Computing Sparse Jacobians and Hessians Using Algorithmic Differentiation

Bradley M. Bell\textsuperscript{1} and Kasper Kristensen\textsuperscript{2}

\textsuperscript{1}IHME, University of Washington, Seattle, USA, bradbell@seanet.com
\textsuperscript{2}DTU Aqua, Technical University of Denmark, DK, kaskr@dtu.dk

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Abstract

Stochastic scientific models and machine learning optimization estimators have a large number of variables; hence computing large sparse Jacobians and Hessians is important. Algorithmic differentiation (AD) greatly reduces the programming effort required to obtain the sparsity patterns and values for these matrices. We present forward, reverse, and subgraph methods for computing sparse Jacobians and Hessians. Special attention is given to the subgraph method because it is new. The coloring and compression steps are not necessary when computing sparse Jacobians and Hessians using subgraphs. Complexity analysis shows that for some problems the subgraph method is expected to be much faster. We compare C++ operator overloading implementations of the methods in the ADOL-C and CppAD software packages using some of the MINPACK-2 test problems. The experiments are set up in a way that makes them easy to run on different hardware, different systems, different compilers, other test problems and other AD packages. The setup time is the time to record the graph, compute sparsity, coloring, compression, and optimization of the graph. If the setup is necessary for each evaluation, the subgraph implementation has similar run times for sparse Jacobians and faster run times for sparse Hessians.

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ACM classifications: F.2.2, G.2.2
1 Introduction

This paper concerns the computation of sparse Jacobians and Hessians for a function $f : \mathbb{R}^n \to \mathbb{R}^m$ that can be evaluated using a computer program. We use $x \in \mathbb{R}^n$ to denote the inputs and $y \in \mathbb{R}^m$ the outputs of the program.

1.1 The Computational Graph Representation

We use $v \in \mathbb{R}^\ell$ to denote all intermediate values that depend on the inputs

$$v = (v_1, \ldots, v_\ell)^T \in \mathbb{R}^n$$

The independent variable subvector (input vector) is

$$x = (v_1, \ldots, v_n)^T \in \mathbb{R}^n.$$ 

The dependent variable subvector (output vector) is

$$y = (v_{\ell-m+1}, \ldots, v_\ell)^T \in \mathbb{R}^m.$$ 

We decompose the computations to a sequence of elementary functions $\phi_k : \mathbb{R}^2 \to \mathbb{R}$. For $k = n + 1$ to $\ell$

$$v_k = \phi_k(v_{a[k]}, v_{b[k]})$$

where the positive integer $a[k]$ and $b[k]$ are the variable index of the left and right operands for the $k$-th elementary function. It follows that $a[k] < k$ and $b[k] < k$, i.e., computation of the $k$-th variable only depends on the independent variables and variables that have been computed previously. The variables are nodes in the computation graph. Each elementary operation corresponds to two arcs, one from variable $v_{a[k]}$ to variable $v_k$ and the other from variable $v_{b[k]}$ to variable $v_k$. We also write $a[k] \prec k$ and $b[k] \prec k$ which means variable $k$ directly depends on variables $a[k]$ and $b[k]$. This is very similar to the notation in [Griewank and Walther, 2008, Section 2.2]. Some references call nodes $a[k], b[k]$ predecessors of node $k$ and node $k$ a successor of $a[k], b[k]$; for example see [Gower and Mello, 2014, Wang et al., 2016].

We represent a unary elementary function using $a[k] = b[k]$ together with a binary function $\phi_k(v_{a[k]}, v_{b[k]})$ that does not depend on its second argument. One example of a unary representation is $\phi_k(v_{a[k]}, v_{b[k]}) = \sin(v_{a[k]})$. Another example is $\phi_k(v_{a[k]}, v_{b[k]}) = v_{a[k]}$ which can be used to set $y_i = v_{\ell-m+i} = v_{a[\ell-m+i]}$. It is not necessary to have the extra node for $v_{\ell-m+i}$ in the graph for this purpose but it makes this presentation simpler.
Example 1.1  Consider the computer program defined by the following pseudo code:

\[
\text{function } y = f(x) \\
(v_1, v_2, v_3) = x \\
v_4 = v_1 + v_2 \\
v_5 = v_3 \ast v_4 \\
y = (v_4, v_5)
\]

The corresponding function \( f : \mathbb{R}^3 \rightarrow \mathbb{R}^2 \) is given by

\[
f_1(x) = x_1 + x_2 \\
f_2(x) = x_3(x_1 + x_2)
\]

The following is a diagram of the corresponding computational graph:

If the last line of the program pseudo code were changed to \( y = v_4 \), then \( f : \mathbb{R}^3 \rightarrow \mathbb{R} \), \( f(x) = x_3(x_1 + x_2) \) and the diagram above would not change.

The dimension of the range of \( \phi_k \) might be greater than one, and its domain might be greater than two. For example, in some operator overloaded AD tools it is possible to record the operations for one function and make that function an elementary operation in another function. This is closely related to checkpointing; see [Griewank and Walther, 2008, Tables 12.3, 12.4]. We only include binary elementary functions in order to simplify this presentation.

1.2  Dependency Relation

There may be a difference between sparsity patterns and dependency patterns. For example, suppose that

\[
\phi_k(v_a[k], v_b[k]) = \begin{cases} 
0 & \text{if } v_a[k] \leq 0 \\
1 & \text{otherwise} 
\end{cases}
\]
It follows that, where \( \phi_k \) is differentiable, its derivative is zero. Some AD packages might return zero for the derivative everywhere while others might return \((+\infty, 0)\) when \( v_{a[k]} = 0 \). In any event, \( \phi_k(v_{a[k]}, v_{b[k]}) \) depends on the value of \( v_{a[k]} \). Hence, a dependency pattern might include more possibly non-zero elements than a Jacobian sparsity pattern. For the purpose of this presentation, we do not distinguish Jacobian sparsity patterns and dependency patterns. We use the notation \( a[k] \prec k \) and \( b[k] \prec k \) to denote the fact that \( v_k \) directly depends on \( v_{a[k]} \) and \( v_{b[k]} \). Furthermore, we use \( \prec^* \) to denote the transitive closure of this relation; e.g., if \( p \prec q \) and \( q \prec k \) then \( p \prec^* k \); see [Griewank and Walther, 2008, Section 2.2]. Note that the \( \phi_k(v_{a[k]}, v_{b[k]}) \) defined above does not depend on \( v_{b[k]} \); i.e., it represents a unary function. In the text below, unary functions correspond to the case where \( \phi_k \) does not depend on its second argument and \( a[k] = b[k] \).

