mathbb{R}\). For a spherical joint, \(q_i \in SO(3)\) while \(\dot{q}_i = \dot{q}_i/\lambda(i) \in \mathbb{R}^3\) as the relative angular velocity between neighboring bodies. For a 6-DoF free motion joint, \(q_i \in SE(3)\) while \(\dot{q}_i = \dot{q}_i/\lambda(i) \in \mathbb{R}^6\). Thus, \(\dot{q}\) is not strictly the time derivative of \(q\) in general.

The spatial velocities of the neighbouring bodies in the tree are then related by \(v_i = v_{\lambda(i)} + S_i \dot{q}_i\), where \(S_i \in \mathbb{R}^{6 \times n_i}\) is the joint motion subspace matrix for joint \(i\) [12] with \(n_i\) its number of DoFs. The velocity \(\dot{v}_i\) can also be written as the sum of joint velocities over predecessors as \(\dot{v}_i = \sum_{\lambda(i) \leq j} S_i \dot{q}_j\). The derivative of the joint motion subspace matrix in local coordinates (often denoted \(S_i\) [12]) is assumed to be zero. The quantity \(S_i = v_i \times S_i\) signifies the rate of change of \(S_i\) due to the local coordinate system moving.

Dynamics: The spatial equation of motion [12] is given for body \(k\) as \(f_k = I_k a_k + v_k \times I_k v_k\), where \(f_k\) is the net spatial force on body \(k\), \(I_k\) is its spatial inertia [12], and \(a_k\) is its spatial acceleration. The development in Ref. [13] presents two additional spatial motion quantities \(\Psi, \Psi\) (Eq. [5]) essential to the derivation in this paper. The quantities \(\Psi, \Psi\) represent the time-derivative of \(S_j\) and \(\Psi_j\), respectively, due to joint \(j\)'s predecessor \(\lambda(j)\) moving.

\[
\begin{align*}
\dot{\Psi} &= v_{\lambda(j)} \times S_j \\
\dot{\Psi} &= a_{\lambda(j)} S_j + v_{\lambda(j)} \times \Psi_j
\end{align*}
\]

The equations for the FO partial derivatives of ID w.r.t \(\dot{q}\) and \(\dot{\dot{q}}\) [13] are shown below. Here \(\tau_i\) and \(\tau_i\) are the joint torques for the joint \(i\) and \(j\) respectively. The quantity \(f^i_j = \sum_{k \geq i} S_i f_k\) is the composite spatial force transmitted across joint \(i\), and \(I^C_i\) is the composite rigid-body inertia of the sub-tree rooted at body \(i\), given as \(I^C_i = \sum_{k \geq i} I_k\). The quantity \(B_k\) is a body-level Coriolis matrix [13, 21].

\[
B_k = \frac{1}{2}[(v_k \times^*) I_k - I_k (v_k \times) + (I_k v_k \bar{\times}^*)] \quad \text{(6)}
\]

while \(B^C_i\) is its composite given by \(B^C_i = \sum_{k \geq i} B_k\).

The next sections extend Eqs. [7][10] for SO derivatives of ID.

\[
\begin{align*}
\frac{\partial \tau_i}{\partial q_j} &= S_i^T [2B^C_i] \dot{\Psi}_j + S_i^T I^C_j \dot{\Psi}_j, (j \preceq i) \\
\frac{\partial \tau_i}{\partial q_i} &= S_i^T [2B^C_i] \dot{\Psi}_j + I^C_i \dot{\Psi}_j + (f^i_j) \bar{\times}^* S_i, (j \preceq i) \\
\frac{\partial \tau_i}{\partial q_j} &= S_i^T [2B^C_i S_j + I^C_i (\dot{\Psi}_j + \dot{S}_j)], (j \preceq i) \\
\frac{\partial \tau_i}{\partial q_i} &= S_i^T [2B^C_i S_j + I^C_i (\dot{\Psi}_j + \dot{S}_j)], (j \preceq i)
\end{align*}
\]

IV. EXTENDING SVA FOR TENSORS USE

The motion space \(M^6\) [12] is extended to a space of spatial-motion matrices \(M^{6 \times n}\), where each column of such a matrix is a usual spatial motion vector. For any \(U \in M^{6 \times n}\) a new spatial cross-product operator \(U \times \) is considered and defined by applying the usual spatial cross-product operator \(\times\) to each column of \(U\). The result is a third-order tensor (Fig. 2) in \(R^{6 \times 6 \times n}\) where each \(6 \times 6\) matrix in the 1-2 dimension is the original spatial cross-product operator on a column of \(U\).

