ON THE COMPUTATIONAL COMPLEXITY OF THE CHAIN RULE OF DIFFERENTIAL CALCULUS

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Abstract. Many modern numerical methods in computational science and engineering rely on derivatives of mathematical models for the phenomena under investigation. The computation of these derivatives often represents the bottleneck in terms of overall runtime performance. First and higher derivative tensors need to be evaluated efficiently.

The chain rule of differentiation is the fundamental prerequisite for computing accurate derivatives of composite functions which perform a potentially very large number of elemental function evaluations. Data flow dependences amongst the elemental functions give rise to a combinatorial optimization problem. We formulate Chain Rule Differentiation and we prove it to be NP-complete. Pointers to research on its approximate solution are given.

Key words. chain rule of differentiation, NP-completeness, algorithmic differentiation, differentiable programming, automatic differentiation

AMS subject classifications. 26B05, 68Q17

1. Introduction. The chain rule is a classic of differential calculus. Hence, it is all the more surprising that first successful steps towards a rigorous computational complexity analysis were taken only in 2008 [19]. A proof of NP-completeness of [Optimal] JACOBIAN ACCUMULATION was presented which is generalized in this paper for derivatives of arbitrary order.

In its simplest form, the chain rule of differentiation reads as

\[ F' = \prod_{i=1}^{q} F'_i \equiv F'_q \cdot F'_{q-1} \cdot \ldots \cdot F'_1. \]

We use = to denote equality and ≡ is the sense of “is defined as.” Differentiability of the elemental functions

\[ F_i : \mathbb{R}^{n_i-1} \to \mathbb{R}^{n_i} : \ z_{i-1} \mapsto z_i = F_i(z_{i-1}) \]

for \( n_0 = n \) and \( n_q = m \) implies differentiability of the composite function

\[ F : \mathbb{R}^n \to \mathbb{R}^m : \ x \mapsto y = F(x) = F_q(F_{q-1}(\ldots F_1(x)\ldots)) \]

where \( z_0 = x \) and \( y = z_q \). Vectors are printed in bold type. The matrix chain product of given elemental Jacobians

\[ F'_i = F'_i(z_{i-1}) \equiv \frac{\partial F_i}{\partial z_{i-1}}(z_{i-1}) \in \mathbb{R}^{n_i \times n_{i-1}} \]

yields

\[ F' = F'(x) \equiv \frac{\partial F}{\partial x}(x) \in \mathbb{R}^{m \times n}, \]

where \( \frac{\partial C}{\partial D} \) denotes the (partial) derivative of the counter \( C \) with respect to the denominator \( D \).

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\[ y = F(x) = F_3(F_2(F_1(x), x), F_1(x)) \Rightarrow \]
\[ \downarrow \]
\[ F' = F'_{3,1}(z_1, z_2) \cdot F'_{1,0}(z_0) + F'_{3,2}(z_1, z_2) \cdot F'_{2,1}(z_0, z_1) \cdot F'_{1,0}(z_0) + F'_{3,1}(z_1, z_2) \cdot F'_{2,0}(z_0, z_1) \]

**Fig. 1. Illustration of Equation (1.7)**

Associativity of matrix multiplication gives rise to the **JACOBIAN CHAIN BRACKETING** problem which can be solved by dynamic programming [2, 10] if the scalar entries of all \( F'_j \) are assumed to be algebraically independent. Potential equality of entries makes the general **JACOBIAN ACCUMULATION** problem NP-complete as shown in [19], where the same problem is referred to as **OPTIMAL JACOBIAN ACCUMULATION**. The proof uses reduction [17] from **ENSEMBLE COMPUTATION** [7]. An extension of the idea is used in this paper for the generalization to derivatives of arbitrary order.