2 Sparse Jacobians

In this section we present a forward algorithm, reverse algorithm, and reverse subgraph algorithm that compute Jacobian sparsity patterns. We also present an algorithm that obtains a sorted subgraph and discuss computing Jacobians and the computational complexity of the subgraph algorithms.

2.1 Forward Mode Sparsity

We use \( J \) to denote the subset of independent variable indices that are of interest, \( J \subset \{1, \ldots, n\} \). For the independent variable indices, \( k \in \{1, \ldots, n\} \), we define \( X_k \) to be the singleton \( \{k\} \), if \( k \in J \), otherwise the empty set. For \( k \geq n \) we define \( X_k \) to be the indices of independent variables in \( J \) that the variable \( v_k \) depends on; i.e.,

\[
X_k = \begin{cases} 
\{k\} & \text{if } k \leq n \text{ and } k \in J \\
\emptyset & \text{if } k \leq n \text{ and } k \notin J \\
\{j : j \in J \text{ and } j \prec^* k\} & \text{otherwise} 
\end{cases}
\]

The forward Jacobian sparsity calculation is given by Algorithm 2.1; see [Griewank and Walther, 2008, Eq. (7.4)]. Note that for unary functions, \( a[k] = b[k] \) and the union in the algorithm is not necessary. The sparsity pattern for the Jacobian \( f^{(1)}(x) \) is given by the observation that for \( i = 1, \ldots, m, j \in J, \text{ and } x \in \mathbb{R}^n, \)

\[
[f^{(1)}_i(x)]_j \neq 0 \Rightarrow j \in X_{i-m+i}.
\]
Algorithm 1 Forward Jacobian Sparsity

\[
\{ X_1, \ldots, X_\ell \} = \text{function}(J) \\
\text{for } k = 1, \ldots, n \\
\quad \text{if } k \in J \text{ set } X_k = \{ k \} \\
\quad \text{else set } X_k = \emptyset \\
\text{for } k = n+1, \ldots, \ell \\
\quad \text{set } X_k = X_a[k] \cup X_b[k]
\]

We note that there are \( \ell \) sets \( X_k \) and at most \(|J|\) elements in each of these sets where \(|J| \leq n\) is the number of elements in set \( J \).

2.2 Reverse Mode Sparsity

We use \( I \) to denote the subset of dependent variable indices that are of interest, \( I \subset \{1, \ldots, m\} \). For the corresponding variable indices \( k \in \{\ell - m + 1, \ldots, \ell\} \) we define \( Y_k \) to be the singleton \( \{k - \ell + m\} \), if \( k - \ell + m \in I \), otherwise the empty set. For \( k \leq \ell - m \) we define \( Y_k \) to be the indices of dependent variables that the variable in \( I \) that are affected by \( v_k \); i.e.,

\[
Y_k = \begin{cases} 
\{k - \ell + m\} & \text{if } k > \ell - m \text{ and } k - \ell + m \in I \\
\emptyset & \text{if } k > \ell - m \text{ and } k - \ell + m \notin I \\
\{i \in I : k \prec \ell - m + i\} & \text{otherwise}
\end{cases}
\]

We use \( \cup \) for the operator that sets the left hand side to the right hand side union the previous value of the left hand side. The reverse Jacobian sparsity calculation is given by Algorithm 2.2 see [Griewank and Walther, 2008, Eq. (7.8)]. Note that for unary functions, \( a[k] = b[k] \) and the second union in the algorithm is not necessary. The sparsity pattern for the Jacobian \( f^{(1)}(x) \) is given by the observation that for \( i \in I, j = 1, \ldots, n, \) and \( x \in \mathbb{R}^n \),

\[
[f^{(1)}_i(x)]_j \neq 0 \Rightarrow i \in Y_j.
\]

We note that there are \( \ell \) sets \( Y_k \) and at most \(|I|\) elements in each of these sets where \(|I| \leq m\) is the number of elements in set \( I \).

2.3 Reverse Subgraph Sparsity

We call this a reverse subgraph method because on each pass through the graph it only visits the nodes that affect a selected dependent variable. (A
2.3 Reverse Subgraph Sparsity

Algorithm 2 Reverse Jacobian Sparsity
\{ Y_1, \ldots, Y_\ell \} = \text{function}(I)
   \begin{align*}
   \text{for} \quad k = \ell, \ldots, \ell - m + 1 \\
   \quad &\text{if} \quad k - \ell + m \in I \quad \text{set} \quad Y_k = \{ k - \ell + m \} \\
   \quad &\text{else} \quad \text{set} \quad Y_k = \emptyset \\
   \text{for} \quad k = \ell - m, \ldots, 1 \\
   \quad &\text{set} \quad Y_k = \emptyset \\
   \text{for} \quad k = \ell - m, \ldots, 1 \\
   \quad &\text{set} \quad Y_{a[k]} \cup Y_k \\
   \quad &\text{set} \quad Y_{b[k]} \cup Y_k
   \end{align*}

forward subgraph method would only visit nodes that are affected by a selected independent variable.) We present two versions of the algorithm. The first is the ‘pattern only’ variant which finds the sparsity pattern of the Jacobian matrix. The second variant is an extension that finds the actual subgraph required to calculate the non-zero values of the Jacobian.

We use $I \subset \{1, \ldots, m\}$ to denote the subset of dependent variable indices that are of interest. We use $J \subset \{1, \ldots, n\}$ to denote the subset of independent variable indices that are of interest. The set $S_i$ accumulates the independent variables in $J$ that affect the dependent variable $y_i = v_{\ell - m + i}$. The stack $K$ contains the nodes in the subgraph that have not yet been processed for this independent variable index $i$. Let $\{X_k\}$ be the output corresponding to Algorithm 2.1 with input $J$. It is not necessary to have the sequence of sets $\{X_k\}$, just the integer sequence $\{c_k\}$ initialized by

$$\begin{align*}
\text{if} \quad X_k = \emptyset &\quad \text{set} \quad c_k = m + 1 \\
\text{else} &\quad \text{set} \quad c_k = 0
\end{align*}$$

The value $c_k = i < m + 1$ is used to indicate that node $k$ has already been processed for this independent variable index $i$. The reverse subgraph Jacobian sparsity calculation is defined by Algorithm 2.3.