Given two spatial motion matrices, \(V \in M^{6 \times n_a}\) and \(U \in M^{6 \times n_b}\), we can now define a cross-product operation between them as \((V \times) U \in M^{6 \times n_a \times n_b}\) via a tensor-matrix product. Such an operation, denoted as \(Z = AB\) is defined as:

\[
Z_{i, j, k} = \sum_j A_{i, j, k} B_{j, l}
\]
for any tensor $A$ and suitably sized matrix $B$. Thus, the $k$-th page, $j$-th column of $V \times U$ gives the cross product of the $k$-th column of $V$ with the $j$-th column of $U$.

In a similar manner, consider a spatial force matrix $F \in F_{6 \times n_j}$. Defining $(V \times *)$ in an analogous manner to in Fig. 2 allows taking a cross-product-like operation $V \times * F$. Again, analogously, we consider a third operator $(\tilde{F} \times *)$ that provides $V \times * F = F \tilde{\times} * V$. In each case, the tilde indicates the spatial-matrix extension of the usual spatial-vector cross products.

For later use, the product of a matrix $B \in \mathbb{R}^{n_1 \times n_2}$, and a tensor $A \in \mathbb{R}^{n_2 \times n_3 \times n_4}$, likewise results in another tensor, denoted as $Y = BA$, and defined as:

$$\mathcal{Y}_{i,k,l} = \sum_j B_{i,j}A_{j,k,l}$$  \hspace{1cm} (12)

Two types of tensor rotations are defined for this paper:

1. $A^\top$: Transpose along the 1-2 dimension. This operation can also be understood as the usual matrix transpose of each matrix (e.g., in Fig. 2) moving along pages of the tensor. If $A^\top = B$, then $A_{i,j,k} = B_{j,i,k}$.

2. $A^\bar{R}$: Rotation of elements along the 2-3 dimension. If $A^\bar{R} = B$, then $A_{i,j,k} = B_{i,k,j}$.

Another notation $(\bar{R}^\top)$ is a combination of $(\bar{R})$ followed by $(\top)$. For example, if $A^{\bar{R}\top} = B$, then $A_{i,j,k} = B_{i,k,j}$.

Properties of the operators are given in Table 1. These properties naturally extend spatial vector properties [12], but with the added book-keeping required from using tensors. For example, the spatial force/vector cross-product operator $\times *$ satisfies $\nu \times * = -\nu \times ^\top$. Property M1 provides the matrix analogy for the spatial matrix operator $\times *$. Property M8 is the spatial matrix analogy of the spatial vector property $u \times v = -v \times u$, where $u$ and $v$ are spatial vectors.

V. SECOND ORDER DERIVATIVES OF INVERSE DYNAMICS

A. Preliminaries

The SO partial derivative of joint torque is also referred to as a dynamics Hessian tensor. This third-order tensor is written in a form $\frac{\partial^2 x}{\partial \theta_i \partial \dot{\theta}_j}$, which signifies taking partial derivative of $\tau_i$ w.r.t $u_j$, followed by $u_k$. The variables $u_j$ and $u_k$ can either be the joint configuration ($q_j$, $q_k$), or joint velocity ($\dot{q}_j$, $\dot{q}_k$). For single-DoF joints, each block of this Hessian tensor is a conventional SO derivative w.r.t joint angles and rates, that reduces to a scalar, and the order of $u_j$ and $u_k$ doesn’t matter. But, for a multi-DoF joint, each entry is a second-order Lie derivative, as defined in Ref. [23], and used in Ref. [13]. Since Lie derivatives may not commute, the order of $u_j$ and $u_k$ matters, and $\frac{\partial^2 \tau_i}{\partial \theta_j \partial \dot{\theta}_k} \neq \frac{\partial^2 \tau_i}{\partial \theta_k \partial \dot{\theta}_j}$ in general. To obtain the partial derivatives of spatial quantities embedded in Eq. 7-10, some identities (App. A) are derived. These are an extension to ones defined in Ref. [13], but use the newly developed spatial matrix operators in Sec. IV.

For example identity K1 (App. A) is an extension of identity J1 in Ref. [13]. The identity J1 (Eq. 13) gives the directional derivative of the joint motion sub-space matrix $S_i$ w.r.t the $p^{th}$ DoF of a previous joint $j$ in the connectivity tree.

$$\frac{\partial S_i}{\partial q_{jp}} = s_{j,p} \times S_i$$  \hspace{1cm} (13)

On the other hand, K1 uses the $\tilde{\times}$ operator to extend it to the partial derivative of $S_j$ w.r.t the full joint configuration $q_j$ to give the tensor $\frac{\partial S_j}{\partial q_{j}}$ as:

$$\frac{\partial S_j}{\partial q_{j}} = S_j \tilde{\times} S_i$$  \hspace{1cm} (14)

The identities K4 and K9 describe the partial derivatives of $\Psi_i$, and $\bar{\Psi}_i$ present in Eq. 7-10. Identities K6, K10, and K12 give the partial derivatives of the composite Inertia ($I^n$), body-level Coriolis matrix ($B^n$), and net composite spatial force on a body ($f^n$) Individual partial derivatives of these quantities allow us to use the plug-and-play approach to simplify the algebra needed for SO partial derivatives of ID.