Numerical simulations in computational science and engineering often result in composite functions of highly complex structure. **Algorithmic differentiation (AD)** [15, 20, 23, 24] (also known as automatic differentiation or differentiable programming) is applicable to differentiable multivariate vector functions \( F : \mathbb{R}^n \to \mathbb{R}^m \) implementing

\[
\begin{align*}
  z_0 &= x \\
  z_j &= F_j((z_i)_{i < j}) & \text{for } j = 1, \ldots, q \\
  y &= z_q,
\end{align*}
\]

where, adopting notation from [15], \( i < j \) if and only if \( z_i \) is an argument of \( F_j \). A directed acyclic graph (dag) \( G = (V, E) \) with integer vertices \( V = \{0, \ldots, q\} \) and edges \( E = \{(i, j) : i < j\} \) is induced. Elemental Jacobians \( F'_{j,i} \) are associated with all edges \( (i, j) \in E \). The (first-order) chain rule becomes

\[
F' = \sum_{(0, \ldots, q)} \prod_{(i,j) \in (0, \ldots, q)} F'_{j,i}
\]

[1]. Equation (1.3) represents a special case. Summation is over all paths \( (0, \ldots, q) \) in \( G \) connecting the input \( z_0 = x \) with the output \( y = z_q \). Products of elemental Jacobians along all paths are evaluated as in Equation (1.1). An example is shown in Figure 1.

For given elemental Jacobians

\[
F'_{j,i} = F'_{j,i}((z_k)_{k < i}) = \frac{\partial F_j}{\partial z_i}((z_k)_{k < i})
\]

the evaluation of Equation (1.7) breaks down into a sequence of fused-multiply-add (fma) operations, where each scalar multiplication is optionally followed by a scalar addition. Higher-order chain rules follow naturally. For example, the second-order chain rule for composite functions as in Equation (1.3) becomes

\[
[F'']_{\delta, \alpha_1, \alpha_2} = \sum_{j=1}^{q} \left( \prod_{i=j+1}^{q} F'_i \right)^{[F'']_{j,\gamma}} \left[ \prod_{i=1}^{j-1} F'_i \right]_{\delta, \gamma, \beta_1, \beta_2} \left[ \prod_{k=1}^{j-1} F_k \right]_{\beta_1, \alpha_1} \left[ \prod_{k=1}^{j-1} F_k \right]_{\beta_2, \alpha_2}
\]
It describes the computation of the Hessian tensor $F'' = [F''_{i,k}]_{s \alpha_1, \alpha_2} \in \mathbb{R}^{m \times n \times n}$ for given elemental Jacobians and Hessians. Index notation (summation over the shared index) is used. The corresponding tensors are enclosed in square brackets. An example can be found in Figure 2.

We are interested in minimizing the number of fma required to evaluate the $p$-th-order chain rule for $p = 1, 2, \ldots$. The indexing in third- and higher-order chain rules becomes rather involved. The corresponding formulas are omitted as they are not required for the following argument.

2. Complexity Analysis. The complexity analysis is conducted for the following decision problem.

**Definition 2.1 (Chain Rule Differentiation).**

**Instance:** A composite function as in Equation (1.6) with given elemental derivatives up to order $p$ and a positive integer $K$.

**Question:** Can the $p$-th derivative of $F$ be computed with at most $K$ fma operations?

Gradual decrease of feasible $K$ yields solutions to the corresponding optimization problem.

Chain Rule Differentiation turns out to be NP-complete. The proof uses reduction from the following combinatorial problem.

**Definition 2.2 (Ensemble Computation).**

**Instance:** A collection $C = \{C_\nu \subseteq A : \nu = 1, \ldots, |C|\}$ of subsets $C_\nu = \{c_\nu^i : i = 1, \ldots, |C_\nu|\}$ of a finite set $A$ and a positive integer $K$.

**Question:** 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 $C_\nu \in C$, $\nu = 1, \ldots, |C|$, 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, for $A = \{a_1, a_2, a_3, a_4\}$, $C = \{\{a_1, a_2\}, \{a_2, a_3, a_4\}, \{a_1, a_3, a_4\}\}$ and $K = 4$ the answer is positive as $C_1 = u_1 = \{a_1\} \cup \{a_2\}$; $u_2 = \{a_3\} \cup \{a_4\}$; $C_2 = u_3 = \{a_2\} \cup u_2$; $C_3 = u_4 = \{a_1\} \cup u_2$. $K = 3$ yields a negative answer identifying $K = 4$ as the solution of the corresponding optimization problem.

**Lemma 2.3.** Ensemble Computation is NP-complete.

**Proof.** See [7].

The proof of the following theorem establishes NP-completeness of Chain Rule Differentiation for derivatives of arbitrary order.

