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Toward Low Static Memory Jacobian Accumulation

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Abstract. Derivatives are essential ingredients of a wide range of numerical algorithms. We focus on the accumulation of Jacobian matrices by Gaussian elimination on a sparse implementation of the extended Jacobian. A symbolic algorithm is proposed to determine the fill-in. The first version of the new algorithm results in a speedup of five compared to the elimination algorithm that does not exploit sparsity. On the given computer architecture we are able to handle problems with roughly four times the original size.

1 Introduction

The context of this paper is *automatic differentiation* [1, 3, 2] of numerical programs. We consider vector functions

$$F : \mathbb{R}^n \supseteq D \rightarrow \mathbb{R}^m, \quad \mathbf{y} = F(\mathbf{x}) \quad , \quad (1)$$

that map a vector $\mathbf{x} \equiv (x_i)_{i=1,\dots,n}$ of *independent* variables onto a vector $\mathbf{y} \equiv (y_j)_{j=1,\dots,m}$ of *dependent* variables. We assume that F has been implemented as a computer program. Hence, it can be decomposed into a sequence of p single assignments of the value of scalar *elemental* functions φ_i to unique *intermediate* variables v_j . This *code list* of F is given as

$$(\mathbb{R} \ni) v_j = \varphi_j(v_i)_{i \prec j} \quad , \quad (2)$$

where $j = n + 1, \dots, q$ and $q = n + p + m$. The binary relation $i \prec j$ denotes a direct dependence of v_j on v_i . So, $P_j = \{i : i \prec j\}$ is the index set of the arguments of φ_j . Similarly, $S_j = \{i : j \prec i\}$ is the index set of the elemental functions that have v_j as an argument. The variables $\mathbf{v} = (v_i)_{i=1,\dots,q}$ are partitioned into the sets X containing the *independent* variables $(v_i)_{i=1,\dots,n}$, Y containing the *dependent* variables $(v_i)_{i=n+p+1,\dots,q}$, and Z containing the intermediate variables $(v_i)_{i=n+1,\dots,n+p}$. The code list of F can be represented as a directed acyclic *computational graph* $G = G(F) = (V, E)$ with integer vertices $V = \{i : i \in \{1, \dots, q\}\}$ and edges $(i, j) \in E$ if and only if $i \prec j$. Moreover, $V = X \cup Z \cup Y$, where $X = \{1, \dots, n\}$, $Z = \{n + 1, \dots, n + p\}$, and $Y = \{n + p + 1, \dots, q\}$. Hence, X , Y , and Z are mutually disjoint. We distinguish between *independent* ($i \in X$), *intermediate* ($i \in Z$), and *dependent* ($i \in Y$) vertices. Under the assumption that all elemental functions are continuously differentiable in some neighborhood of their arguments all edges (i, j) can be labeled with the partial derivatives $c_{j,i} \equiv \frac{\partial v_j}{\partial v_i}$ of v_j w.r.t. v_i . This labeling yields the *linearized* computational graph G of F . From now on we use the notation G to refer to the linearized computational

graph. Equation (2) can be written as a system of nonlinear equation $C(\mathbf{v})$ [5] as follows.

$$\varphi_j(v_i)_{i \prec j} - v_j = 0 \quad \text{for } j = n + 1, \dots, q \quad . \quad (3)$$

Differentiation with respect to \mathbf{v} leads to

$$C' = C'(\mathbf{v}) \equiv (c'_{j,i})_{i,j=1,\dots,q} = \begin{cases} c_{j,i} & \text{if } i \prec j \\ -1 & \text{if } i = j \\ 0 & \text{otherwise} \end{cases} \quad . \quad (4)$$

The *extended Jacobian* C' is lower triangular. Its rows and columns are enumerated as $j, i = 1, \dots, q$. Row j of C' corresponds to vertex j of G and contains the partial derivatives $c_{j,k}$ of vertex j w.r.t. all of its predecessors $k \in P_j$. In the following we refer to a row i as *independent* for $i \in \{1, \dots, n\}$, as *intermediate* for $i \in \{n + 1, \dots, n + p\}$, and as *dependent* if $i \in \{n + p + 1, \dots, q\}$.

