OPTIMIZATION OF GENERALIZED JACOBIAN CHAIN PRODUCTS WITHOUT MEMORY CONSTRAINTS

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Abstract. The efficient computation of Jacobians represents a fundamental challenge in computational science and engineering. Large-scale modular numerical simulation programs can be regarded as sequences of evaluations of in our case differentiable modules with corresponding local Jacobians. The latter are typically not available. Tangent and adjoint versions of the individual modules are assumed to be given as results of algorithmic differentiation instead. The classical (Jacobian) matrix chain product formulation is extended with the optional evaluation of matrix-free Jacobian-matrix and matrix-Jacobian products as tangents and adjoints. We propose a dynamic programming algorithm for the minimization of the computational cost of such generalized Jacobian chain products without considering constraints on the available persistent system memory. In other words, the naive evaluation of an adjoint of the entire simulation program is assumed to be a feasible option. No checkpointing is required. Under the given assumptions we obtain optimal solutions which improve the best state of the art methods by factors of up to seven on a set of randomly generated problem instances of growing size.

1. Introduction. This paper extends our prior work on computational cost-efficient accumulation of Jacobian matrices. The corresponding combinatorial Optimal Jacobian Accumulation (OJA) problem was shown to be NP-complete in [18]. Elimination techniques yield different structural variants of (OJA) discussed in [17]. Certain special cases turn out to be computationally tractable as described in [12] and [20].

Relevant closely related work by others includes the introduction of VERTEX ELIMINATION (VE) [13], an integer programming approach to VE [5], computational experiments with VE [6], and the formulation of OJA as LU factorization [22].

Let the multivariate vector function \( y = F(x) : \mathbb{R}^n \to \mathbb{R}^m \) (in the following referred to as the primal function) be continuously differentiable over the domain of interest and let \( F = F_q \circ F_{q-1} \circ \ldots \circ F_2 \circ F_1 \) be such that \( z_i = F_i(z_{i-1}) : \mathbb{R}^{n_i} \to \mathbb{R}^{m_i} \) for \( i = 1, \ldots, q \) and \( z_0 = x, y = z_q \). According to the chain rule of differential calculus the Jacobian \( F' = F'(x) \) of \( F \) is equal to

\[
F' \equiv \frac{dF}{dx} = F'_q \cdot F'_{q-1} \cdot \ldots \cdot F'_1 \in \mathbb{R}^{m \times n}.
\]

We discuss the minimization of the computational cost in term of fused multiply-add (fma) operations of the evaluation of Equation (1.1).

Algorithmic differentiation [14, 19] offers two fundamental modes for preaccumulation of the local Jacobians \( F'_i = F'_i(z_{i-1}) \in \mathbb{R}^{m_i \times n_i} \) prior to the evaluation of the matrix chain product in Equation (1.1). Directional derivatives are computed in scalar tangent mode as

\[
\dot{z}_i = F'_i \cdot \dot{z}_{i-1} \in \mathbb{R}^{m_i}.
\]

Accumulation of the entire Jacobian requires evaluation of \( n_i \) tangents in the Cartesian basis directions in \( \mathbb{R}^{n_i} \) if \( F'_i \) is dense. Potential sparsity can and should be detected [11] and exploited [8, 15]. We denote the computational cost of evaluating a subchain \( F'_j \cdot \ldots \cdot F'_i \),

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\( j > i \), of Equation (1.1) as \( \text{fma}_{j,i} \). The computational cost of evaluating \( F'_i \) in tangent mode is denoted as \( \text{fma}_{i,i} = \text{fma}_i \).

**Scalar Adjoint mode** yields

\[
(1.3) \quad \bar{z}_{i-1} = \bar{z}_i \cdot F'_i \in \mathbb{R}^{1 \times n_i}
\]

and hence dense Jacobians by \( m_i \) reevaluations of Equation (1.3) with \( \bar{z}_i \) ranging over the Cartesian basis directions in \( \mathbb{R}^{m_i} \). The scalar adjoint of \( \bar{z}_i \) can be interpreted as the derivative of some scalar objective with respect to \( z_i \) yielding \( \bar{z}_i \in \mathbb{R}^{1 \times m_i} \) as a row vector. The computational cost of evaluating \( F'_i \) in adjoint mode is denoted as \( \text{fma}_{i,i} = \text{fma}_i \). Further formalization of this cost estimate will follow in Section 2. Combinatorially more challenging Jacobian accumulation methods based on elimination techniques applied to computational graphs [17] will not be considered here. While they may yield a further reduction of \( \text{fma}_{i,i} \) the resulting irregularity of memory accesses makes actual gains in computational performance hard to achieve.

**The Jacobian Chain Product Bracketing problem** asks for a bracketing of the right-hand side of Equation (1.1) which minimizes the number of \( \text{fma} \) operations. **Jacobian Chain Bracketing** can be solved by dynamic programming [3, 9] even if the individual factors are sparse. Sparsity patterns of all subproducts need to be evaluated symbolically in this case [12]. The following recurrence yields an optimal bracketing at a computational cost of \( O(q^3) \):

\[
(1.4) \quad \text{fma}_{j,i} = \begin{cases} 
\min(\text{fma}_{i,i}, \text{fma}_i) & j = i \\
\min_{k<j} (\text{fma}_{j,k+1} + \text{fma}_{k,i} + \text{fma}_{j,k,i}) & j > i
\end{cases}
\]

Facilitated by the overlapping subproblems and optimal substructure properties of Jacobian Chain Product Bracketing the optimization of enclosing chains look up tabulated solutions to all subproblems at constant time complexity. For example, a Jacobian chain product of length \( q = 4 \) with \( F'_1 \in \mathbb{R}^4 \), \( F'_2 \in \mathbb{R}^{1 \times 4} \), \( F'_3 \in \mathbb{R}^{4 \times 5} \), \( F'_4 \in \mathbb{R}^{5 \times 3} \) and \( \text{fma}_{4,4} = 21 \), \( \text{fma}_{3,3} = 5 \), \( \text{fma}_{2,2} = 192 \), \( \text{fma}_{1,1} = 84 \) yields the optimal bracketing \( F' = F'_4 \cdot (F'_3 \cdot F'_2) \cdot F'_1 \) with a cumulative cost of 349 \( \text{fma} \).

The more general Jacobian Chain Product problem asks for some \( \text{fma} \)-optimal way to compute \( F' \) without the restriction of the search space to valid bracketings of Equation (1.1). For example, the matrix product

\[
\begin{pmatrix}
6 & 0 \\
0 & 7
\end{pmatrix}
\begin{pmatrix}
7 & 0 \\
0 & 6
\end{pmatrix}
= \begin{pmatrix}
42 & 0 \\
0 & 42
\end{pmatrix}
\]

[1] can be evaluated at the expense of a single \( \text{fma} \) as opposed to two by exploiting commutativity of scalar multiplication. Jacobian Chain Product Bracketing is NP-complete; see [16] as well as the upcoming proof of Theorem 2.1.