The input value for the sequence $\{c_k\}$ can be computed using Algorithm 2.1 with the sets $X_k$ replaced by integer values $c_k$ that are $m + 1$ for empty $X_k$ and 0 for non-empty $X_k$. The complexity of this calculation is $O(\ell)$, $\ell$ is the number of nodes in the graph. Note that for unary functions, $a[k] = b[k]$ and the condition for the second if block in the algorithm is false. The sparsity pattern for the Jacobian $f^{(1)}(x)$ is given by the observation that for $i \in I$, $j \in J$, and $x \in \mathbb{R}^n$,

$$[f_i^{(1)}(x)]_j \neq 0 \Rightarrow j \in S_i.$$
Algorithm 3 Reverse Subgraph Jacobian: Return Sparsity Pattern

\[ \{ S_i : i \in I \} = \text{function}(I, c_1, \ldots, c_\ell) \]

for \( i \in I \)
  set \( \text{done} = i \), \( \text{ignore} = m + 1 \)
  set \( K = \emptyset \)
  set \( S_i = \emptyset \)
  push \( \ell - m + i \) into \( K \)

while \( K \neq \emptyset \)
  pop \( k \) from \( K \)
  if \( c_a[k] \notin \{ \text{done}, \text{ignore} \} \)
    set \( c_a[k] = \text{done} \)
    if \( a[k] \leq n \) set \( S_i \cup \{ a[k] \} \)
    else push \( a[k] \) into \( K \)
  if \( c_b[k] \notin \{ \text{done}, \text{ignore} \} \)
    set \( c_b[k] = \text{done} \)
    if \( b[k] \leq n \) set \( S_i \cup \{ b[k] \} \)
    else push \( b[k] \) into \( K \)

We note that there are \(|I|\) sets \( S_i \), at most \(|J|\) elements in each of these sets, and \(|I| \leq m \), \(|J| \leq n \). We contrast this with the forward and reverse mode sparsity patterns which have \( \ell \) sets; i.e., a set for each node in the graph.

Remark 2.1 Algorithm 3 is a non-recursive depth-first search in reverse direction from each dependent variable. It uses a mark vector \( c \), of already processed nodes, to avoid multiple placements of the same node in the stack \( K \). The mark vector need not be cleared between consecutive searches because the dependent variable index is used as unique mark for each search. This is important when the subgraph is much smaller than the full graph. The ‘pop \( k \) from \( K \)’ in the algorithm could be replaced by extracting any element from \( K \) and the algorithm would still work. However, extracting the most recently pushed element (the pop) reduces the worst case space requirement for \( K \) from \( l \), the size of the full graph, to the maximum vertex depth of the graph.

2.4 Reverse Subgraph Sorting

Algorithm 3 computes the sparsity patterns \( \{ S_i : i \in I \} \). For each \( i \), the subgraph corresponding to the node order of the pops from \( K \) would have to
be sorted in dependency order to be used for computations. For example, to calculate reverse mode derivatives along the subgraph a dependency order is required. In a worst case scenario, the subgraphs are as big as the full graph and the cost of a reverse sweep is $O(l)$. The cost of sorting the subgraph is $O(l \times \log(l))$. Hence, the sorting could asymptotically become expensive compared to other parts of the algorithm. It is therefore relevant to avoid the sort. With a minor modification of Algorithm 2.3 we can directly obtain a dependency sorted subgraph. If $v_{d[1]}, \ldots, v_{d[|G|]}$ is the ordering for a subgraph $G$, we say that $G$ is dependency sorted or topologically sorted if

$$v_{d[p]} \prec v_{d[q]} \Rightarrow p < q .$$

The main change to the algorithm is as follows: When the top of the stack is a node, for which all the nodes it depends on are already in the subgraph, the top node of the stack is moved to the end of the subgraph. A new mark $-i$ is used to signify that a node has been moved to the subgraph. The result is that the nodes in the subgraph are always dependency sorted.

**Remark 2.2** Algorithm 2.4 can be used to find all the subgraphs, one by one, as needed to perform a full Jacobian calculation. When a $G_i$ has been used for a sweep it is not needed anymore and can be discarded. Note that $G_i$ is only guaranteed to be dependency sorted. In particular, one cannot assume that the independent variable indices (node indices $\leq n$) in the sparsity pattern of the $i$-th row of the Jacobian are at the beginning of $G_i$.

### 2.5 Computing Jacobians

Once a sparsity pattern for a Jacobian is available, a row (column) compression technique could be used to by reverse mode (forward mode) to multiple rows (columns) of the Jacobian during one pass of the computational graph. This requires an approximate solution of a graph coloring problem; see [Griewank and Walther, 2008, Eq. 8.6 and Section 8.3], [Coleman and Verma, 1998].

The reverse subgraph Jacobian method does not require coloring or a compression step. In this way it is similar to the edge pushing algorithm; see [Petra et al., 2018], [Gower and Mello, 2014]. Reference [Gower and Mello, 2014] defines the apex-induced subgraph corresponding to a fixed node as the nodes that the fixed node depends on (plus the corresponding arcs). The subgraphs in this paper are apex-induced subgraphs corresponding to dependent variables. The subgraph Jacobian calculation method for a selected dependent variable is the same as for normal reverse pass, except that only
Algorithm 4 Reverse Subgraph Jacobian: Return Sorted Subgraph
\[ \{G_i : i \in I\} = \text{function}(I, c_1, \ldots, c_\ell) \]
\begin{verbatim}
for i ∈ I
    set visited = i, done = −i, ignore = m + 1
    set \( G_i = \emptyset, K = \emptyset \)
    push \( \ell - m + i \) into K
while K ≠ ∅
    set \( k = \text{top}(K) \)
    comment If all inputs to node \( k \) are done move \( k \) to \( G_i \)
    if \( c_a[k] \in \{\text{done, ignore}\} \) and \( c_b[k] \in \{\text{done, ignore}\} \)
        pop \( k \) from \( K \)
        push \( k \) into \( G_i \)
        set \( c_k = \text{done} \)
    else
        comment \( v_{\text{max}} \) may depend on \( v_{\text{min}} \)
        for \( \nu = \max(a[k], b[k]), \min(a[k], b[k]) \)
            if \( c_\nu \notin \{\text{visited, done, ignore}\} \)
                if \( \nu \leq n \)
                    push \( \nu \) into \( G_i \)
                    set \( c_\nu = \text{done} \)
                else
                    push \( \nu \) into \( K \)
                    set \( c_\nu = \text{visited} \)
        endfor
    endelse
endwhile
endfor
endfunction
\end{verbatim}
2.6 Complexity of the Subgraph Methods