To calculate the SO partial derivatives, we take subsequent partial derivatives of the terms $\frac{\partial \tau_i}{\partial \theta_j}$, $\frac{\partial \tau_i}{\partial \dot{\theta}_j}$, and $\frac{\partial \tau_i}{\partial q_{j}}$ w.r.t joint configuration ($q$), and joint velocity ($\dot{q}$) for joint $k$. We consider three cases, by changing the order of index $k$ as:

- **Case A:** $k \leq j \leq i$
- **Case B:** $j < k \leq i$
- **Case C:** $j \leq i < k$

### Table 1: Spatial Matrix Algebra Identities

$\nu \in M^{6 \times 6}, F \in F^{6 \times n_j}, V \in M^{6 \times 1}, B \in \mathbb{R}^{n_1 \times n_2}, Y \in \mathbb{R}^{n_2 \times n_3 \times n_4}$.

| Identity | Expression |
|----------|------------|
| M1       | $U \times * = - (U \times V)^\top$ |
| M2       | $-V^\top (U \times *) = (U \times V)^\top F$ |
| M3       | $-V^\top (U \times *) F = (U \times V)^\top F$ |
| M4       | $(U \times v) = -\nu \times U$ |
| M5       | $U \times * F = (F \times U)^\bar{R}$ |
| M6       | $F \times U = (U \times F)^\bar{R}$ |
| M7       | $(\lambda U) \times \lambda (U \times \nu)$ |
| M8       | $U \times v = - (V \times U)^\bar{R}$ |
| M9       | $(v \times U) \times = v \times U \times - U \times \nu \times$ |
| M10      | $(v \times U) \times = v \times U \times - U \times \nu \times$ |
| M11      | $(\nu \times U) \times = U \times v \times - v \times U \times$ |
| M12      | $(U \times F)^\bar{R} = - F^\top (U \times)$ |
| M13      | $V^\top (U \times * F) = (V \times U)^\bar{R} F = (F^\top (V \times U)^\bar{R})^\top$ |
| M14      | $\nu \times * F = F \tilde{\times} \nu$ |
| M15      | $f^\tilde{\times} U = U \times f$ |
| M16      | $V^\top (U \times * F)^\bar{R} = [(V \times U)^\bar{R} F]}^\bar{R}$ |
| M17      | $V^\top (U \times * F)^\bar{R} = (-U^\top (V \times F))^\bar{R}$ |
| M18      | $V^\top (U \times * F)^\bar{R} = (V^\top (U \times *) F)^\bar{R}$ |
| M19      | $(B \nu)^\top = Y \times B^\top$ |
The sections below outline the approach taken for calculating the SO partial derivatives. Only some cases are shown to illustrate the main idea, while a detailed summary of all the cases can be found in App. B with step-by-step derivations in Ref. [19] for full documentation.

B. Second order partial derivatives with respect to \( q \)

For SO partials of ID w.r.t \( q \), we take the partial derivatives of Eq. 7 and 8 w.r.t. \( q_k \) for cases A, B, and C mentioned above. Although, the symmetric blocks in the Hessian allow us to re-use three of those six cases. For any of the cases, the partial derivatives of Eq. 7 and 8 can be taken, as long as the accompanying conditions on the equations are met. For example, for Case B \( (j \prec k \preceq i) \), since \( j \prec i \), only Eq. 8 can be used. A derivation for Case C \( (j \preceq i \prec k) \) is shown here as an example. We take the partial derivative of Eq. 7 w.r.t \( q_k \).

Applying the product rule, and using the identities K4, K9, and K13 as:

\[
\frac{\partial^2 \tau_j}{\partial q_j \partial q_k} = 2S_i^T \left( \frac{\partial B_i^C}{\partial q_k} \dot{\Psi} + \frac{\partial I_i^C}{\partial q_k} \ddot{\Psi} \right) \tag{15}
\]

The quantities \( \frac{\partial B_i^C}{\partial q_k} \) and \( \frac{\partial I_i^C}{\partial q_k} \) are third-order tensors where the partial derivatives of matrices \( B_i^C \) and \( I_i^C \) w.r.t each DoF of joint \( k \) are stacked as matrices along the pages of the tensor. Using the identities K6 and K10 to expand:

\[
\frac{\partial^2 \tau_j}{\partial q_j \partial q_k} = 2S_i^T \left( B_i^C [\dot{\Psi}_k] + S_i \times \dot{B}_i^C - B_i^C (S_i \times \dot{\Psi}_k) \right) \dot{\Psi}_j \\
+ S_i^T \left( S_i \times \dot{I}_i^C - I_i^C \right) \dot{\Psi}_j \tag{16}
\]

where the tensor \( B_i^C [\dot{\Psi}_k] \) is a composite calculated for the sub-tree as \( B_i^C [\dot{\Psi}_k] = \sum_{k \geq i} B_i \dot{\Psi}_k \) with:

\[
B_i [\dot{\Psi}_k] = \frac{1}{2} \left[ \left( \dot{\Psi}_k \times \right) I_i - I_i(\dot{\Psi}_k \times) + I_i(\dot{\Psi}_k) \times \right] \tag{17}
\]