2. **Generalized Jacobian Chain Product.** Any \( F_i = F_i(z_{i-1}) \) induces a labeled directed acyclic graph (DAG) \( G_i = G_i(z_{i-1}) = (V_i, E_i) \) for \( i = 1, \ldots, q \). Vertices in \( V_i = \{ v^j_i : j = 1, \ldots, |V_i| \} \) represent the elemental arithmetic operations \( \varphi^j_i \in \{ +, \sin, \ldots \} \) executed by the implementation of \( F_i \) for given \( z_{i-1} \). Edges in \( (j,k) \in E_i \subseteq V_i \times V_i \) mark data dependencies between arguments and results of elemental operations. They are labeled with local partial derivatives

\[
\frac{\partial \varphi^j_i}{\partial v^k_j}, \quad k : (j,k) \in E_i
\]

of the elemental functions with respect to their arguments. An example is shown in Figure 2.1. Note that a single evaluation of the adjoint in Figure 2.1 (d) delivers both gradient entries for \( \bar{z}^{i+1}_i = 1 \) while two evaluations of the tangent with \( \bar{z}' = (1 \ 0)^T \) and \( \bar{z}' = (0 \ 1)^T \) are required to complete the same task.
Preaccumulation of local Jacobians $F'_{i} \in \mathbb{R}^{m_{i} \times n_{i}}$ requires either $n_{i}$ evaluations of the scalar tangent or $m_{i}$ evaluations of the scalar adjoint. In order to avoid unnecessary reevaluation of the function values and of the local partial derivatives we switch to vectorized versions tangent and adjoint modes.

For given $z_{i-1} \in \mathbb{R}^{n_{i}}$ and $\bar{z}_{i-1} \in \mathbb{R}^{m_{i} \times n_{i}}$ the Jacobian-free evaluation of

$$Z_{i} = F'_{i}(z_{i-1}) \cdot \bar{z}_{i-1} \in \mathbb{R}^{m_{i}, n_{i}},$$

in vector tangent mode is denoted as

$$(2.1) \quad \dot{Z}_{i} := F_{i}(z_{i-1}) \cdot \bar{Z}_{i-1}.$$  

Preaccumulation of a dense $F'_{i}$ requires $\dot{Z}_{i-1}$ to be equal to the identity $I_{n_{i}} \in \mathbb{R}^{n_{i}, n_{i}}$. Equation (2.1) amounts to the simultaneous propagation of $n_{i}$ tangents through $G_{i}$. Explicit construction (and storage) of $G_{i}$ is not required as the computation of tangents augments the primal arithmetic locally. For example, the codes in Figure 2.1 (b) and (c) can be interleaved as $v_{j} = \ldots ; v_{j} = \ldots$ for $j = 1, \ldots, 4$. Tangent propagation induces a computational cost of $n_{i} \cdot |E_{i}|$ in addition to the invariant cost of the primal function evaluation ($|V_{i}|$) augmented with the computation of all local partial derivatives ($|E_{i}|$). The invariant memory requirement of the primal function evaluation is increased by the memory requirement of the tangents the minimization of which turns out to be NP complete as a variant of the DIRECTED BANDWIDTH problem [21]. In the following the invariant part of the computational cost will not be included in cost estimates. The memory requirements of all instances of the discrete search spaces of the combinatorial optimization problems considered in this paper are assumed to be feasible.

Equation (2.1) can be interpreted as the “product” of the DAG $G_{i}$ with the matrix $\dot{Z}_{i-1}$. If $\dot{Z}_{i-1}$ is dense, then its DAG becomes the directed acyclic version of the complete bipartite graph $K_{n_{i-1}, m_{i-1}}$. The computation of $\dot{Z}_{i}$ amounts to the application of the chain rule to the composite DAG [2]. Forward vertex elimination [13] yields a computational cost of $\tilde{n}_{i-1} \cdot |E_{i}|$.

For given $z_{i-1} \in \mathbb{R}^{n_{i}}$ and $\bar{z}_{i} \in \mathbb{R}^{m_{i} \times n_{i}}$ the Jacobian-free evaluation of

$$Z_{i-1} = \bar{Z}_{i} \cdot F'_{i}(z_{i-1}) \in \mathbb{R}^{m_{i} \times n_{i}},$$

in vector adjoint mode is denoted as

$$(2.2) \quad Z_{i-1} := \bar{Z}_{i} \cdot F_{i}(z_{i-1}).$$  

Preaccumulation of a dense $F'_{i}$ requires $\bar{Z}_{i}$ to be equal to the identity $I_{m_{i}} \in \mathbb{R}^{m_{i}, m_{i}}$. Equation (2.2) represents the simultaneous reverse propagation of $m_{i}$ adjoints through $G_{i}$. Without constraints on the total memory requirement the cost-optimal propagation of adjoints amounts to storage of $G_{i}$ thus avoiding unnecessary reevaluation of (parts of) the
primal function in the context of checkpointing methods [10]. For example, the reversal of the data flow requires the adjoint code in Figure 2.1 (d) to be preceded by (the relevant parts of) the primal code in Figure 2.1 (b) (computation of \( v_3 \)). Vector adjoint propagation induces an (additional) computational cost of \( \tilde{m}_i \cdot |E_i| \). The minimization of the additional memory requirement amounts to a variant of the NP complete DIRECTED BANDWIDTH problem [21].

Equation (2.2) can be interpreted as the "product" of the matrix \( Z_i \) with the DAG \( G_i \). If \( Z_i \) is dense, then its DAG becomes the directed acyclic version of the complete bipartite graph \( K_{\tilde{m}_i, m_i} \). The computation of \( Z_{i-1} \) amounts to the application of the chain rule to the composite DAG [2]. Backward vertex elimination [13] yields a computational cost of \( \tilde{m}_i \cdot |E_i| \).

Vector tangent and vector adjoint modes belong to the fundamental set of functionalities offered by the majority of mature algorithmic differentiation software solutions. Hence, we assume them to be available for all \( F_i \) and refer to them simply as tangents and adjoints.