The asymptotic complexity of the subgraph algorithms 2.3 and 2.4 is easy to assess. Both algorithms loop across subgraphs and nodes in each subgraph. For each subgraph, each subgraph node is visited once in Algorithm 2.3 and twice in Algorithm 2.4. The work per node is bounded by a constant independent of the computational graph because there are no more than two arguments (incoming edges) and one result (variable) for each node. It follows that the complexity of both algorithms is

\[ O \left( \sum_{i \in I} |G_i| \right) + O(\ell), \]

whether computing patterns only or numerical entries of the Jacobian. The set \( I \) is the independent variables of interest and \( |I| \) is less than or equal \( m \).

The term \( O(\ell) \) is for the complexity of initializing the sequence \( c_1, \ldots, c_\ell \). If few independent variables are of interest, the term \( \sum_{i \in I} |G_i| \) could be less than \( \ell \), the number of nodes in the entire graph.

The formula above tells us that, for a given problem, the efficiency of the subgraph method is not directly determined by sparsity of the Jacobian matrix. What really matters is the amount of overlap between the subgraphs. The less overlap (smaller \( |G_i \cap G_j| \)) the faster are the algorithms. This is in contrast with the graph coloring approach for which the efficiency is determined by the sparsity pattern of the Jacobian. We highlight these differences by two simple examples:

Example 2.1 The Jacobian \( f^{(1)}(x) \) for this example is a dense matrix. Let \( A \) be a random \( n \)-by-\( n \) matrix and consider the matrix vector multiplication function \( f(x) = Ax \). The computational graph essentially consists of \( n^2 \) multiply-add instructions. The size of the full graph is thus \( O(n^2) \). The size of the \( i \)-th subgraph is \( O(n) \) because \( y_i \) is only affected by row \( i \) of \( A \). The time to calculate the Jacobian by each of the methods using \( n \) reverse sweeps is:
Clearly, no method can be faster than $O(n^2)$ for this problem. Although this example was chosen to show the benefit of the subgraph methods, it demonstrates that there exist non-sparse problems where Algorithm 2.4 is asymptotically optimal.

**Example 2.2** The Jacobian $f^{(1)}(x)$ for this example is the identity matrix plus a matrix that is zero except for column $n$. Suppose that for $k = 1, \ldots, n$, $\phi_k$ is a unary function (in the sense of this paper) and

$$v_{n+k} = \phi_k(v_{n+k-1}, v_{n+k-1}).$$

Recall that $v_n = x_n$ and define $f : \mathbb{R}^n \rightarrow \mathbb{R}^n$ by

$$y_k = v_{2n} + x_k,$$

for $k = 1, \ldots, n$. The computational graph of $f$ and all its subgraphs are of size $O(n)$. The sparsity pattern of the Jacobian is $\{n\}$ for the $n$-th row and $\{n, k\}$ for rows $k = 1, \ldots, n - 1$. This Jacobian can be recovered using a combination of one forward pass and one reverse pass. The asymptotic complexity of the different methods is:

| Method        | Bound          |
|---------------|----------------|
| $n$ full sweeps | $O(n^3)$       |
| Coloring      | $O(n^3)$       |
| Algorithm 2.3 | $O(n^2 \log(n))$ |
| Algorithm 2.4 | $O(n^2)$       |

The subgraph method is inefficient for this problem because of the high subgraph overlap. The coloring approach is most efficient for this example because of the special sparsity pattern.

The examples 2.1 and 2.2 are also useful for testing that implementations of a subgraph algorithm scales as expected for various values of $n$. 
3 Sparse Hessians

In this section we consider computing the sparsity pattern for the Hessian of
\[ g(x) = \sum_{i=1}^{m} w_i f_i(x), \]
where \( w \in \mathbb{R}^m \). We use \( I \) to denote the dependent variable indices for which \( w_i \neq 0 \); i.e.,
\[ i \in I \iff i \in \{1, \ldots, m\} \text{ and } w_i \neq 0. \]

In addition, we use \( J \) to denote the subset of independent variables that are of interest, \( J \subset \{1, \ldots, n\} \). Let \( \{X_k\} \) be the output corresponding to Algorithm 2.1 with input \( J \). Let \( \{Y_k\} \) be the output corresponding to Algorithm 2.2 with input \( I \). It is not necessary to have the sequence of sets \( \{Y_k\} \), just the reverse mode activity analysis Boolean sequence \( \{d_k\} \) defined by
\[ d_k = (Y_k \neq \emptyset). \]

Here and below \( \partial_p h(u) \) is the partial of \( h \) with respect to the \( p \)-th component of its argument vector evaluated at \( u \). We use \( \partial_{p,q} \) to abbreviate \( \partial_p \partial_q \). We say that the elementary function \( \phi_k \) is left nonlinear if \( \partial_{1,1} \phi_k(u) \) is possibly non-zero for some \( u \). It is right nonlinear if \( \partial_{2,2} \phi_k(u) \) is possibly non-zero for some \( u \). It is jointly nonlinear if \( \partial_{1,2} \phi_k(u) = \partial_{2,1} \phi_k(u) \).