**Theorem 2.4.** Chain Rule Differentiation is NP-complete.

**Proof.** Consider an arbitrary instance $(A, C, K)$ of Ensemble Computation and a bijection $A \leftrightarrow \hat{A}$, where $\hat{A}$ consists of $|A|$ mutually distinct primes $^1 \in \{2, 3, 5, \ldots\}$. A corresponding bijection $C \leftrightarrow \hat{C}$ is implied. Create an extended version $(\hat{A} \cup \hat{B}, \hat{C}, K + |\hat{B}|)$ of Ensemble Computation by adding unique entries from a sufficiently large set $\hat{B}$ of primes not in $\hat{A}$ to the $\hat{C}_j$ such that they end up having the same cardinality $q$.

$^1$The proof in [19] does not mention primes explicitly. However, their use in connection with the uniqueness property due to the fundamental theorem of arithmetic [8] turns out to be crucial for the correctness of the overall argument.
Note that a solution for this extended instance of **ENSEMBLE COMPUTATION** implies a solution of the original instance as each entry of $\tilde{B}$ appears exactly once.

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

$$F : \mathbb{R} \to \mathbb{R}^{|\tilde{C}|} : \quad y = z_q = F(x)$$

with $F(x) = F_q(F_{q-1}(\ldots F_1(x) \ldots))$ defined as

$$F_1 : \mathbb{R} \to \mathbb{R}^{|\tilde{C}|} : \quad z_1 = F_1(x) : \quad z_j^1 = \frac{\tilde{c}_1^j}{p!} \cdot x^p$$

and

$$F_i : \mathbb{R}^{|\tilde{C}|} \to \mathbb{R}^{|\tilde{C}|} : \quad z_i = F_i(z_{i-1}) : \quad z_j^i = \tilde{c}_i^j \cdot z_j^{i-1}$$

where $z_i = (z_j^i)$. The $p$-th derivative of $F_1$ becomes equal to

$$F_1^{[p]} = \left( \tilde{c}_1^j \right)_{j=1}^{p} \in \mathbb{R}^{|\tilde{C}|} = \mathbb{R}^{|\tilde{C}| \times \ldots \times (p \text{ times}) \times 1}.$$

The remaining Jacobians ($i = 2, \ldots, q$)

$$F_i^{[1]} = F'_i = (\tilde{a}_{j,k}^i) \in \mathbb{R}^{|\tilde{C}| \times |\tilde{C}|},$$
turn out to be diagonal matrices with

\[ d_{j,k}^i = \begin{cases} c_j^i & \text{if } j = k \\ 0 & \text{otherwise} \end{cases} \]

for \( j = 1, \ldots, |\tilde{C}| \). From \( F_i^{[p]} = 0 \) for \( p > 1 \) it follows that the chain rule of order \( p \) simplifies to

\[ F^{[p]} = \prod_{i=2}^{q} F_i^{[1]} \cdot F_i^{[p]} \tag{2.13} \]

which follows by induction over \( p \): Obviously, the claim holds for \( p = 1 \). Refer to Figure 2, Equation (2.1) for illustration for \( q = 3 \).

For \( p = 2 \) we get Equation (1.8), where all terms with \( j > 1 \) vanish identically as they contain \( F_j^{[2]} = F_j'' = 0 \) as a factor. The remaining term (for \( j = 1 \)) yields Equation (2.13). See Figure 2, Equations (2.2)–(2.4) for illustration.

Suppose that the claim holds for \( p - 1 \), that is,

\[ F^{[p-1]} = \prod_{i=2}^{q} F_i^{[1]} \cdot F_i^{[p-1]} . \]

Application of the (first-order) chain rule yields terms containing \( F_i^{[2]} = 0 \) due to differentiation of the \( F_i^{[1]} \) for \( i = 2, \ldots, q \). They all vanish identically under the given reduction. Only the last term due to differentiation of \( F_i^{[p-1]} \) remains. It is equal to the right-hand side of Equation (2.13). Further illustration is provided in Figure 2 for \( p = 3 \) yielding Equations (2.5)–(2.12).

According to the fundamental theorem of arithmetic [8] the elements of \( \tilde{C} \) correspond to unique (up to commutativity of scalar multiplication) factorizations of the \( |\tilde{C}| \) nonzero entries of \( F^{[p]} \in \mathbb{R}^{|\tilde{C}|} \). This uniqueness property extends to arbitrary subsets of the \( \tilde{C} \) considered during the exploration of the search space of CHAIN RULE DIFFERENTIATION. A solution implies a solution of the associated extended instance of ENSEMBLE COMPUTATION and, hence, of the original instance.