Analogous to JACOBIAN CHAIN PRODUCT the GENERALIZED JACOBIAN CHAIN PRODUCT problem asks for an algorithm for computing \( F' \) with a minimum number of fma operations for given tangents and adjoints for all \( F_i \) in Equation (1.1). As a generalization of an NP-complete problem GENERALIZED JACOBIAN CHAIN PRODUCT must be computationally intractable too. The corresponding proof turns out to be very similar to the arguments presented in [18] and [16]. It uses reduction from ENSEMBLE COMPUTATION which was shown to be NP-complete in [7]:

Given a collection \( C = \{ C_\nu \subseteq A : \nu = 1, \ldots, |C| \} \) of subsets \( C_\nu = \{ c''_i : i = 1, \ldots, |C_\nu| \} \) of a finite set \( A \) and a positive integer \( K \) is there a sequence \( u_i = s_i \cup t_i \) for \( i = 1, \ldots, k \) of \( k \leq K \) union operations, where each \( s_i \) and \( t_i \) is either \( \{ a \} \) for some \( a \in A \) or \( u_j \) for some \( j < i \), such that \( s_i \) and \( t_i \) are disjoint for \( i = 1, \ldots, k \) and such that for every subset \( C_\nu \subseteq C \), \( \nu = 1, \ldots, |C| \), there is some \( u_i, 1 \leq i \leq k \), that is identical to \( C_\nu \). Instances of ENSEMBLE COMPUTATION are given as triplets \((A, C, K)\).

For example, let \( A = \{ a_1, a_2, a_3, a_4 \} \), \( C = \{ \{ a_1, a_2 \}, \{ a_2, a_3, a_4 \}, \{ a_1, a_3, a_4 \} \} \) and \( K = 4 \). The answer to the decision version of this instance of ENSEMBLE COMPUTATION is positive with a corresponding solution given by \( C_1 = u_1 = \{ a_1 \} \cup \{ a_2 \}; u_2 = \{ a_3 \} \cup \{ a_4 \}; C_2 = u_3 = \{ a_2 \} \cup u_2; C_3 = u_4 = \{ a_1 \} \cup u_2 \). \( K = 3 \) yields a negative answer identifying \( K = 4 \) as the solution of the corresponding minimization version of ENSEMBLE COMPUTATION.

A decision version of GENERALIZED JACOBIAN CHAIN PRODUCT can be formulated as follows:

Let tangents \( \tilde{F}_i \cdot \tilde{Z}_i \) and adjoints \( Z_{i+1} \cdot \tilde{F}_i \) be given for all elemental functions \( F_i \), \( i = 1, \ldots, q \), in Equation (1.1) as well as a positive integer \( K \). Is there a sequence of fma operations of length \( k \leq K \) which yields all nonzero entries of \( F' \)?

An example can be found in Figure 2.2 with further explanation to follow.

**Theorem 2.1.** GENERALIZED JACOBIAN CHAIN PRODUCT is NP-complete.

**Proof.** Consider an arbitrary instance \((A, C, K)\) of ENSEMBLE COMPUTATION and a bijection \( A \leftrightarrow \tilde{A} \), where \( \tilde{A} \) consists of \(|A|\) mutually distinct primes. A corresponding bijection \( C \leftrightarrow \tilde{C} \) is implied. Create an extension \((A \cup \tilde{B}, \tilde{C}, K + |B|)\) by adding unique entries from a sufficiently large set \( \tilde{B} \) of primes not in \( A \) to the \( \tilde{C} \) such that they all have the same cardinality \( q \). Note that a solution for this extended instance of ENSEMBLE COMPUTATION implies a solution of the original instance of ENSEMBLE COMPUTATION as each entry of \( \tilde{B} \) appears exactly once.

Fix the order of the elements of the \( \tilde{C}_j \) arbitrarily yielding \( \tilde{C}_j = (\tilde{c}_j)_{i=1}^{\tilde{|C|}} \) for \( j = 1, \ldots, |\tilde{C}| \).

Let

\[
F_i : \mathbb{R}^{C_i} \to \mathbb{R}^{\tilde{C}_i} : \quad z_i = F_i(z_{i-1}) : \quad z^j_i = \tilde{c}^j_i \cdot z^j_{i-1}.
\]

Equation (1.1) becomes a diagonal matrix chain product \( F' = F'_q \cdot \ldots \cdot F'_1 = D_q \cdot \ldots \cdot D_1 \) with \( d_{i,j} = \tilde{c}^j_i \) for \( j = 1, \ldots, |\tilde{C}| \) and \( i = 1, \ldots, q \). By construction \( \text{fma}_{i,j} = \text{fma}_q = \text{fma}_0 = 0 \) through exploitation of bipartiteness of the \( G_i \). According to the fundamental theorem of arithmetic [4] the elements of \( \tilde{C} \) correspond to unique (up to commutativity of scalar multiplication) factorizations of the \(|\tilde{C}|\) nonzero diagonal entries of \( F' \). This uniqueness
property extends to arbitrary subsets of the \( \tilde{C}_j \) considered during the exploration of the search space of the Generalized Jacobian Chain Product problem.

Note that the given family of problem instances are also instances of Jacobian Chain Product as \( \text{fma}_{i,i} = 0 \) for \( i = 1, \ldots, q \). A solution implies a solution of the associated extended instance of Ensemble Computation and, hence, of the original instance of Ensemble Computation.

A proposed solution for Generalized Jacobian Chain Product is easily validated by counting the at most \( |\tilde{C}| \cdot q \) scalar multiplications performed.

A graphical illustration of the reduction is given in Figure 2.2 for a problem instance that corresponds to the example presented for Ensemble Computation.

\[
A = \{a_1, a_2, a_3, a_4\} \Rightarrow \bar{A} = \{2, 3, 5, 7\}
\]
\[
\bar{B} = \{11\}
\]
\[
C = \{\{a_1, a_2\}, \{a_2, a_3, a_4\}, \{a_1, a_3, a_4\}\} \Rightarrow \bar{C} = \{\{2, 3, 11\}, \{3, 5, 7\}, \{2, 5, 7\}\}
\]
\[
K + |\bar{B}| = K + 1 = 5.
\]
The three nonzero diagonal entries of \( F' = (f'_j,i) \in \mathbb{R}^{3 \times 3} \) are computed at the expense of 5 \text{fma} (no additions involved) yielding a positive answer to the given decision version of Generalized Jacobian Chain Product.

3. Generalized Dense Jacobian Chain Product Bracketing. The formulation of Jacobian Chain Product Bracketing assumes availability of all factors of the Jacobian chain product \( F' = F'_q \cdot F'_{q-1} \cdots \cdot F'_1 \). Locally, the choice is between multiplying \( F'_i \) with a factor on its left or on its right within the chain. Generalized Dense Jacobian Chain Product Bracketing assumes availability of implementations of tangents \( \tilde{F}_i \cdot \tilde{Z}_i \) and adjoints \( Z_{i+1} \cdot F_i \). The number of local choices increases. Tangents or adjoints of \( F_i \) can be evaluated or either of them can be used to preaccumulate \( F'_i \). All \( F'_i \) are assumed to be dense.