3.1 Forward Mode Sparsity

Forward mode for function, derivative, and Hessian values starts with the zero, first, and second order values for the independent variables; i.e., \( x_j, \dot{x}_j, \ddot{x}_j \) for \( j = 1, \ldots, n \). It computes the zero, first, and second order values for the other variables using the following equations for \( k = n + 1, \ldots, \ell \):
\begin{align*}
v_k &= \phi_k(v_a[k], v_b[k]) \\
\dot{v}_k &= \partial_1 \phi_k(v_a[k], v_b[k]) \dot{v}_a[k] + \partial_2 \phi_k(v_a[k], v_b[k]) \dot{v}_b[k] \\
\ddot{v}_k &= \partial_1 \phi_k(v_a[k], v_b[k]) \ddot{v}_a[k] + \partial_2 \phi_k(v_a[k], v_b[k]) \ddot{v}_b[k] \\
&\quad + \partial_{1,1} \phi_k(v_a[k], v_b[k]) v_a^2[k] + \partial_{2,2} \phi_k(v_a[k], v_b[k]) v_b^2[k] \\
&\quad + 2 \partial_{1,2} \phi_k(v_a[k], v_b[k]) \dot{v}_a[k] \dot{v}_b[k].
\end{align*}

The forward mode Hessian sparsity calculation is defined by Algorithm 3.1. This is similar to the algorithm [Walther, 2008] Algorithm II. One difference is using \( \{d_k\} \) to avoid the ‘dead end’ nodes mentioned in the reference.
and nodes that are not included in the Hessian because the corresponding \( w_i \) is zero; see Eq 1 and Eq 2. This is probably the reason that the adolc implementation has a larger \( nnz \) (more possibly non-zero values) than the other implementations in Table 5 and Table 7.

The set \( N_j \), in the algorithm, accumulates the nonlinear interactions between the \( j \)-th independent variable and other independent variables. The nonlinear interactions are initialized as empty. This corresponds to the second order values for the independent variables being zero; i.e., \( 0 = \ddot{x} \in \mathbb{R}^\ell \). In the case where \( \phi_k \) is jointly nonlinear and left nonlinear, the algorithm [Walther, 2008, Algorithm II] uses the fact that \( X_k = X_{a[k]} \cup X_{b[k]} \) to combine two of the unions into one. A similar optimization is done for the case where \( \phi_k \) is jointly nonlinear and right nonlinear.

The sparsity pattern for the Hessian \( g^{(2)}(x) \) is given by the observation that for \( j \in J, p \in J, \) and \( x \in \mathbb{R}^n \),

\[
[g^{(2)}(x)]_{j,p} \neq 0 \Rightarrow p \in N_j .
\]

Given the second order forward mode equation for \( \bar{v}_k \) in Eq 3 a proof for this assertion would be similar to the proof for Algorithm 3.2. The Boolean vector \( d \) has length \( \ell \). There are \( \ell \) sets \( X_k \) and at most \( |J| \) elements in each of these sets. There are \( n \) sets \( N_j \) and at most \( |J| \) elements in each of these sets.
3.2 Reverse Mode Sparsity

The reverse mode Hessian sparsity calculation is defined by Algorithm 3.2. This is similar to the table [Griewank and Walther, 2008, Table 7.4], but includes more general nonlinear binary functions; e.g., \( \text{pow}(x, y) = x^y \). In addition, the algorithm and proof show how to extend the algorithm to functions with more than two arguments.

Algorithm 6 Reverse Hessian Sparsity

\[
\{ M_1, \ldots, M_\ell \} = \text{function}(X_1, d_1, \ldots, X_\ell, d_\ell)
\]

for \( k = 1, \ldots, \ell \) set \( M_k = \emptyset \)

for \( k = \ell, \ldots, n + 1 \) if \( d_k \)

set \( M_a[k] \cup M_k \)

set \( M_b[k] \cup M_k \)

if \( \phi_k \) is left nonlinear

set \( M_a[k] \cup X_a[k] \)

set \( M_b[k] \cup X_a[k] \)

if \( \phi_k \) is right nonlinear

set \( M_a[k] \cup X_b[k] \)

set \( M_b[k] \cup X_b[k] \)

if \( \phi_k \) is jointly nonlinear

set \( M_a[k] \cup X_b[k] \)

set \( M_b[k] \cup X_a[k] \)

As with Algorithm 3.1 when \( \phi_k \) is both left nonlinear and jointly nonlinear (or right nonlinear and jointly nonlinear) two of the unions in Algorithm 3.2 can be combined into one. We include a theorem and proof for this algorithm below.

**Theorem 3.1** For \( j \in J, p \in J, \) and \( x \in \mathbb{R}^n \),

\[
[g^{(2)}(x)]_{j,p} \neq 0 \Rightarrow p \in M_j .
\]

**Proof:** We define the sequence of scalar valued functions \( F_\ell, \ldots, F_n \) by

\[
F_\ell(v_1, \ldots, v_\ell) = \sum_{i=1}^{m} w_i v_{\ell-m+i} ,
\]
and for $k = \ell, \ldots, n + 1$,

$$F_{k-1}(v_1, \ldots, v_{k-1}) = F_k[v_1, \ldots, v_{k-1}, \phi_k(v_a[k], v_b[k])].$$

The function $F_n(x)$ is the same as $g(x)$. Reverse mode computes the derivatives $F_k$ with respect to its arguments for $k = \ell - 1, \ldots, n$. The derivative of $F_n$ with respect to its arguments is equal to $g^{(1)}(x)$ and is the final value for $\dot{x} = (\ddot{v}_1, \ldots, \ddot{v}_n)$ in the algorithm below. We use $\dot{+}$ for the operator that sets the left hand side to the right hand side plus the previous value of the left hand side.

for $k = 1, \ldots, \ell - m$ set $\ddot{v}_k = 0$
for $i = 1, \ldots, m$ set $\ddot{v}_{\ell-m+i} = w_i$
for $k = \ell, \ldots, n + 1$
set $\ddot{v}_{a[k]} = \partial_1 \phi_k(v_a[k], v_b[k]) \ddot{v}_k$
set $\ddot{v}_{b[k]} = \partial_2 \phi_k(v_a[k], v_b[k]) \ddot{v}_k$