Eq. (17) is a natural tensor extension of the body-level Coriolis matrix (Eq. 6) with a matrix argument.

For efficient implementation, all the cases are converted to an index order of \( k \preceq j \preceq i \). First we switch the indices \( k \) and \( j \), followed by \( j \) and \( i \) in Eq. 15 to get \( \frac{\partial^2 \tau_j}{\partial q_i \partial q_k} \) as:

\[
\frac{\partial^2 \tau_j}{\partial q_i \partial q_k} = 2S_i^T \left( B_i^C [\dot{\Psi}_j] + S_i \times \dot{B}_i^C - B_i^C (S_i \times \dot{\Psi}_j) \right) \dot{\Psi}_k \\
+ S_i^T \left( S_i \times \dot{I}_i^C - I_i^C \right) \dot{\Psi}_k \tag{18}
\]

For the term \( \frac{\partial^2 \tau_j}{\partial q_i \partial q_k} \), the symmetric property of a Hessian block is exploited:

\[
\frac{\partial^2 \tau_j}{\partial q_i \partial q_k} = \left[ \frac{\partial^2 \tau_j}{\partial q_k \partial q_i} \right]^\top (k \preceq j \prec i) \tag{19}
\]

The 2-3 tensor rotation in Eq. 19 occurs due to symmetry along the 2nd and 3rd dimensions. Expressions for other cases are in App. B with full derivation in Ref. [19, Sec. IV].

C. Second order partial derivatives with respect to \( \dot{q} \)

For SO partials w.r.t \( \dot{q} \), we take the partial derivatives of Eq. 2 and 10 w.r.t \( \dot{q}_k \). Here, the Case A is split into two cases: 1) \( k \prec j \preceq i \), and 2) \( k = j \preceq i \). This split arises due to the condition for using identity K15 (App. A), and makes the associated algebra easier to follow. A similar split also occurs for Case B into 1) \( j \prec k \preceq i \), and 2) \( j \prec k = i \). The total number of cases is five and results in eight expressions, where some of the expressions exploit symmetry of the Hessian blocks. A list of expressions is given in App. B with full derivation in Ref. [19, Sec. V].

D. Cross Second order partial derivatives with respect to \( q, \dot{q} \)

For cross SO partials, the partial derivative of Eqs. 2,10 w.r.t \( q_k \) to get \( \frac{\partial^2 \tau_j}{\partial q \partial q_k} \). The three cases A,B, and C (Sec. V-A) for Eq. 10 result in six expressions, which are then also used for the symmetric term \( \frac{\partial^2 \tau_j}{\partial \dot{q} \partial \dot{q}_k} \) as:

\[
\frac{\partial^2 \tau_j}{\partial \dot{q} \partial \dot{q}_k} = \left[ \frac{\partial^2 \tau_j}{\partial \dot{q}_k \partial \dot{q}} \right]^\top \tag{20}
\]

Here, we solve all the three cases A,B and C for both Eq. 9 and Eq. 10. Pertaining to Case A \( (k \preceq j \preceq i) \), since \( j \preceq i \), Eq. 9 can be safely used to get \( \frac{\partial^2 \tau_j}{\partial \dot{q} \partial \dot{q}_k} \). However, the \( j \neq i \) requirement on Eq. 10 constrains the condition in Case A to \( k \preceq j \preceq i \). Similarly, for Case C \( (j \preceq i \prec k) \), taking partial derivative of Eq. 10 results in a stricter case \( j \preceq i \prec k \). The indices in the final expressions are switched to order \( k \preceq j \preceq i \) for efficient implementation. Appendix B lists the six expressions with full derivation in Ref. [19, Sec. VI].