The focus of this paper is on reducing the static memory requirement of Jacobian accumulation by Gaussian elimination on C' . We aim to reuse memory freed due to so called *fill-out* to store *fill-in* generated during the elimination process. The structure of the paper is as follows: In Section 2 we review *compressed row storage* (CRS) for storing C' . In Section 3 we introduce a *symbolic* algorithm that uses a sparse bit pattern to detect fill-in and fill-out. Furthermore, we present first ideas on how to make use of fill-out to further reduce memory requirement. Section 5 shows some runtime and memory analysis.

1.1 Elimination Techniques

The *Jacobian matrix* (or simply *Jacobian*) of F as defined in Equation (1) at point \mathbf{x}_0 is defined as follows:

$$(I\!\!R^{m \times n} \ni) F' = F'(\mathbf{x}_0) \equiv \left(\frac{\partial y_i}{\partial x_j}(\mathbf{x}_0) \right)_{j=1,\dots,n}^{i=1,\dots,m} \quad .$$

F' can be obtained by eliminating all intermediate vertices $j \in Z$ from G as introduced in [6]. Each predecessor $i \in P_j$ of j is connected with all successors $k \in S_j$. If $(i, k) \notin E$, then it has to be generated and labeled with $c_{k,i} := c_{k,j} \cdot c_{j,i}$. Otherwise the value of $c_{k,i}$ is updated as $c_{k,i} := c_{k,i} + c_{k,j} \cdot c_{j,i}$. In the former case we say that *fill-in* is generated whereas *absorption* takes place in the latter. The elimination of vertex j can be understood as some sort of *Gaussian* elimination of all non-zero entries in row/column j of C' . Therefore one has to find all those rows k with $j \prec k$. In order to eliminate row/column j we perform the following transformation on C' .

Definition 1 (Row/Column Elimination in C')

$$c_{k,i} := c_{k,i} + c_{k,j} \cdot c_{j,i} \quad \forall i \prec j \wedge \forall k : j \prec k \quad (5)$$

$$c_{j,i} := 0 \quad \forall i \prec j \quad (6)$$

$$c_{k,j} := 0 \quad \forall k : j \prec k \quad (7)$$

$$c_{j,j} := 0 \quad . \quad (8)$$

Note that $c_{k,i} = 0$ if $i \not\prec k$. The new partial derivatives of v_k , $j \prec k$, with respect to v_i , $i \prec j$, are computed by applying the chain rule in Equation (5). Hence, any sensitivities of the v_k on v_j as well as of v_j on any of the v_i are removed in Equation (6) and Equation (7), respectively. Fill-out is generated. Setting the diagonal entry $c_{j,j}$ to zero in Equation (8) leads to the removal of the j -th row and column in C' . If $c_{k,i} = 0$ then Equation (5) leads to fill-in otherwise it yields absorption.

1.2 Example

Consider the vector function $F : R^3 \rightarrow R^3$ whose code list is given in Figure 1(a). The corresponding G and C' are shown in Figure 1 (b) and (c), respectively. The

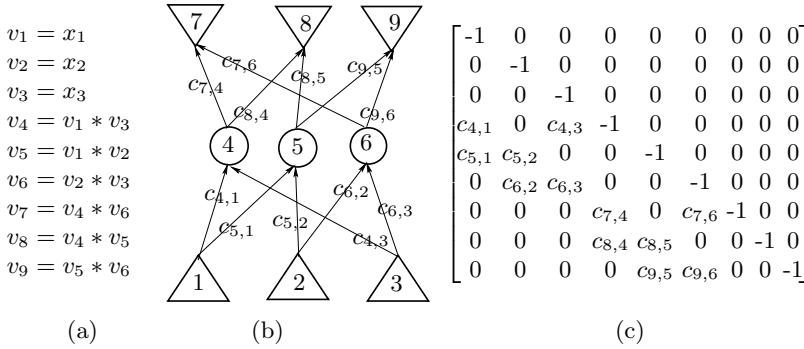


Fig. 1. Code list (a); linearized computational graph G (b); C' (c) of F .