Differentiating the algorithm above with respect to $x$, and using the forward mode equation for $\ddot{v}_k$ in Eq [3] we obtain

for $k = 1, \ldots, \ell$ set $\ddot{v}_k = 0$
for $k = \ell, \ldots, n + 1$
comment differentiate setting of $\ddot{v}_{a[k]}$
set $\dot{\ddot{v}}_{a[k]} = \partial_1 \phi_k(v_a[k], v_b[k]) \ddot{v}_k$
set $\dot{\ddot{v}}_{a[k]} = \partial_1, \phi_k(v_a[k], v_b[k]) \ddot{v}_k \ddot{v}_{a[k]}$
set $\dot{\ddot{v}}_{a[k]} = \partial_1, \phi_k(v_a[k], v_b[k]) \ddot{v}_k \ddot{v}_{b[k]}$
comment differentiate setting of $\ddot{v}_{b[k]}$
set $\dot{\ddot{v}}_{b[k]} = \partial_2 \phi_k(v_a[k], v_b[k]) \ddot{v}_k$
set $\dot{\ddot{v}}_{b[k]} = \partial_2 \phi_k(v_a[k], v_b[k]) \ddot{v}_k \ddot{v}_{a[k]}$
set $\dot{\ddot{v}}_{b[k]} = \partial_2 \phi_k(v_a[k], v_b[k]) \ddot{v}_k \ddot{v}_{b[k]}$

Suppose that in Eq [3] $\dot{x}$ is the $j$-th elementary vector. It follows that $\dot{x}_p = \partial_{p,j} g(x)$ for $p = 1, \ldots, n$. We claim that at the beginning of the iteration $k$, in the algorithm above and in Algorithm [3.2] for $p = 1, \ldots, k$

$$\dot{\ddot{v}}_p \neq 0 \Rightarrow j \in M_p .$$

Proving this claim will complement the proof of the theorem. For the first iteration, $k = \ell$ and $\dot{\ddot{v}}_p = 0$ for all $p$. Hence the claim is true for $k = \ell$. 

15
3.2 Reverse Mode Sparsity

Suppose the claim is true at the beginning of the $k$-th iteration, it suffices to show it is true at the beginning of iteration $k-1$. If $p \neq a[k]$ and $p \neq b[k]$ then $\dot{v}_p$ and $M_p$ are the same at the beginning of iteration $k$ and $k-1$, so we are done. The two cases $p = a[k]$ and $p = b[k]$ are symmetric. It suffices to show the case $p = a[k]$; i.e., at the end of iteration $k$

$$\dot{v}_{a[k]} \neq 0 \Rightarrow j \in M_{a[k]}.$$  

If $\dot{v}_{a[k]} \neq 0$ at the beginning of iteration $k$ then by induction $j \in M_{a[k]}$ at the beginning of iteration $k$ and by Algorithm 3.2 it also true at the end of iteration $k - 1$.

Consider the remaining case where $\dot{v}_{a[k]} = 0$ at the beginning of iteration $k$ and $\dot{v}_{a[k]} \neq 0$ at the end of iteration $k$. This implies that the right hand side was non-zero in one of the three assignments to $\dot{v}_{a[k]}$ above. This in turn implies that $d_k$ is true (otherwise $\dot{v}_k$ and $\dot{v}_k$ would be zero). Suppose the first assignment to $\dot{v}_{a[k]}$ is non-zero,

$$0 \neq \partial_1 \phi_k(v_{a[k]}, v_{b[k]}) \hat{v}_k.$$  

This implies that all three terms in the product on the right hand side are non-zero. Hence $\dot{v}_{a[k]} = \partial_1 v_{a[k]}(x)$ is non-zero and $j \in X_{a[k]}$. Furthermore $\phi_k$ is left nonlinear. Hence, at the end of iteration $k$, $X_{a[k]} \subset M_{a[k]}$ and $j \in M_{a[k]}$. This completes the case where the first assignment to $\dot{v}_{a[k]}$ is non-zero.

Suppose the second assignment to $\dot{v}_{a[k]}$ is non-zero,

$$0 \neq \partial_{1,1} \phi_k(v_{a[k]}, v_{b[k]}) \hat{v}_k \dot{v}_{a[k]}.$$  

This implies that all three terms in the product on the right hand side are non-zero. Hence $\dot{v}_{a[k]} = \partial_2 v_{a[k]}(x)$ is non-zero and $j \in X_{a[k]}$. Furthermore $\phi_k$ is left nonlinear. Hence, at the end of iteration $k$, $X_{a[k]} \subset M_{a[k]}$ and $j \in M_{a[k]}$. This completes the case where the second assignment to $\dot{v}_{a[k]}$ is non-zero.

Suppose the third assignment to $\dot{v}_{a[k]}$ is non-zero,

$$0 \neq \partial_{1,2} \phi_k(v_{a[k]}, v_{b[k]}) \hat{v}_k \dot{v}_{b[k]}.$$  

This implies that all three terms in the product on the right hand side are non-zero. Hence $\dot{v}_{b[k]} = \partial_2 v_{b[k]}(x)$ is non-zero and $j \in X_{b[k]}$. Hence, at the end of iteration $k$, $X_{b[k]} \subset M_{a[k]}$ and $j \in M_{a[k]}$. This completes the case where the third assignment to $\dot{v}_{a[k]}$ is non-zero. Q.E.D.

**Remark 3.1** The edge pushing algorithm [Gower and Mello, 2014, Algorithm 3.1] is an alternative reverse mode algorithm for computing Hessian
3.3 Subgraph Sparsity

We are given a function $f : \mathbb{R}^n \rightarrow \mathbb{R}^m$ and define $g : \mathbb{R}^n \rightarrow \mathbb{R}$ by

$$g(x) = \sum_{i=1}^{m} w_i f_i(x).$$

Using reverse mode we can compute $g^{(1)}(x)$ in $O(\ell)$ operations. In addition we can obtain the corresponding computational graph; for example see Kristensen et al., 2016, Tape T2 on pp. 7], [Wang et al., 2016, Section 3.1].

We use this computational graph to define the function $h : \mathbb{R}^n \rightarrow \mathbb{R}^n$

$$h(x) = g^{(1)}(x) = \sum_{i=1}^{m} w_i f_i^{(1)}(x).$$

The Jacobian of $h(x)$ is the Hessian of $g(x)$. We can apply the reverse subgraph Jacobian algorithm to the computational graph for $h(x)$ to obtain the sparsity pattern for the Hessian $g^{(2)}(x)$.