E. Cross Second Order Partial derivatives with respect to \( \dot{q} \) and \( \ddot{q} \)

As explained before, the cross-SO partial derivatives of ID w.r.t \( \dot{q} \) and \( \ddot{q} \) results in \( \frac{\partial M}{\partial \dot{q}} \). The lower-triangle of the mass matrix \( M(q) \) for the case \( j \preceq i \) is given as [12]:

\[
M_{ji} = S_i^j I_i^C S_i \tag{21}
\]

Since \( M(q) \) is symmetric [12], \( M_{ij} = M_{ji} \). We apply the three cases A, B, and C discussed above. As an example, for Case B \( (j \prec k \preceq i) \), we take the partial derivative of \( M_{ji} \) w.r.t \( q_k \) and use the product rule, along with identity K13 as:

\[
\frac{\partial M_{ji}}{\partial q_k} = S_i^j \left( \frac{\partial I_i^C}{\partial q_k} S_i + I_i^C \frac{\partial S_i}{\partial q_k} \right) \tag{22}
\]

Using with identities K1 and K6, and canceling terms gives:

\[
\frac{\partial M_{ji}}{\partial q_k} = S_i^j \left( S_i \times I_i^C \right) S_i \tag{23}
\]

Switching indices \( k \) and \( j \) lead to the index order \( k \prec j \preceq i \). Using property M5 leads to:

\[
\frac{\partial M_{ki}}{\partial q_j} = S_k^j \left( (I_i^C S_i) \times S_j \right)^\top \tag{24}
\]

Symmetry of \( M(q) \) gives us \( \frac{\partial M_{ki}}{\partial q_j} \) as:

\[
\frac{\partial M_{ki}}{\partial q_j} = \left[ \frac{\partial M_{ki}}{\partial q_j} \right]^\top \tag{25}
\]

In this case, since the symmetry is along the 1st and the 2nd dimension of the tensor \( \frac{\partial M_{ki}}{\partial q_j} \), the tensor 1-2 rotation takes...
place. Expressions for other cases are listed in App. [B] with
details of derivation at Ref. [19, Sec. VII]

VI. EFFICIENT IMPLEMENTATION AND ALGORITHM

The expressions for SO partials of ID (App. [B]) are first
reduced to matrix form to avoid tensor operations keeping in
mind the lack of stable tensor support in the C++ Eigen library.
The reduction to matrix form is achieved by considering the expressions for
a single DoF of joint \( i \), one at a time. This results in dropping
out of the tensor rotations defined earlier and is explained with
the help of two examples.

Example 1: Considering the case \( k \prec j \preceq i \) the expression

\[
\frac{\partial^2 \tau_{1}}{\partial q_{j} \partial q_{k}} = - \left[ S_{j}^{T} (2B_{i}^{C}[S_{i}][S_{k}]^{R})^{\top} \right]
\]

is studied for the \( p^{th} \) DoF of joint \( i \). The tensor term \( B_{i}^{C}[S_{i}] \)
(denoted by Eq. [17]) reduces to a matrix \( B_{i}^{C} \) where \( s_{i,p} \) is
\( p \)-th column of \( S_{i} \). This term represents the value \( B_{i}^{C} \) would
take if all bodies in the subtree at \( i \) moved with velocity \( s_{i,p} \). The
above reduction enables dropping the 3D tensor rotation \((\hat{R})\). On the other hand, the rotation \((\hat{R})\), originally operating
on a third-order tensor, now operates on a matrix, reducing to
the usual matrix transpose:

\[
\frac{\partial^2 \tau_{1}}{\partial q_{j} \partial q_{k}} = - \left[ 2S_{j}^{T} B_{i}^{C}[s_{i,p}]S_{k} \right]^{T}
\] (26)

Example 2: The term \( \frac{\partial^2 \tau_{1}}{\partial q_{j} \partial q_{i}} \) for the \( p^{th} \) DoF of the joint \( i \) is evaluated in this case. Note the \( 2 \times 3 \)
tensor rotation \((\hat{R})\) results in a matrix transpose, since the matrix
\( \frac{\partial^2 \tau_{1}}{\partial q_{j} \partial q_{i}} \) is a slice in the \( 2 \times 3 \) dimension.

\[
\frac{\partial^2 \tau_{1}}{\partial q_{j} \partial q_{i}} = \left[ \frac{\partial^2 \tau_{1}}{\partial q_{j} \partial q_{i}} \right]^{T}
\] (27)

Algorithm [IDSVA SO] (IDSVA SO) is detailed in App. [B] and returns
all the SO partials explained in Sec. [V] The algorithm has a
computational complexity of \( O(N^d_{\text{fs}}} \), where \( d \) is the
depth of the kinematic tree. It is implemented with all kinematic
and dynamic quantities represented in the ground frame. When
body \( i \) is a successor of \( j \), instead of solving the SO expressions for
joint \( i \), they can be evaluated for the entire sub-tree of body
\( j \) at the same time. In this regard, the index order \( k \preceq j \preceq i \) converts to \( k \to j \preceq \nu(j) \), and \( k \to j \prec i \to k \to j \preceq \varpi(j) \). This
ordering results in the partial derivatives for the vectors
\( \varpi_{\nu(j)} \) and \( \varpi_{\varpi(j)} \) instead of \( \tau_{1} \), and saves an inner loop.