A proposed solution for CHAIN RULE DIFFERENTIATION is easily validated by counting the at most \( |\tilde{C}| \cdot q \) scalar multiplications performed.

For illustration consider the extended version of the example presented for ENSEMBLE COMPUTATION:

\[
A = \{a_1, a_2, a_3, a_4\} \Rightarrow \tilde{A} = \{2, 3, 5, 7\} \\
B = \{11\} \\
C = \{\{a_1, a_2\}, \{a_2, a_3, a_4\}, \{a_1, a_3, a_4\}\} \Rightarrow \tilde{C} = \{\{2, 3, 11\}, \{3, 5, 7\}, \{2, 5, 7\}\} \\
K + |\tilde{B}| = K + 1 = 5 .
\]

The three nonzero entries of

\[
F^{[p]} = F_3^{[1]} \cdot F_2^{[1]} \cdot F_1^{[p]} = \begin{pmatrix} 11 & 3 \\ 7 & 5 \end{pmatrix} \cdot \begin{pmatrix} 2 \\ 3 \end{pmatrix} \cdot \begin{pmatrix} 2 \\ 3 \end{pmatrix}
\]
are computed as
\[
\begin{align*}
\frac{dz_1^2}{dx} &= \frac{dz_2^2}{dz_1^3} \cdot \frac{dp^3z_1}{dz_1^2} = 3 \cdot 2 = 6 \\
\frac{dz_2^3}{dz_2^3} &= \frac{dz_2^3}{dz_2^3} \cdot \frac{dp^3z_2}{dz_3^3} = 5 \cdot 3 = 15 \\
\frac{dz_3^2}{dz_3^3} &= \frac{dz_3^2}{dz_3^3} \cdot \frac{dp^3z_3}{dz_3^3} = 7 \cdot 5 = 35 \\
F_1^{[p]} &= \bar{y}_1 \cdot \left(\frac{dz_2^2}{dz_1^3} \cdot \frac{dp^3z_1}{dz_1^2}\right) = 11 \cdot 6 = 66 \\
F_2^{[p]} &= \frac{dz_3^2}{dz_3^3} \cdot \frac{dp^3z_3}{dz_3^3} = 35 \cdot 3 = 105 \\
F_3^{[p]} &= \frac{dz_3^2}{dz_3^3} \cdot \frac{dp^3z_3}{dz_3^3} = 35 \cdot 2 = 70.
\end{align*}
\]

at the expense of five fma (no additions involved) yielding a positive answer to this instance of the decision version of Chain Rule Differentiation. A corresponding answer to the decision version of Ensemble Computation is implied. Figure 3 depicts the corresponding dag.

3. Tangents and Adjoints. As an immediate consequence of Theorem 2.4 the fma-optimal evaluation of tangents and adjoints of arbitrary order turns out to be computationally intractable. Tangents and adjoints result from algorithmic differentiation applied to given implementations of sufficiently often differentiable multivariate vector functions $\mathbf{y} = \mathbf{F}(\mathbf{x})$ as in Equation (1.6).

The $p$-th-order tangent of $\mathbf{F}$ is defined as
\[
\tilde{\mathbf{y}}_p = \left[F^{[p]}(\mathbf{x})\right]_{k,j_1,\ldots,j_p} \cdot \prod_{i=1}^{p} [\bar{\mathbf{x}}_i]_{j_i},
\]

for given input $\mathbf{x} \in \mathbb{R}^n$ and input tangents $\bar{\mathbf{x}}_i \in \mathbb{R}^n$. It enables the computation of $\mathbf{F}^{[p]}$ with a relative (with respect to the cost of evaluating $\mathbf{F}$) computational cost of $\mathcal{O}(n^p)$ by letting the input tangents range independently over the Cartesian basis vectors in $\mathbb{R}^n$. Exploitation of sparsity is likely to reduce the computational effort [9].