3.4 Computing Hessians

Once a sparsity pattern for a Hessian is available, the values in the Hessian are computed in a manner similar to how the Jacobians are calculated; see Section 2.5.

4 Experiments

The speed tests reported below were run using the following hardware and software:
### 4.1 CSV File

Each run of the speed test program adds a row to a csv file with the following columns:

- **KB**: This is the average memory usage, in kilobytes, where each kilobyte is 1000 bytes (not 1024 bytes). A separate run of the speed test program by valgrind’s massif tool is used to determine these values.

- **implement**:
  - **adolc**: A forward or reverse algorithm implemented by the ADOL-C package
  - **cppad**: A forward or reverse algorithm implemented by the CppAD package
  - **subgraph**: A CppAD implementation of Algorithm 2.3. Note that the potentially faster Algorithm 2.4 is not implemented in CppAD and therefore not part of the test.

- **problem**: This is the minpack2 test source code used to compute $f(x)$; see [Averick et al., 1992]. The source code was converted to C using f2c and then to C++ so it could be used with ADOL-C and CppAD. The available problem values are:
  - **dficfj**: The flow in a channel Jacobian problem
  - **dierfj**: The incompressible elastic rod Jacobian problem
  - **deptfg**: The elastic-plastic torsion Hessian problem
dgl1fg One Dimensional Ginzburg-Landau Hessian problem

colpack: If true, the ColPack package was used to solve the coloring subproblem. Otherwise a greedy distance two coloring algorithm (inspired by the algorithm [Gebremedhin et al., 2005] Algorithm 3.2 and implemented in the CppAD package) is used. In either case, if this is a Hessian problem, a special version of the coloring algorithm that takes advantage of the symmetry, is used. The colpack option must be true when implement is adolc. It must be false when implement is subgraph because it does not use coloring.

indirect: If this is true, an indirect method was used to get more compression out of the coloring problem. It can only be true when implement is adolc and problem corresponds to computing a Hessian. This must be false when implement is cppad because it does not support this recovery option. It must also be false when implement is subgraph because it does not use a compression technique.

optimize: Was the computation graph was optimized. This must be false when implement is adolc because it does not have this option.

setup: Does the sec result include the setup time; e.g., recording the graph, computing sparsity, coloring, compression, and optimization of the graph. If the computational graph (see Section 1.1) corresponding to a function does not depend on the argument to the function, the setup operations can be performed once and re-used for any argument value. Note that optimization is not included in the setup time when implement is adolc. Coloring and compression are not included when implement is subgraph.

reverse: If true (false) reverse mode (forward mode) was used for computing both the sparsity pattern and derivative values. This option must be true when implement is subgraph.

onepass: If true, the derivative values were computed using one pass of graph with multiple directions at the same time. Otherwise, each directional derivative is computed using a separate pass. This option must be false when implement is subgraph. The onepass option must be true when implement is adolc and reverse is false.

n: This is the size of the domain space for f(x).

m: This is the size of the range space for f(x). If m = 1 (m > 1), this is a Hessian (Jacobian) problem.

nnz: This is the number of possibly non-zero values in sparse matrix calculated by the implementation. For a Jacobian problem, the matrix is
the entire Jacobian. For a Hessian problem, the matrix is the upper triangle of the Hessian. Note that one implementation may compute a more efficient sparsity pattern than another (have fewer possibly non-zero values).

\textit{sec}: This is the number of seconds for each calculation of the sparse Jacobian or Hessian.

4.2 Result Tables

There is one table for each \textit{problem} and value for \textit{setup}. For each \textit{implement}, only the combination of options that result in the smallest \textit{sec} (smallest time and fastest execution) is included in the table. Given this selection, options that are the same for all the implementations in a table are reported in the caption at the top of the table. The other options are reported in each row of the table. The rows for each table are sorted so that the \textit{sec} column is monotone non-decreasing.

4.2.1 Jacobian Without Setup

Table 1: \textit{problem=\texttt{dficfj}}, \textit{setup=false}, \textit{indirect=false}, \textit{n=3200}, \textit{m=3200}, \textit{nnz=24787}

| KB   | implement | colpack | optimize | reverse | onepass | sec   |
|------|-----------|---------|----------|---------|---------|-------|
| 12108| adolc     | true    | false    | false   | true    | 0.00186 |
| 13361| cppad     | true    | true     | false   | true    | 0.00233 |
| 6480 | subgraph  | false   | true     | true    | false   | 0.00586 |

Table 2: \textit{problem=\texttt{dierfj}}, \textit{setup=false}, \textit{indirect=false}, \textit{n=3003}, \textit{m=3003}, \textit{nnz=31600}

| KB   | implement | colpack | optimize | reverse | onepass | sec   |
|------|-----------|---------|----------|---------|---------|-------|
| 11561| adolc     | true    | false    | false   | true    | 0.0015 |
| 5797 | cppad     | true    | true     | false   | true    | 0.00182 |
| 4049 | subgraph  | false   | true     | true    | false   | 0.00411 |

Table 1 (Table 2) compares the time, \textit{sec}, and memory, \textit{KB}, required to compute the Jacobian where \textit{problem} is \texttt{dficfj} (\texttt{dierfj}) and \textit{setup} is false. The \texttt{adolc} and \texttt{cppad} implementations use the same algorithms, hence their similar run times is not surprising. The \texttt{subgraph} implementation takes
4 EXPERIMENTS

4.2 Result Tables

about twice as long. (The subgraph implementation does not require a
sparsity calculation or solving a coloring sub-problem and these tasks are
part of the setup for the adolc and cppad implementations.) The number
of possibly non-zeros in the Jacobian sparsity pattern, \( nnz \), depends on the
problem but does not depend on the implementation; i.e., the sparsity pat-
tern efficiency is the same for all the implementations. The fastest option
choices for the cppad implementation are optimize true, reverse false, and
onepass true. Using colpack true with the cppad implementation is faster
for one problem and slower for the other. The indirect true option is not
available for Jacobian problems. The onepass true option results in more
memory usage but we have not included those details in the result tables.
The subgraph implementation uses less memory than the other implemen-
tations.