The forward pass in Alg. [IDSVA SO] solves for kinematic and dynamic
quantities like \( a_{i}, B_{i}^{C}, f_{i}^{C}, \dot{\psi}_{i}, \) and \( \dot{\Psi}_{i} \), for the entire
tree. The backward pass then cycles from leaves to root of the tree
and consists of two nested loops: 1) The first loops over all the
DoFs of joint \( j \) to calculate intermediate variables 2) The
second loop then uses these variables to get the SO partials for
the entire sub-tree. The index \( d \) (Alg. [IDSVA SO] Line 13, 30) cycles
over all the DoFs of the joint \( j \) (i.e., from 1 to \( n_{j} \)), and similarly
\( c \) for joint \( k \). The index \( d' \) (Line 14, 32) is the index of the \( d^{th} \)
DoF of joint \( j \) in the kinematic tree (i.e., from 1 to \( n \)), with \( d' \)
for joint \( k \).

The algorithm also makes use of the property that \( u^{T} B v = \text{Trace}(u v^{T} B) \) for vectors \( u, v \) and matrix \( B \). The colon notation represents reshaping a matrix into a vector. In this
regard, if \( A = u^{T} B v \) then \( u^{T} B v = A(:,)^{T} B(:,). \) Consider the
implementation of Eq. [23] as an example. In line 27, the \( 6 \times 6 \)
matrix \( B_{j}^{C}[s_{i,d}] \) is reshaped into a 36-vector for building
columns of a \( 36 \times 6 \) matrix \( D_{3} \). This reshaping is key to the
algorithm, since it allows using \( B_{i}^{C}[s_{i,d}] \) for all \( i \in \nu(j) \) at the
same time to implement [26] on line 55. The matrix transpose
is also dropped since the result \( \frac{\partial^2 \tau_{w}(a)}{\partial q_{\nu} \partial q_{\nu}} \) is a vector.

While the algorithm is complex, an open-source MATLAB version of it can be found at [24], and is integrated with
Featherstone’s spatial v2 library [12].

VII. ACCURACY AND PERFORMANCE

A complex-step method [25] was used to calculate the
SO partials of ID and verify the accuracy for the proposed
algorithm. The complex-step approach was applied to FO
derivatives of ID [13] and verified derivatives accurate to
machine precision. For run-time comparison, the automatic differentiation tool
CasADi [20] in MATLAB was used. AD was used to take the
Jacobians of \( \frac{\partial^2 \tau_{1}}{\partial q_{j} \partial q_{i}} \), using the algorithm presented in
Ref. [13] for the FO derivatives. Since CasADi is not
compatible with functions defined on a Lie group, systems with
single DoF revolute joints were considered. Fig. 5 shows a comparison of IDSVA with the AD and complex-step approach
for serial and branched chains with a branching factor \( b f \) [12].
For serial chains, IDSVA outperforms AD for all \( N \) with
speedups between 1.5 and 3× for models with \( N > 5 \). For
branched chains, the AD computational graph is highly
efficient, resulting in performance gains beyond a critical \( N \). For
\( b f = 2 \) chains, this critical \( N \) lies at \( N = 70 \). The complex-step
method is accurate but slow in run-time, as seen from the
plot in Fig. 3.

A preliminary run-time analysis is also performed with
an implementation extending the Pinocchio [26] open-source
library. Fig. 4 gives run-time numbers (in \( \mu s \)) for several
fixed/float base models for the IDSVA SO algorithm, implemented in C/C++ within the Pinocchio framework [26].
For reference, the run-times for the IDSVA FO algorithm given in [13] are also provided. All computations were performed on an Intel (R) Xeon CPU with 3.07 Ghz, with turbo boost off. From Fig. 4, SO partial derivatives of a floating base 18-DoF HyQ quadruped model take 0.403 ms (or 403 µs) in the C/C++ implementation.

VIII. CONCLUSIONS

In this paper, SO partial derivatives of rigid-body inverse dynamics w.r.t. \( q \), \( \dot{q} \), and \( \ddot{q} \) were derived using Spatial Vector Algebra (SVA) for models with multi-DoF Lie group joints. SVA was extended for spatial matrices to enable tensor operations. This extension was done using three cross-product operators for spatial matrices. An efficient recursive algorithm was also developed to calculate the SO partial derivatives of ID by exploiting common expressions and the structure of the connectivity tree. A MATLAB run-time comparison with AD using CasADi shows a speedup between 1.5-3× for serial chains with \( N > 5 \). Future work will focus on closed-chain structures and more efficient C/C++ implementation for use in optimization.