symbols \triangle represent independent, \triangledown dependent, and \circlearrowleft intermediate vertices. Consider row 5 in Figure 1 (c) containing $c_{5,1}$ and $c_{5,2}$. These are labels of incoming edges (1, 5) and (2, 5) of vertex 5 in Figure 1 (b). Column 5 contains the partial derivatives $c_{8,5}$ and $c_{9,5}$ that are the labels of outgoing edges (5, 8) and (5, 9) of vertex 5. In the context of symbolic elimination we are merely interested in the sparsity structure of C' . Hence, \times represents fill-in, \circlearrowleft represents fill-out, and blanks represent zeros in C' . Eliminating $c_{5,1}$ in C' is equivalent to *front-elimination* [7] of (1, 5) as shown in Figure 2 (a). Fill-in is generated as $c_{8,1}$ [(1, 8)] and $c_{9,1}$ [(1, 9)] since rows [vertices] 8 and 9 have non-zeros [incoming edges] in [from] column [vertex] 5. The elimination of the row/column [vertex] 5 in C' [G] can be done by elimination [front-elimination] of all non-zeros [incoming edges] in [to] row/column [vertex] 5. The resulting fill-in, namely $c_{8,1}$, $c_{8,2}$, $c_{9,1}$, and $c_{9,2}$ [(1, 8), (2, 8), (1, 9), and (2, 9)] in C' [G] is shown in Figure 3 (b) [(a)]. A total of $p!$ different row [vertex] elimination orderings in C' [G] are possible. In this paper we focus on *reverse elimination* ($n + p, \dots, n + 1$). Hence, the Jacobian F' [the bipartite graph G'] is derived from C' [G] by elimination of all intermediate rows [vertices] in order (6, 5, 4). The result is shown in Figure 4 (b) [(a)].

2 The Problem

In order to exploit the sparsity of C' we use compressed row storage [4]. Fill-in and fill-out may result in additional memory allocation and lost memory in CRS,

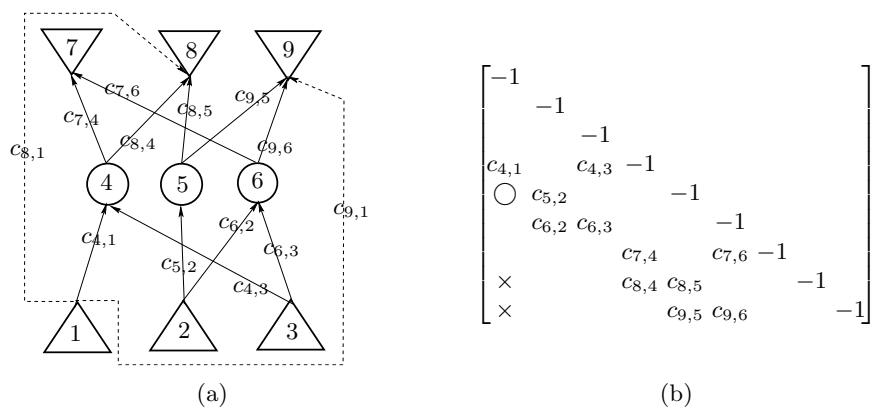


Fig. 2. $G [C']$ after front-elimination [elimination] of $(1, 5)$ [$c_{5,1}$] (a) [(b)].