4.2.2 Jacobian With Setup

Table 3: \( \text{problem}=\text{dficfj}, \text{setup}=\text{true}, \text{indirect}=\text{false}, \text{optimize}=\text{false}, \)
\( n=3200, m=3200, nnz=24787 \)

| KB  | implement | colpack | reverse | onepass | sec   |
|-----|-----------|---------|---------|---------|-------|
| 9807| adolc     | true    | false   | true    | 0.0109|
| 18430| cppad    | true    | false   | true    | 0.013 |
| 8859| subgraph  | false   | true    | false   | 0.0141|

Table 4: \( \text{problem}=\text{dierfj}, \text{setup}=\text{true}, \text{indirect}=\text{false}, \text{optimize}=\text{false}, \)
\( n=3003, m=3003, nnz=31600 \)

| KB  | implement | colpack | reverse | onepass | sec   |
|-----|-----------|---------|---------|---------|-------|
| 9585| adolc     | true    | false   | true    | 0.00862|
| 5151| cppad     | false   | true    | false   | 0.00887|
| 13645| subgraph | false   | true    | true    | 0.0116|

Table 3 (Table 4) is similar to Table 1 (Table 2) with the difference
being that setup is true instead of false. The time for the adolc, cppad and
subgraph implementations are all close. The fastest option choices for the
cppad implementation are optimize false, reverse false, and onepass true.
Using colpack true with the cppad implementation is faster for one problem
and slower for the other. The subgraph implementation uses less memory
than the other implementations.

### 4.2.3 Hessian Without Setup

Table 5: \(\text{problem} = \text{deptfg}, \text{setup} = \text{false}, \text{onepass} = \text{false}, n = 3600, m = 1\)

| KB  | KB  | colpack | indirect | optimize | reverse | nnz  | sec  |
|-----|-----|---------|----------|----------|---------|------|------|
| 5207| subgraph | false  | false   | true     | true    | 10680| 0.00499 |
| 4364| cppad   | true   | false   | true     | false   | 10680| 0.00523 |
| 15115| adolc  | true   | true    | false    | false   | 14161| 0.0226   |

Table 6: \(\text{problem} = \text{dgl1fg}, \text{setup} = \text{false}, \text{onepass} = \text{false}, n = 5000, m = 1, nnz = 10000\)

| KB  | KB  | colpack | indirect | optimize | reverse | sec  |
|-----|-----|---------|----------|----------|---------|------|
| 6086| cppad | true    | false   | true     | true    | 0.00535 |
| 9806| subgraph | false  | false   | true     | true    | 0.00982 |
| 16679| adolc | true   | true    | false    | false   | 0.0243  |

Table 5 (Table 6) compares the time, \(\text{sec}\), and and memory, \(\text{KB}\), required to compute the Hessian where \(\text{problem}\) is \(\text{deptfg}\) (\(\text{dgl1fg}\)) and \(\text{setup}\) is false. The \(\text{cppad}\) and \(\text{subgraph}\) implementations have similar times and the \(\text{adolc}\) implementation takes twice as long. The number of possibly non-zero\(s\) in the \(\text{adolc}\) implementation for the \(\text{deptfg}\) problem is significantly larger than in the other implementations; i.e., its sparsity pattern is not as efficient as the other implementations. The fastest option choices for the \(\text{cppad}\) implementation are \(\text{colpack} \text{ true}, \text{optimize} \text{ true}, \text{and} \text{reverse} \text{ true}\). The \(\text{indirect} \text{ true} \text{option} \text{is} \text{not} \text{available} \text{with} \text{the} \text{cppad} \text{implementation. No implementation uses less memory for both problems.}

### 4.2.4 Hessian With Setup

Table 7 (Table 8) is similar to Table 5 (Table 6) with the difference being that \(\text{setup}\) is true instead of false. The \(\text{subgraph}\) implementation is the fastest for this case and the \(\text{cppad}\) implementation is significantly slower. The fastest option choices for the \(\text{cppad}\) implementation are \(\text{colpack} \text{ true}, \text{optimize} \text{ false}, \text{and} \text{reverse} \text{ true}\). The \(\text{adolc}\) implementation uses less memory than the other implementations.
5 CONCLUSIONS

Table 7: \textit{problem=deptfg, setup=true, onepass=false, n=3600, m=1}

| KB   | implement | colpack | indirect | optimize | reverse | nnz | sec  |
|------|-----------|---------|----------|----------|---------|-----|------|
| 7809 | subgraph  | false   | false    | true     | true    | 10680 | 0.0258 |
| 15299| adolc     | true    | true     | false    | false   | 14161 | 0.0453 |
| 4921 | cppad     | true    | false    | true     | false   | 10680 | 0.0843 |

Table 8: \textit{problem=dgl1fg, setup=true, onepass=false, n=5000, m=1, nnz=10000}

| KB   | implement | colpack | indirect | optimize | reverse | sec  |
|------|-----------|---------|----------|----------|---------|------|
| 33709| subgraph  | false   | false    | false    | true    | 0.0603 |
| 7917 | cppad     | true    | false    | true     | false   | 0.111 |
| 19144| adolc     | true    | false    | true     | false   | 0.114 |

4.2.5 Reproducing Results

The source code that produced the results corresponds to the tag 20210803 of the following git repository:

[https://github.com/bradbell/sparse_ad](https://github.com/bradbell/sparse_ad).

5 Conclusions

If the computational graph (see Section 1.1) corresponding to a function does not depend on the argument to the function, the setup can be done once and reused many times. In the other case, when the setup operations are computed for each argument to a sparse Jacobian, all the implementation have similar timing results. When computing the setup operations for each argument to a sparse Hessian, the \texttt{subgraph} implementation is significantly faster and \texttt{cppad} is significantly slower.

Further testing is called for. We have provided a GitHub repository with the source code used to obtain the results in this paper. This facilitates reproduction of the results as well as extension of the tests to other cases. Other cases include different computer hardware, operating systems, compilers, and versions of the AD packages. The tests can also be extended to other AD packages as well as other problems and problem sizes. The tests also provide example source code that implements the algorithms presented in this paper.
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