Formally, the Generalized Dense Jacobian Chain Product Bracketing reads as follows:

Let tangents \( \tilde{F}_i \cdot \tilde{Z}_i \) and adjoints \( \tilde{Z}_{i+1} \cdot \tilde{F}_i \) be given for all elemental functions \( F_i \), \( i = 1, \ldots, q \), in Equation (1.1) whose respective Jacobians are assumed to be dense. For a given positive integer \( K \) there is a sequence of evaluations of the tangents and/or adjoints which minimizes the number of \text{fma} operations required for the accumulation of the Jacobian \( F' \).

Example. A generalized dense Jacobian chain product of length two yields the following eight different bracketings:
- \( F' = F_2 \cdot F_1 = F_2 \cdot (F_1 \cdot I_{n_0}) \)

Fig. 2.2. Reduction from Ensemble Computation to (Generalized) Jacobian Chain Product
\[ F' = F_1' = F_1 = (I_{n_1} \cdot F_1) \]
\[ F' = F_2' \cdot F_3' = (I_{n_3} \cdot F_2) \cdot F_3 \]
\[ F' = F_3' \cdot F_4' = (I_{n_4} \cdot F_3) \cdot F_4 \]
\[ F' = F_2' \cdot F_3' = (I_{n_3} \cdot F_2) \cdot (I_{n_1} \cdot F_3) \]
\[ F' = F_2' \cdot F_3' = (I_{n_3} \cdot F_2) \cdot F_3 \]
\[ F' = F_2' \cdot F_3' = (F_2 \cdot I_{n_2}) \cdot F_3 \]
\[ F' = F_2' \cdot F_3' = F_2 \cdot (I_{n_1} \cdot F_3) \]
\[ F' = F_2' \cdot F_3' = (F_2 \cdot I_{n_1}) \cdot F_3 \]

Theorem 3.1. A solution to Generalized Dense Jacobian Chain Product Bracketing can be computed by the following dynamic programming recurrence:

\[
\begin{align*}
|E_j| \cdot \min\{n_j, m_j\} & \quad j = i \\
\text{fma}_{j,i} = \begin{cases} 
|E_j| \cdot \min\{n_j, m_j\} & \quad j = i \\
\min_{1 \leq k < j} \begin{cases} 
\text{fma}_{j,k+1} + \text{fma}_{k,i} + m_j \cdot m_k \cdot n_i, \\
\text{fma}_{j,k+1} + m_j \cdot \sum_{\nu=1}^{k} |E_{\nu}|, \\
\text{fma}_{k,i} + n_i \cdot \sum_{\nu=k+1}^{j} |E_{\nu}| 
\end{cases} & \quad j > i.
\end{cases}
\end{align*}
\]

Proof. We enumerate the four different conditions in Equation (3.1) as

(a) \[|E_j| \cdot \min\{n_j, m_j\}\]
(b) \[\min_{1 \leq k < j} \text{fma}_{j,k+1} + \text{fma}_{k,i} + m_j \cdot m_k \cdot n_i,\]
(c) \[\min_{1 \leq k < j} \text{fma}_{j,k+1} + m_j \cdot \sum_{\nu=1}^{k} |E_{\nu}| \text{ and}\]
(d) \[\min_{1 \leq k < j} \text{fma}_{k,i} + n_i \cdot \sum_{\nu=k+1}^{j} |E_{\nu}|.\]

The proof proceeds by induction over \(l = j - i\).

0 \leq l \leq 1. All local Jacobians \(F' = F'_{j,j}\) need to be computed in either tangent or adjoint modes at computational costs of \(n_j \cdot |E_j|\) or \(m_j \cdot |E_j|\). The respective minima are tabulated. Special structure of the underlying DAGs \(G_i = (V_i, E_i)\) such as bipartiteness is not exploited. It could result in lower values for \(\text{fma}_{i,i}\), e.g. zero in case of bipartiteness.

The search space for the product of two dense Jacobians \(F'_{i+1} \cdot F'_i\) for given tangents and adjoints of \(F_{i+1}\) and \(F_i\) consists of the following configurations:

1. \((I_{n_{i+1}} \cdot F_{i+1}) : \text{Homogeneous tangent mode yields a computational cost of} \]
   \[\text{fma}_{i+1,i} = n_i \cdot |E_i| + n_i \cdot |E_{i+1}|.\]
   Equivalently, this scenario can be interpreted as preaccumulation of \(F'_i\) in tangent mode followed by evaluation of \((I_{n_{i+1}} \cdot F_{i+1}) \cdot F'_i\). This case is covered by Equation 3.1 (a) and (d) with \(n_i \leq m_i\).

2. \((I_{n_{i+1}} \cdot F_{i+1}) : \text{Preaccumulation of } F'_i\text{ in adjoint mode followed by evaluation of} \]
   \[\text{fma}_{i+1,i} = n_i \cdot |E_i| + n_i \cdot |E_{i+1}|.\]
   This case is covered by Equation 3.1 (a) and (d) with \(n_i \geq m_i\).

3. \((I_{m_{i+1}} \cdot F_{i+1}) : \text{Homogeneous adjoint mode yields a computational cost of} \]
   \[\text{fma}_{i+1,i} = m_{i+1} \cdot |E_{i+1}| + m_{i+1} \cdot |E_i|.\]
   Equivalently, the preaccumulation of \(F'_{i+1}\) in adjoint mode is followed by evaluation of \((I_{m_{i+1}} \cdot F_{i+1}) \cdot F'_i\). This case is covered by Equation 3.1 (a) and (c) with \(n_{i+1} \geq m_{i+1}\).

4. \((I_{m_{i+1}} \cdot F_{i+1}) : \text{Preaccumulation of } F'_{i+1}\text{ in tangent mode followed by evaluation of} \]
   \[\text{fma}_{i+1,i} = n_{i+1} \cdot |E_{i+1}| + m_{i+1} \cdot |E_i|.\]
   This case is covered by Equation 3.1 (a) and (c) with \(n_{i+1} \leq m_{i+1}\).
5. \((\hat{F}_{i+1} \cdot I_{n_{i+1}}) \cdot (I_{m_i} \cdot \hat{F}_i)\) : Preaccumulation of \(F'_i\) in adjoint mode followed by preaccumulation of \(F'_{i+1}\) in tangent mode and evaluation of the dense matrix product \(F'_{i+1} \cdot F'_i\) yields a variant of homogeneous preaccumulation with a computational cost of
\[
fma_{i+1,i} = m_i \cdot |E_i| + n_{i+1} \cdot |E_{i+1}| + m_{i+1} \cdot n_{i+1} \cdot n_i.
\]
This case is covered by Equation 3.1 (a) and (b) with \(n_i \geq m_i\) and \(n_{i+1} \leq m_{i+1} \).
The remaining three homogeneous preaccumulation options cannot improve the optimum.