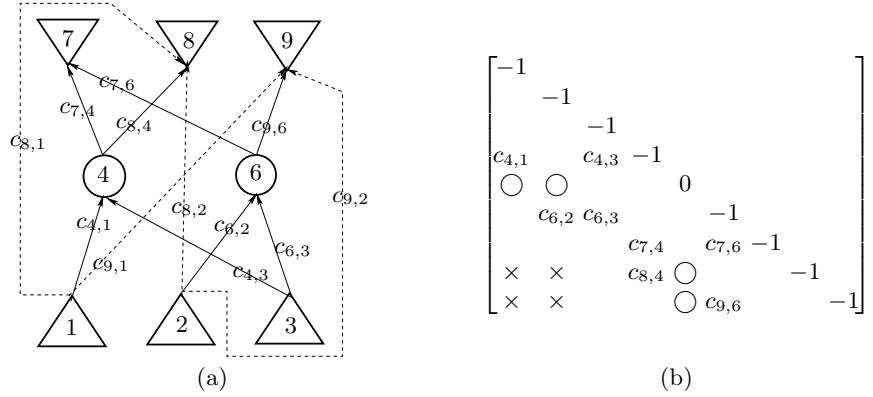
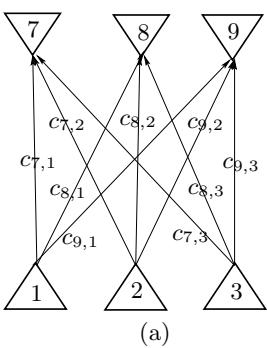


Fig. 3. $G [C']$ after elimination of vertex [row/column] 5 (a) [(b)].

respectively. As mentioned above F' can be computed from C' by reverse elimination. Different elimination orderings may yield different amounts of fill-in and fill-out. Finding an optimal (or near optimal) elimination ordering is the subject of ongoing work. In this paper we are merely interested in the computation of F' while exploiting the sparsity of C' by using CRS. Our objective is to allocate (once) static memory for accumulation of F' from a given C' in CRS format by reverse elimination. The extended Jacobian C' of F as in Figure 1 (a) has the following CRS representation:

$$\begin{aligned} \alpha &= [c_{4,1}, c_{4,3}, c_{5,1}, c_{5,2}, c_{6,2}, c_{6,3}, c_{7,4}, c_{7,6}, c_{8,4}, c_{8,5}, c_{9,5}, c_{9,6}] \\ \kappa &= [1, 3, 1, 2, 2, 3, 4, 6, 4, 5, 5, 6] \\ \rho &= [1, 1, 1, 1, 3, 5, 7, 9, 11, 13] \quad . \end{aligned}$$

The CRS currently does not contain memory for potential fill-in. Therefore we need a fill-in detection procedure to allocate enough memory in our CRS structure. The corresponding symbolic elimination algorithm (see Section 3) yields the following CRS structure:



$$\begin{bmatrix} -1 & -1 & -1 \\ \circ & \circ & 0 \\ \circ & \circ & 0 \\ \times & \times & \circ \\ \times & \times & \circ \\ \times & \times & \circ \end{bmatrix} \quad \begin{bmatrix} 0 & -1 & -1 \\ 0 & -1 & -1 \\ -1 & -1 & -1 \end{bmatrix}$$

(b)

Fig. 4. Bipartite graph G' (a) and the corresponding structure of C' (b) after reverse elimination; The Jacobian is the 3×3 matrix in the lower left corner of C' after the elimination procedure.

$$\begin{aligned}\alpha &= [c_{4,1}, c_{4,3}, c_{5,1}, c_{5,2}, c_{6,2}, c_{6,3}, 0, 0, 0, c_{7,4}, c_{7,6}, 0, 0, 0, c_{8,4}, c_{8,5}, 0, 0, 0, c_{9,5}, c_{9,6}] \\ \kappa &= [1, 3, 1, 2, 2, 3, 1, 2, 3, 4, 6, 1, 2, 3, 4, 5, 1, 2, 3, 5, 6] \\ \rho &= [1, 1, 1, 1, 3, 5, 7, 12, 17, 22]\end{aligned}$$

Elimination of 6 yields :

$$\begin{aligned}\alpha &= [c_{4,1}, c_{4,3}, c_{5,1}, c_{5,2}, \mathbf{0}, \mathbf{0}, 0, c_{7,2}, c_{7,3}, c_{7,4}, \mathbf{0}, 0, 0, 0, c_{8,4}, c_{8,5}, 0, c_{9,2}, c_{9,3}, c_{9,5}, \mathbf{0}] \\ \kappa &= [1, 3, 1, 2, -1, -1, 1, 2, 3, 4, -1, 1, 2, 3, 4, 5, 1, 2, 3, 5, -1] \\ \rho &= [1, 1, 1, 1, 3, -1, 12, 17, 22]\end{aligned}$$

where

$$\begin{aligned}c_{7,2} &:= c_{6,2} \cdot c_{7,6}; & c_{7,3} &:= c_{6,3} \cdot c_{7,6}; \\ c_{9,2} &:= c_{6,2} \cdot c_{9,6}; & c_{9,3} &:= c_{6,3} \cdot c_{9,6}\end{aligned}$$