The special case in Equation (2.13) resulting from the reduction in the proof of Theorem 2.4 yields
\[
\tilde{\mathbf{y}}_p = \prod_{i=2}^{q} F_i^{[1]} \cdot F_1^{[p]} \cdot \prod_{j=1}^{p} \bar{x}_j,
\]

where $\bar{x}_j \in \mathbb{R}$ and $\tilde{\mathbf{y}}_p \in \mathbb{R}^{[C]}$. A solution for $\bar{x}_j = 1$, $j = 1,\ldots,p$, implies a solution of Chain Rule Differentiation. The corresponding Tangent Differentiation problem is hence at least as hard as Chain Rule Differentiation.

Adjoints of order $p$ of $\mathbf{F}$ are defined as
\[
[\tilde{\mathbf{y}}_t]_{j_1,\ldots,j_p} = [\tilde{\mathbf{x}}_t]_{j_1,\ldots,j_p} \cdot \left[F^{[p]}(\mathbf{x})\right]_{k,j_1,\ldots,j_p} \prod_{i=1}^{p} [\bar{\mathbf{x}}_i]_{j_i},
\]

for given input $\mathbf{x} \in \mathbb{R}^n$, output adjoint $\tilde{\mathbf{y}}_t \in \mathbb{R}^m$ and input tangents or adjoints $\bar{\mathbf{x}}_i \in \mathbb{R}^n$ yielding the input adjoint $\tilde{\mathbf{x}}_t \in \mathbb{R}^n$. They allow for $\mathbf{F}^{[p]}$ to be evaluated with a relative computational cost of $\mathcal{O}(mn^{p-1})$ by letting $\tilde{\mathbf{y}}_t$ and the $\tilde{\mathbf{x}}_t$, $l \neq i = 1,\ldots,p$, range independently over the Cartesian basis vectors in $\mathbb{R}^m$ and $\mathbb{R}^n$, respectively. Again,
potential sparsity of $F[p]$ should be exploited. The prime use case for adjoints is the computation of gradients ($p = 1$ and $m = 1$) with a relative computational cost of $O(1)$. This method is also known as “back-propagation” in the context of deep neural networks.

Equation (2.13) yields

$$\bar{x}_l = \bar{y}_l^T \cdot \prod_{i=2}^{q} F_i[1] \cdot F_1[p] \cdot \prod_{l \neq j=1}^{p} \bar{x}_j$$

where $\bar{x}_j \in \mathbb{R}$ for $j = 1, \ldots, p$ and $\bar{y}_l \in \mathbb{R}^{\bar{C}_l}$. A solution for $\bar{y}_l = 1 \in \mathbb{R}^{\bar{C}_l}$ and $\bar{x}_j = 1$, $l \neq j = 1, \ldots, p$, implies a solution of Chain Rule Differentiation. The number of additions performed on top of the scalar multiplications is invariant and equal to $|\bar{C}| - 1$. The corresponding Adjoint Differentiation problem becomes at least as hard as Chain Rule Differentiation.

Refer to the literature on algorithmic differentiation for a comprehensive discussion of first- and higher-order tangents and adjoints.

4. Conclusion. The understanding of the computational complexity of discrete problems is a crucial prerequisite for the development of effective algorithms for their (approximate) solution. The efficient computation of first and higher derivatives of numerical simulations has been both a major challenge and fundamental motivation of research and development within the intersection of numerical analysis and theoretical computer science for many decades. Algorithmic progress has largely been based on the assumption about Chain Rule Differentiation being computationally intractable. A formal proof has been missing so far. This gap in the theoretical foundations of algorithmic differentiation is filled by this paper.

A substantial body of known results on discrete problems in algorithmic differentiation exists. It comprises, for example, coloring methods for the compression of sparse derivative tensors [9], algorithms for efficient data flow reversal in adjoint simulations [13] and elimination methods on dags [18]. Refer to the proceedings of so far seven international conferences on algorithmic differentiation, e.g., [3, 5, 6], for a comprehensive survey of numerical, e.g., [14], discrete, e.g., [4], and implementation, e.g., [22], issues as well as for reports on a large number number of successful applications in computational science and engineering, e.g., [12, 16, 21]. Research and development efforts due to the recent increase in interest in artificial intelligence and machine learning [11] are expected to benefit tremendously from this rich collection of results. The algorithmic differentiation community’s web portal www.autodiff.org contains further links in addition to a comprehensive bibliography on the subject.

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