APPENDIX A: MULTI-DOF JOINT IDENTITIES

The following spatial vector/matrix identities are derived by taking the partial derivative w.r.t. the full joint configuration \( q_j \), or joint velocity \( \dot{q}_j \) of the joint \( j \). The identities apply when \( j \leq i \), and equal zero, unless otherwise stated.

\[
\begin{align*}
\frac{\partial S_j}{\partial q_j} & = S_j \times S_i, \\
\frac{\partial \dot{S}_j}{\partial q_j} & = \dot{\Psi}_j \times S_i + S_j \times \dot{S}_i, \\
\frac{\partial (S_j \dot{q}_j \times S_i)}{\partial q_j} & = S_j \times (S_j \dot{q}_j \times S_i), \\
\frac{\partial \Psi_i}{\partial q_j} & = \dot{\Psi}_j \times S_i + S_j \times \dot{\Psi}_i, \\
\frac{\partial \dot{\Psi}_i}{\partial q_j} & = \ddot{\Psi}_j \times S_i + S_j \times \ddot{\Psi}_i + \dot{\Psi}_j \dot{q}_j, \\
\frac{\partial I_C}{\partial q_j} & = \begin{cases} S_j \times \dot{I}_C - \dot{I}_C (S_j \times), & \text{if } j \leq i \\ S_j \times \dot{I}_C + S_j \times \dot{I}_C (S_j \times), & \text{if } j > i \end{cases}
\end{align*}
\]
\[
\frac{\partial^2 \tau_i}{\partial q_j \partial q_k} = \left[-\left[S_i^\top \left( A_i S_k \right) \dot{S}_j \right] \right]^\top, (k = j \leq i)
\]

\[
\frac{\partial^2 \tau_k}{\partial q_j \partial q_j} = S_k \left[ 2B_C \left[ S_i \right] S_j \right]^\top, (k < j \leq i)
\]

\[
\frac{\partial^2 \tau_i}{\partial q_j \partial q_i} = \left[ \frac{\partial^2 \tau_{ij}}{\partial q_j \partial q_i} \right]^\top, (k < j \leq i)
\]

\[
\frac{\partial^2 \tau_j}{\partial q_j \partial q_j} = S_j \left[ \left( I_C^\top S_i \right) \dot{S}_j \right]^\top, (k < j \leq i)
\]

\[
\frac{\partial^2 \tau_k}{\partial q_j \partial q_i} = S_k \left[ 2B_C \left[ S_i \right] \dot{S}_j \dot{S}_j \right]^\top, (k \leq j < i)
\]

**Cross SO Partial w.r.t \( q \) and \( \dot{q} \):**

\[
\frac{\partial^2 \tau_i}{\partial q_j \partial q_k} = \left[ -\left[S_i^\top \left( A_i S_k \right) \dot{S}_j \right] \right]^\top, (k = j \leq i)
\]

**FO Partial of \( M(q) \) w.r.t \( \dot{q} \):**

\[
\frac{\partial M_{ij}}{\partial q_i} = 0, (k \leq j \leq i)
\]

\[
\frac{\partial M_{ki}}{\partial q_j} = S_k \left[ \left( I_C^\top S_i \right) \dot{S}_j \right]^\top, (k < j \leq i)
\]

\[
\frac{\partial M_{ik}}{\partial q_j} = \left[ \frac{\partial M_{ki}}{\partial q_j} \right]^\top, (k < j \leq i)
\]

\[
\frac{\partial M_{kj}}{\partial q_i} = S_k A_j S_j, (k < j \leq i)
\]

\[
\frac{\partial M_{ij}}{\partial q_i} = \left[ \frac{\partial M_{ij}}{\partial q_i} \right]^\top, (k \leq j \leq i)
\]

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[2] J. Koennemann, A. Del Prete, Y. Tassa, E. Todorov, O. Stasse, M. Bennewitz, and N. Mansard, “Whole-body model-predictive control applied to the hrp-2 humanoid,” in *IEEE/RSJ Int. Conf. on Intelligent Robots and Systems*, 2015, pp. 3346–3351.
Require: \( q, \dot{q}, \ddot{q}, \) model