Elimination of 5 yields :

$$\begin{aligned}\alpha &= [c_{4,1}, c_{4,3}, \mathbf{0}, \mathbf{0}, \mathbf{0}, 0, c_{7,2}, c_{7,3}, c_{7,4}, \mathbf{0}, c_{8,1}, c_{8,2}, 0, c_{8,4}, \mathbf{0}, c_{9,1}, c_{9,2}, c_{9,3}, \mathbf{0}, \mathbf{0}] \\ \kappa &= [1, 3, -1, -1, -1, -1, 1, 2, 3, 4, -1, 1, 2, 3, 4, -1, 1, 2, 3, -1, -1] \\ \rho &= [1, 1, 1, 1, -1, -1, 12, 17, 22]\end{aligned}$$

where

$$\begin{aligned}c_{8,1} &:= c_{5,1} \cdot c_{8,5}; & c_{8,2} &:= c_{5,2} \cdot c_{8,5}; \\ c_{9,1} &:= c_{5,1} \cdot c_{9,5}; & c_{9,2} &:= c_{9,2} + c_{5,2} \cdot c_{9,5}\end{aligned}$$

Elimination of 4 yields :

$$\begin{aligned}\alpha &= [\mathbf{0}, \mathbf{0}, \mathbf{0}, \mathbf{0}, \mathbf{0}, c_{7,1}, c_{7,2}, c_{7,3}, \mathbf{0}, \mathbf{0}, c_{8,1}, c_{8,2}, c_{8,3}, \mathbf{0}, \mathbf{0}, c_{9,1}, c_{9,2}, c_{9,3}, \mathbf{0}, \mathbf{0}] \\ \kappa &= [-1, -1, -1, -1, -1, -1, 1, 2, 3, -1, -1, 1, 2, 3, -1, -1, 1, 2, 3, -1, -1] \\ \rho &= [1, 1, 1, -1, -1, -1, 12, 17, 22]\end{aligned}$$

where

$$\begin{aligned} c_{7,1} &:= c_{4,1} \cdot c_{7,4}; & c_{7,3} &:= c_{7,3} + c_{4,3} \cdot c_{7,4}; \\ c_{8,1} &:= c_{8,1} + c_{4,1} \cdot c_{8,4}; & c_{8,3} &:= c_{4,3} \cdot c_{8,4} . \end{aligned}$$

Bold **0**'s in α represent fill-out. Bold **-1**'s in κ and ρ mark eliminated entries and rows, respectively. For our example this approach leads to 9 additional memory allocations for fill-in and 12 fill-out's. Compared to the memory needed for storing the whole extended Jacobian we observe a decrease in memory requirement by less than a factor of 2. The savings are more substantial for larger problems as illustrated in Section 5. Moreover, we expect to decrease the memory further by reusing fill-out.

3 Symbolic Elimination Algorithm

Our symbolic fill-in detection algorithm uses a bit pattern $B = B(F)$ to hold the sparsity structure of C' . Figure 5 (a) shows the corresponding integer matrix for the extended Jacobian C' in Figure 1 (c). The binary representation is shown in Figure 5 (b). The symbolic algorithm is implemented in C++. Therefore we start counting with zero. Whenever we refer to the j -th row in B we mean the row with index $j - 1$.

$$\begin{array}{c} \left(\begin{array}{c} 0 \\ 0 \\ 0 \\ 40960 \\ \mathbf{49152} \\ 24576 \\ 5120 \\ 6144 \\ 3072 \end{array} \right) \\ \text{(a)} \end{array} \quad \begin{array}{c} \left(\begin{array}{cccccccc} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ \mathbf{1} & \mathbf{1} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} \\ 0 & 1 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 1 & 0 & 0 \end{array} \right) \\ \text{(b)} \end{array}$$

Fig. 5. Bit pattern B as an integer matrix (a) and binary representation of C' (b).