1. \((\hat{F}_{i+1} \cdot I_{n_{i+1}}) \cdot (\hat{F}_i \cdot I_{n_i})\) : Preaccumulation of both \(F'_i\) and \(F'_{i+1}\) in tangent mode and evaluation of the dense matrix product \(F'_{i+1} \cdot F'_i\) yields a computational cost of
\[
fma_{i+1,i} = n_i \cdot |E_i| + n_{i+1} \cdot |E_{i+1}| + m_{i+1} \cdot n_{i+1} \cdot n_i.
\]
It follows that \(n_i \leq m_i\) and \(n_{i+1} \leq m_{i+1}\) as the computational cost would otherwise be reduced by preaccumulation of either \(F'_i\) or \(F'_{i+1}\) (or both) in adjoint mode. Superiority of homogeneous tangent mode follows immediately from \(n_i \leq m_i\) \(\leq n_{i+1} \leq m_{i+1}\) implying
\[
n_i \cdot |E_i| + n_{i+1} \cdot |E_{i+1}| \leq n_i \cdot |E_i| + n_{i+1} \cdot |E_{i+1}|
\]
\[
< n_i \cdot |E_i| + m_{i+1} \cdot |E_{i+1}| + m_{i+1} \cdot n_{i+1} \cdot n_i.
\]

2. \((I_{m_{i+1}} \cdot \hat{F}_{i+1}) \cdot (I_{m_i} \cdot \hat{F}_i)\) : Preaccumulation of both \(F'_i\) and \(F'_{i+1}\) in adjoint mode and evaluation of the dense matrix product \(F'_{i+1} \cdot F'_i\) yields a computational cost of
\[
fma_{i+1,i} = m_i \cdot |E_i| + n_{i+1} \cdot |E_{i+1}| + m_{i+1} \cdot n_{i+1} \cdot n_i.
\]
It follows that \(m_i \geq n_i\) and \(m_{i+1} \geq n_{i+1}\) as the computational cost would otherwise be reduced by preaccumulation of either \(F'_i\) or \(F'_{i+1}\) (or both) in tangent mode. Superiority of homogeneous adjoint mode follows immediately from \(m_i \geq n_i\) \(\geq m_{i+1}\) implying
\[
m_{i+1} \cdot |E_{i+1}| + m_{i+1} \cdot |E_{i}| \leq m_i \cdot |E_i| + m_{i+1} \cdot |E_{i+1}|
\]
\[
< m_i \cdot |E_i| + m_{i+1} \cdot |E_{i+1}| + m_{i+1} \cdot n_{i+1} \cdot n_i.
\]

3. \((I_{m_{i+1}} \cdot \hat{F}_{i+1}) \cdot (\hat{F}_i \cdot I_{n_i})\) : Preaccumulation of \(F'_i\) in tangent mode followed by preaccumulation of \(F'_{i+1}\) in adjoint mode and evaluation of the dense matrix product \(F'_{i+1} \cdot F'_i\) yields a computational cost of
\[
fma_{i+1,i} = n_i \cdot |E_i| + m_{i+1} \cdot |E_{i+1}| + m_{i+1} \cdot n_{i+1} \cdot n_i.
\]
It follows that \(n_i \leq m_i\) and \(n_{i+1} \geq m_{i+1}\) as the computational cost would otherwise be reduced by preaccumulation of either \(F'_i\) in adjoint mode or by preaccumulation of \(F'_{i+1}\) in tangent mode (or both). This scenario turns out to be inferior to either homogeneous tangent or adjoint modes. For \(n_i \leq m_{i+1}\)
\[
n_i \cdot |E_i| + n_{i+1} \cdot |E_{i+1}| \leq n_i \cdot |E_i| + m_{i+1} \cdot |E_{i+1}|
\]
\[
< n_i \cdot |E_i| + m_{i+1} \cdot |E_{i+1}| + m_{i+1} \cdot n_{i+1} \cdot n_i
\]
while for \(n_i \geq m_{i+1}\)
\[
m_{i+1} \cdot |E_{i+1}| + m_{i+1} \cdot |E_{i}| \leq m_{i+1} \cdot |E_{i+1}| + n_i \cdot |E_i|
\]
\[
< n_i \cdot |E_i| + m_{i+1} \cdot |E_{i+1}| + m_{i+1} \cdot n_{i+1} \cdot n_i.
\]
1 \leq l \Rightarrow l+1. \textbf{Generalized Dense Jacobian Chain Product Bracketing} inherits the overlapping subproblems property from Dense Jacobian Chain Product Bracketing. It adds two choices at each split location \( i \leq k < j \). Splitting at position \( k \) implies the evaluation of \( F_{j,i} \) as \( F_{j,k+1} \cdot F_{k,i} \). In addition to both \( F_{j,k+1} \) and \( F_{k,i} \) being available there are the following two options: \( F_{j,k,i} \) is available and it enters the tangent \( \dot{F}_{j,k+1} \cdot F_{k,i} \) as argument; \( F_{j,k,i+1} \) is available and it enters the adjoint \( F_{j,k+1} \cdot \dot{F}_{k,i} \) as argument. All three options yield \( F_{j,i} \) and they correspond to Equation 3.1 (b)-(d).

The \textit{optimal substructure} property remains to be shown. It implies feasibility of tabulating solutions to the \( \sum_{i=2}^{l+1} \) subproblems for constant-time lookup during the exhaustive search of the \( 3 \cdot l \) possible scenarios corresponding to the \( l \) split locations.

Let the \textit{optimal substructure} property not hold for an optimal \( \text{fma}_{l+1,1} \) obtained at split location \( 1 \leq k < l + 1 \). Three cases need to be distinguished that correspond to Equation 3.1 (b)-(d).

\begin{itemize}
\item[(b)] \( \text{fma}_{j,k+1} + \text{fma}_{k,i} + m_j \cdot m_k \cdot n_1 \): The optimal substructure property holds for the preaccumulation of both \( F_{j,k+1} \) and \( F_{k,i} \) given as chains of length \( \leq l \). The cost of the dense matrix product \( F_{j,k+1} \cdot F_{k,i} \) is independent of the respective preaccumulation methods. For the \textit{optimal substructure} property to not hold either the preaccumulation \( F_{j,k+1} \) or the preaccumulation of \( F_{k,i} \) must be suboptimal. However, replacement of this suboptimal preaccumulation method with the tabulated optimum would reduce the overall cost and hence yield the desired contradiction.