1: \( v_0 = 0; \ a_0 = -a_p \)
2: for \( j = 1 \) to \( N \) do
3: \( v_i = v_{i-1} + S_i \dot{q}_i \)
4: \( a_i = a_{i-1} + S_i \ddot{q}_i + v_i \times S_i \dot{q}_i \)
5: \( \dot{S}_i = v_i \times S_i \)
6: \( \dot{\dot{S}}_i = a_i \times S_i \)
7: for \( d = 1 \) to \( n_j \) do
8: \( I^C_i = I_i \)
9: \( B_i^C = \frac{1}{2}(v_i \times \dot{v}_i)I_i - I_i (v_i \times) + (I_i v_i) \dot{v}_i \)
10: \( f_i^C = I_i a_i + (v_i \times \dot{v}_i)I_i v_i \)
11: end for
12: for \( j = 1 \) to \( N \) do
13: \( \dot{d}' = \nabla \text{DofIndex}(d, d) \)
14: \( s_d = S_{j,d} ; \dot{\psi}_d = \dot{\psi}_{j,d} ; \ddot{\psi}_d = \ddot{\psi}_{j,d} ; \dot{s}_d = \dot{S}_{j,d} \)
15: \( B_i^C [s_d] = \frac{1}{2}[(s_d \times \dot{v}_i) - I_i^C - I_i^C (s_d \times) + (I_i^C s_d) \dot{v}_i] \)
16: \( B_i^C [\dot{\psi}_d] = \frac{1}{2}[(\dot{\psi}_d \times \dot{v}_i)I_i^C - I_i^C (\dot{\psi}_d \times) + (I_i^C \dot{\psi}_d) \dot{v}_i] \)
17: \( B_i^C [\ddot{\psi}_d] = \frac{1}{2}[(\ddot{\psi}_d \times \dot{v}_i)I_i^C - I_i^C (\ddot{\psi}_d \times) + (I_i^C \ddot{\psi}_d) \dot{v}_i] \)
18: \( A_1 = s_d \times I_i^C - I_i^C (s_d \times) \)
19: \( A_2 = B_i^C [s_d] + s_d \times B_i^C [s_d] \)
20: \( A_3 = (I_i^C s_d) \dot{v}_i \)
21: \( T_1 (\cdot ; d') = I_i^C s_d \)
22: \( T_2 (\cdot ; d') = -B_i^C (\cdot ; s_d) \)
23: \( T_3 (\cdot ; d') = B_i^C [\dot{\psi}_d] + I_i^C \dot{\psi}_d + f_j \dot{v}_i \times s_d \)
24: \( T_4 (\cdot ; d') = B_i^C [\ddot{\psi}_d] + I_i^C \ddot{\psi}_d + s_d \)
25: \( D_1 (\cdot ; d') = A_1 (\cdot) \)
26: \( D_2 (\cdot ; d') = A_2 (\cdot) \)
27: \( D_3 (\cdot ; d') = B_i^C [s_d] (\cdot) \)
28: \( D_4 (\cdot ; d') = A_3 (\cdot) \)
29: end for
30: for \( d = 1 \) to \( n_j \) do
31: \( \dot{k} = j \)
32: \( d' = \nabla \text{DofIndex}(j, d) \)
33: \( s_d = S_{j,d} ; \dot{\psi}_d = \dot{\psi}_{j,d} ; \ddot{\psi}_d = \ddot{\psi}_{j,d} ; \dot{s}_d = \dot{S}_{j,d} \)
34: while \( k > 0 \) do
35: for \( c = 1 \) to \( n_k \) do
36: \( \dot{c}' = \nabla \text{DofIndex}(k, c) \)
37: \( s_c = S_{k,c} ; \dot{\psi}_c = \dot{\psi}_{k,c} ; \ddot{\psi}_c = \ddot{\psi}_{k,c} ; \dot{s}_c = \dot{S}_{k,c} \)
38: \( t_1 (s_c \dot{\psi}_c) (\cdot) \)
39: \( t_2 (s_c \ddot{\psi}_c) (\cdot) \)
40: \( t_3 (\dot{\psi}_c \dot{\psi}_c) (\cdot) \)
41: \( t_4 (s_c \ddot{\psi}_c) (\cdot) \)
42: \( t_5 (s_c \dot{\psi}_c \dot{\psi}_c) (\cdot) \)
43: \( t_6 (s_c \dot{s}_c) (\cdot) \)
44: \( p_1 = \dot{\psi}_c \times s_d \)
45: \( p_2 = \ddot{\psi}_c \times s_d \)
46: \( \frac{\partial^2 \tau_{\dot{q}}}{\partial q \partial q} = -t_1^T D_3 (\cdot, \nu (j)) + p_1 T_1 (\cdot, \nu (j)) \)
47: \( \frac{\partial^2 \tau_{\ddot{q}}}{\partial q \partial q} = -t_2^T D_3 (\cdot, \nu (j)) \)
48: if \( k < j \) then
49: \( t_6 = (s_c \dot{\psi}_c) (\cdot) \)
50: \( t_7 = (s_c \ddot{\psi}_c) (\cdot) \)
51: \( p_3 = s_c \times s_d \)
52: \( p_4 = \nu (j) \)
53: \( p_5 = s_c \times s_d \)
54: \( \frac{\partial^2 \tau_{\dot{q}}}{\partial q \partial q} = \frac{\partial^2 \tau_{\ddot{q}}}{\partial q \partial q} = \frac{\partial^2 \tau_{\ddot{q}}}{\partial q \partial q} = -t_2^T D_3 (\cdot, \nu (j)) \)