\item[(c)] \( \text{fma}_{j,k+1} + m_j \cdot \sum_{i=1}^{k} |E_i| \): The optimal substructure property holds for the preaccumulation of \( F_{j,k+1} \). The cost of the adjoint \( F_{j,k+1} \cdot \dot{F}_{k,i} \) is independent of the preaccumulation method. The replacement of a suboptimal preaccumulation of \( F_{k,i} \) with the tabulated optimum would reduce the overall cost and hence yield the desired contradiction.

\item[(d)] \( \text{fma}_{k,i} + n_1 \cdot \sum_{i=k+1}^{v} |E_i| \): The optimal substructure property holds for the preaccumulation of \( F_{k,i} \). The cost of the tangent \( \dot{F}_{j,k+1} \cdot F_{k,i} \) is independent of the preaccumulation method. The replacement of a suboptimal preaccumulation of \( F_{k,i} \) with the tabulated optimum would reduce the overall cost and hence yield the desired contradiction.
\end{itemize}

**Example.** We present examples for the previously discussed generalized dense Jacobian chain product of length two. Five configurations are considered with their solutions corresponding to the five instances of the search space investigated in the proof of Theorem 3.1. Optimal values are highlighted.

1. \( n_1 = 2, m_1 = n_2 = 4, m_2 = 8, |E_1| = |E_2| = 100: \)
   \[
   \begin{align*}
   \text{fma} \left( \dot{F}_2 \cdot (I_{n_1}) \right) &= 400, \quad \text{fma} \left( \dot{F}_2 \cdot (I_{m_1} \cdot \dot{F}_1) \right) = 600, \\
   \text{fma} \left( (I_{m_2} \cdot \dot{F}_2) \cdot \dot{F}_1 \right) &= 1600, \quad \text{fma} \left( (I_{m_2} \cdot \dot{F}_2) \cdot (I_{m_1} \cdot \dot{F}_1) \right) = 1200, \\
   \text{fma} \left( (I_{m_2} \cdot \dot{F}_2) \cdot (I_{m_1} \cdot \dot{F}_1) \right) &= 864, \quad \text{fma} \left( (I_{m_2} \cdot \dot{F}_2) \cdot (I_{m_1} \cdot \dot{F}_1) \right) = 664, \\
   \text{fma} \left( (I_{m_2} \cdot \dot{F}_2) \cdot (I_{m_1} \cdot \dot{F}_1) \right) &= 1264, \quad \text{fma} \left( (I_{m_2} \cdot \dot{F}_2) \cdot (I_{m_1} \cdot \dot{F}_1) \right) = 1064.
   \end{align*}
   \]

2. \( n_1 = 4, m_1 = n_2 = 2, m_2 = 32, |E_1| = |E_2| = 100: \)
   \[
   \begin{align*}
   \text{fma} \left( \dot{F}_2 \cdot (I_{n_1}) \right) &= 800, \quad \text{fma} \left( \dot{F}_2 \cdot (I_{m_1} \cdot \dot{F}_1) \right) = 600, \\
   \text{fma} \left( (I_{m_2} \cdot \dot{F}_2) \cdot \dot{F}_1 \right) &= 6400, \quad \text{fma} \left( (I_{m_2} \cdot \dot{F}_2) \cdot (I_{m_1} \cdot \dot{F}_1) \right) = 3400, \\
   \text{fma} \left( (I_{m_2} \cdot \dot{F}_2) \cdot (I_{m_1} \cdot \dot{F}_1) \right) &= 656, \quad \text{fma} \left( (I_{m_2} \cdot \dot{F}_2) \cdot (I_{m_1} \cdot \dot{F}_1) \right) = 856, \\
   \text{fma} \left( (I_{m_2} \cdot \dot{F}_2) \cdot (I_{m_1} \cdot \dot{F}_1) \right) &= 3656, \quad \text{fma} \left( (I_{m_2} \cdot \dot{F}_2) \cdot (I_{m_1} \cdot \dot{F}_1) \right) = 3856.
   \end{align*}
   \]
3. \( n_1 = 8, m_1 = n_2 = 4, m_2 = 2 \), \(|E_1| = |E_2| = 100\):
\[
\text{fma} \left( \hat{F}_2 \cdot (\hat{F}_1 \cdot I_{n_1}) \right) = 1600, \quad \text{fma} \left( \hat{F}_2 \cdot (I_{m_1} \cdot \hat{F}_1) \right) = 1200, \\
\text{fma} \left( (I_{m_2} \cdot \hat{F}_2) \cdot \hat{F}_1 \right) = 400, \quad \text{fma} \left( (\hat{F}_2 \cdot I_{n_2}) \cdot \hat{F}_1 \right) = 600, \\
\text{fma} \left( (\hat{F}_2 \cdot I_{n_2}) \cdot (I_{m_1} \cdot \hat{F}_1) \right) = 864, \quad \text{fma} \left( (I_{m_2} \cdot \hat{F}_2) \cdot (I_{m_1} \cdot \hat{F}_1) \right) = 1264, \\
\text{fma} \left( (I_{m_2} \cdot \hat{F}_2) \cdot (\hat{F}_1 \cdot I_{n_1}) \right) = 664, \quad \text{fma} \left( (\hat{F}_2 \cdot I_{n_2}) \cdot (\hat{F}_1 \cdot I_{n_1}) \right) = 1064.
\]

4. \( n_1 = 32, m_1 = n_2 = 2, m_2 = 4 \), \(|E_1| = |E_2| = 100\):
\[
\text{fma} \left( \hat{F}_2 \cdot (\hat{F}_1 \cdot I_{n_1}) \right) = 6400, \quad \text{fma} \left( \hat{F}_2 \cdot (I_{m_1} \cdot \hat{F}_1) \right) = 3400, \\
\text{fma} \left( (I_{m_2} \cdot \hat{F}_2) \cdot \hat{F}_1 \right) = 800, \quad \text{fma} \left( (\hat{F}_2 \cdot I_{n_2}) \cdot \hat{F}_1 \right) = 600, \\
\text{fma} \left( (\hat{F}_2 \cdot I_{n_2}) \cdot (I_{m_1} \cdot \hat{F}_1) \right) = 656, \quad \text{fma} \left( (I_{m_2} \cdot \hat{F}_2) \cdot (I_{m_1} \cdot \hat{F}_1) \right) = 3656, \\
\text{fma} \left( (I_{m_2} \cdot \hat{F}_2) \cdot (\hat{F}_1 \cdot I_{n_1}) \right) = 856, \quad \text{fma} \left( (\hat{F}_2 \cdot I_{n_2}) \cdot (\hat{F}_1 \cdot I_{n_1}) \right) = 3856.
\]

5. \( n_1 = 4, m_1 = n_2 = 2, m_2 = 4 \), \(|E_1| = |E_2| = 100\):
\[
\text{fma} \left( \hat{F}_2 \cdot (\hat{F}_1 \cdot I_{n_1}) \right) = 800, \quad \text{fma} \left( \hat{F}_2 \cdot (I_{m_1} \cdot \hat{F}_1) \right) = 600, \\
\text{fma} \left( (I_{m_2} \cdot \hat{F}_2) \cdot \hat{F}_1 \right) = 800, \quad \text{fma} \left( (\hat{F}_2 \cdot I_{n_2}) \cdot \hat{F}_1 \right) = 600, \\
\text{fma} \left( (\hat{F}_2 \cdot I_{n_2}) \cdot (I_{m_1} \cdot \hat{F}_1) \right) = 432, \quad \text{fma} \left( (I_{m_2} \cdot \hat{F}_2) \cdot (I_{m_1} \cdot \hat{F}_1) \right) = 632, \\
\text{fma} \left( (I_{m_2} \cdot \hat{F}_2) \cdot (\hat{F}_1 \cdot I_{n_1}) \right) = 632, \quad \text{fma} \left( (\hat{F}_2 \cdot I_{n_2}) \cdot (\hat{F}_1 \cdot I_{n_1}) \right) = 832.
\]

4. Implementation and Numerical Results. Our reference implementation can be downloaded from [www.github.com/un10076/ADMission/GDJCPB](http://www.github.com/un10076/ADMission/GDJCPB) together with the sample problems referred to in this section. It comes in two parts: `gdjcpb_generate.exe` generates problem instances randomly for a given length \( n \) of the chain and upper bound \( \text{max}_\mathbf{m}_n \) on the number of rows and columns of the individual factors. The output can be redirected into a text file which serves as input to `gdjcpb_solve.exe`. The latter computes one solution to the given problem instance. This solution is compared with the costs of the homogeneous tangent, adjoint and preaccumulation methods. The latter implies a solution of the resulting Dense Jacobian Chain Product Bracketing problem.

The source code is written in simple C++. It should compile under arbitrary operating systems assuming availability of a C++14 standard compliant compiler. The `Makefile` provided covers Linux and gcc++ (e.g., version 7.4.0). A `README` contains essential instructions for building and running.

**Example.** Running `gdjcpb_generate.exe 3 3` yields, for example,

3 3 29
1 3 14
2 1 7

desccribing the problem instance \( F' = F'_3 \cdot F'_2 \cdot F'_1 \), where

\[
F'_1 \in \mathbb{R}^{2 \times 3} \rightarrow G_1 = (V_1, E_1) : \ |E_1| = 29 \\
F'_2 \in \mathbb{R}^{1 \times 3} \rightarrow G_2 = (V_2, E_2) : \ |E_2| = 14 \\
F'_3 \in \mathbb{R}^{2 \times 1} \rightarrow G_3 = (V_3, E_3) : \ |E_3| = 7.
\]
Let this problem description be stored in the text file problem.txt. Running
gdjcpb_solve.exe problem.txt

generates the following output:

Dynamic Programming Table:

fma{1,1}=87; Split=0; Operation=Tangent
fma{2,2}=14; Split=0; Operation=Adjoint
fma{2,1}=43; Split=1; Operation=Adjoint
fma{3,3}=7; Split=0; Operation=Tangent
fma{3,2}=27; Split=2; Operation=Preaccumulation
fma{3,1}=56; Split=2; Operation=Preaccumulation

Optimal Cost=56

Cost of homogeneous tangent mode=150
Cost of homogeneous adjoint mode=100
Cost of optimal homogeneous preaccumulation=108+15=123

$F_1'$ is optimally accumulated in tangent mode at the expense of $3 \cdot 29 = 87 \text{fma}$ (similarly, $F_2'$ in adjoint mode at $1 \cdot 14 = 14 \text{fma}$ and $F_3'$ in tangent mode at $1 \cdot 7 = 7 \text{fma}$). Splitting is not applicable (Split=0). The optimal method to compute $F_2' \cdot F_1$ at cost $14+1 \cdot 29 = 43 \text{fma}$. Preaccumulation of $F_2'$ and $F_3'$ followed by the dense matrix product $F_3' \cdot F_2'$ turns out to be the optimal method for computing $F_3,2$. The entire problem instance is evaluated optimally as

$$F' = (\hat{F}_3 \cdot I_1) \cdot (\hat{F}_2 \cdot \hat{F}_1)$$

yielding a computational cost of $7 \cdot 1 + (14 + 29) \cdot 1 + 2 \cdot 1 \cdot 3 = 56 \text{fma}$.

Homogeneous tangent mode

$$F' := \hat{F}_3 \cdot (\hat{F}_2 \cdot (\hat{F}_1 \cdot I_n))$$

yields a cost of $n_1 \cdot \sum_{i=1}^{3} |E_i| = 3 \cdot (29 + 14 + 7) = 150 \text{fma}$. Homogeneous adjoint mode

$$F' := ((I_{m_3} \cdot \hat{F}_3) \cdot \hat{F}_2) \cdot \hat{F}_1$$

yields a cost of $m_3 \cdot \sum_{i=1}^{3} |E_i| = 2 \cdot (29 + 14 + 7) = 100 \text{fma}$. Optimal preaccumulation of $F'_i$ for $i = 1, 2, 3$ takes $\sum_{i=1}^{3} |E_i| \cdot \min(m_i, n_i) = 1 \cdot 7 + 1 \cdot 14 + 3 \cdot 29 = 108 \text{fma}$ followed by optimal bracketing as

$$F' = F'_3 \cdot (F'_2 \cdot F'_1)$$

adding $9 + 6 = 15 \text{fma}$ and yielding a total cost of the optimal homogeneous preaccumulation method of $108 + 15 = 123 \text{fma}$. The dynamic programming solution of the Generalized Dense Jacobian Chain Product Bracketing problem yields an improvement of nearly 50 percent over homogeneous adjoint mode.

In Table 4.1 we present further results for problem instances of growing size generated by calling gdjcpb_generate.exe len max_mn. The dynamic programming solutions improve the best homogeneous method by factors between two and seven. Full specifications of all five test problems can be found in the github repository.

5. Conclusion and Outlook. This paper generalizes prior work on (Jacobian) matrix chain products in the context of algorithmic differentiation (AD) [14, 19]. Tangents and adjoints of modules of numerical simulation programs are typically available rather than the corresponding local Jacobian matrices. Optimal combination of tangents and adjoints yield sometimes impressive reductions of the overall operations count (factors of up to 60 are reported in Section 4). Dynamic programming makes the underlying abstract combinatorial problem formulation computationally tractable.
Applicability of the algorithmic results of this paper to real world applications requires further generalization. Rigorous minimization of the computational cost of an AD task must be based on information about elemental data dependences and resulting Jacobian sparsity patterns. Constraints on the available persistent memory need to be taken into account. Coarser grain data dependence patterns yield matrix DAGs rather than matrix chains. See below for further illustration. These aspects are the subject of ongoing development efforts of the AD Mission Planning software framework.

**Exploitation of Local DAG Structure and Jacobian Sparsity.** Exploitation of sparsity of the $F_i$ in Equation (1.1) impacts the computational cost estimate for their preaccumulation. For example, the nonzero entries of a diagonal matrix $F_i' \in \mathbb{R}^{n \times n}$ can be obtained at the expense of $|E_i|$ fma in either tangent or adjoint modes. Various Jacobian compression techniques based on coloring of different representations of the sparsity patterns as graphs have been proposed for general Jacobian sparsity patterns [8]. The minimization of the overall computational cost becomes intractable as a consequence of intractability of the underlying coloring problems.

Further exploitation of data dependence patterns through structural properties of the concatenation of the local DAGs may lead to further decrease of the computational cost. Vertex, edge, and face elimination techniques have been proposed to allow for applications of the chain rule beyond Jacobian chain multiplication [17]. For example, the following sparse Jacobian chain product was used in [16] to illustrate superiority of vertex elimination [13]:

$$
\begin{pmatrix}
  m_{0,0}^2 & 0 & 0 \\
  0 & m_{1,1}^2 & m_{1,2}^2
\end{pmatrix}
\begin{pmatrix}
  m_{0,0}^1 & m_{0,1}^1 & 0 \\
  0 & m_{1,1}^1 & m_{1,2}^1 \\
  0 & 0 & m_{2,2}^1
\end{pmatrix}
\begin{pmatrix}
  m_{0,0}^0 & 0 \\
  m_{0,1}^0 & m_{1,0}^0 \\
  0 & m_{2,1}^0
\end{pmatrix}
$$

It is straight forward to verify that both bracketings yield a computational cost of $9fma$. Full exploitation of distributivity enables computation of the resulting matrix as

$$
\begin{pmatrix}
m_{0,0}(m_{0,0}^0 + m_{0,1}^1 m_{1,0}^1) \\
 m_{1,0}^1 m_{1,1}^1 m_{1,2}^1
\end{pmatrix}
\begin{pmatrix}
m_{0,0}^0 \\
 m_{0,1}^0 \\
 0
\end{pmatrix}
\begin{pmatrix}
m_{1,0}^0 \\
 m_{1,1}^1 \\
 m_{1,2}^2 + m_{2,1}^2 m_{2,2}^1
\end{pmatrix}
$$

at the expense of only $8fma$.

**Adding Memory Constraints.** Let $F = F_3 \circ F_2 \circ F_1 : \mathbb{R}^8 \to \mathbb{R}$ such that $F_1 : \mathbb{R}^8 \to \mathbb{R}^4$, $F_2 : \mathbb{R}^4 \to \mathbb{R}^2$, $F_3 : \mathbb{R}^2 \to \mathbb{R}^1$ and $|E_i| = 16$ for $i = 1, 2, 3$. Execution of `gdjcpb_solve.exe` for a corresponding problem specification yields the following output:

**Dynamic Programming Table:**

| len | max_mn | Tangent | Adjoint | Preaccumulation | Optimum |
|-----|--------|---------|---------|-----------------|---------|
| 10  | 10     | 3,708   | 5,562   | 2,618           | 1,344   |
| 50  | 50     | 1,283,868 | 1,355,194 | 1,687,575       | 71,668  |
| 100 | 100    | 3,677,565 | 44,866,293  | 40,880,996      | 1,471,636 |
| 250 | 250    | 585,023,794 | 1,496,126,424 | 1,196,618,622   | 9,600,070 |
| 500 | 500    | 21,306,718,862 | 19,518,742,454 | 1,027,696,225   | 149,147,898 |

**Test Results: Cost in fma**

Optimal Cost=48
Cost of homogeneous tangent mode=384
Cost of homogeneous adjoint mode=48
Cost of optimal homogeneous preaccumulation=112+40=152

Obviously, homogeneous adjoint mode turns out to be optimal, which is also recovered by the dynamic programming algorithm. Let the persistent memory requirement of adjoint mode applied to \( F_i \) be estimated as \( |E_i| \). The total memory requirement of homogeneous adjoint mode is equal to \( 3 \cdot 16 = 48 \). Let the size of the available persistent memory requirement be bounded from above by \( M = 40 \). Homogeneous adjoint mode becomes infeasible.

Feasible alternatives include the preaccumulation of \( F_3' \) in tangent mode with no extra persistent memory required and followed by adjoint mode applied to \( F_2 \) and \( F_1 \) yielding

\[
F' = ((\dot{F}_3 \cdot I_2) \cdot \dot{F}_2) \cdot \dot{F}_1
\]

at the expense of \( 2 \cdot 16 + 1 \cdot 16 + 1 \cdot 16 = 64 \text{fma} \) and with feasible persistent memory requirement of \( 16 + 16 = 32 \).

The **optimal substructure** property does not hold anymore. Corresponding optimization methods are under development.

**From Matrix Chains to Matrix DAGs.** Let

\[
F = \left( \begin{array}{c}
F_2 \circ F_1 \\
F_3 \circ F_1
\end{array} \right) : \mathbb{R}^2 \rightarrow \mathbb{R}^3
\]

such that \( F_1 : \mathbb{R}^2 \rightarrow \mathbb{R}^4, F_2 : \mathbb{R}^4 \rightarrow \mathbb{R}^3, F_3 : \mathbb{R}^4 \rightarrow \mathbb{R}^4 \) and \( |E_i| = 16 \) for \( i = 1, 2, 3 \). Assuming availability of sufficient persistent memory homogeneous adjoint mode turns out to be optimal for \( F_2 \circ F_1 \). The Jacobian of \( F_3 \circ F_1 \) is optimally computed in homogeneous tangent mode which yields a conflict for \( F_1' \). Separate optimization of the two Jacobian chain products \( F_2' \cdot F_1' \) and \( F_3' \cdot F_1' \) yields a cumulative computational cost of \( 1 \cdot (16+16) + 2 \cdot (16+16) = 96 \text{fma} \). A better solution is

\[
F' = \left( \begin{array}{c}
\dot{F}_2 \cdot \dot{F}_1 \\
(I_1 \cdot \dot{F}_3) \cdot (\dot{F}_1 \cdot F_2)
\end{array} \right)
\]

yielding a slight decrease in the computational cost to \( 2 \cdot 16 + 2 \cdot 16 + 1 \cdot 16 + 1 \cdot 4 \cdot 8 = 88 \text{fma} \). More significant savings can be expected for less simple DAGs.

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