Algorithm 1 (Symbolic Algorithm)

IN : B — bit pattern of C'
OUT: B — filled bit pattern after reverse elimination

```
[1] FOR  $i = n + p - 1, \dots, n$ 
[2]   FOR  $j = q - 1, \dots, i$ 
[3]      $k := i \gg 4;$ 
[4]     IF ( $B[j][k] \wedge 1 \ll (15 - i \% 16)$ )
[5]       FOR  $m = 0, \dots, k$ 
[6]          $B[j][m] := B[j][m] \vee B[i][m];$ 
```

Consider the symbolic elimination of row 6 in Figure 5 (a) using Algorithm 1 with $i = 5$ and $j = 8$ in line [1] and [2], respectively. The integer values corresponding to rows 6 and 9 are stored in column $k = 0$ (line [3]) with $B[5][0] = 24576$ and

$B[8][0] = 3072$. $6 \prec 9$ as in line [4] $24576 \wedge 2^{15-5} = true$. Hence, $B[8][0] = 27648 = 24576 \vee 3072$. Line [5] in Algorithm 1 performs the bitwise *OR* for all affected columns of B .

In the following we apply Algorithm 1 to the bit pattern of F shown in Figure 5 (a). The result is shown in Figure 6 (b). Symbolic elimination proceeds as follows:

$$\begin{array}{c|c|c|c} & \begin{pmatrix} 0 \\ 0 \\ 0 \\ 40960 \\ 49152 \\ 24576 \\ 5120 \\ 6144 \\ 3072 \end{pmatrix} & \begin{pmatrix} 0 \\ 0 \\ 0 \\ 40960 \\ 49152 \\ 24576 \\ \mathbf{29696} \\ 6144 \\ \mathbf{27648} \end{pmatrix} & \begin{pmatrix} 0 \\ 0 \\ 0 \\ 40960 \\ 49152 \\ 24576 \\ 29696 \\ \mathbf{55296} \\ \mathbf{60416} \end{pmatrix} & \begin{pmatrix} 0 \\ 0 \\ 0 \\ 40960 \\ 49152 \\ 24576 \\ \mathbf{62464} \\ \mathbf{63488} \\ 60416 \end{pmatrix} \\ \xrightarrow{\text{elim}(6)} & & \xrightarrow{\text{elim}(5)} & \xrightarrow{\text{elim}(4)} & \end{array}$$

where

$$29696 = 2^{14} + 2^{13} + 5120; \quad 27648 = 2^{14} + 2^{13} + 3072;$$

$$55296 = 2^{15} + 2^{14} + 6144; \quad 60416 = 2^{15} + 27648;$$

$$62464 = 2^{15} + 29696; \quad 63488 = 2^{13} + 55296.$$

$$\begin{array}{c|c} \begin{pmatrix} 0 \\ 0 \\ 0 \\ 40960 \\ 49152 \\ 24576 \\ \mathbf{62464} \\ 63488 \\ 60416 \end{pmatrix} & \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 1 & 0 & 0 & 0 & 0 & 0 \\ \mathbf{1} & \mathbf{1} & \mathbf{1} & \mathbf{1} & 0 & 0 & 0 & 0 \\ 1 & 1 & 1 & 1 & 0 & 0 & 0 & 0 \\ 1 & 1 & 1 & 0 & 1 & 1 & 0 & 0 \end{pmatrix} \\ (a) & (b) \end{array}$$

Fig. 6. B (a) and the corresponding binary representation (b) after symbolic elimination.

4 First Ideas on Fill-out

We introduce two different methods for reusing fill-out. The symbols \otimes [\bigcirc] represent fill-out that is [not] reused, $*$ represents a non-zero entry and \times represents fill-in in C' .

4.1 Technique 1

We exploit the fact that the elimination of any $c_{j,i}$ yields fill-out in the current memory location. Consider the situation illustrated in Figure 7. The fill-in $c_{j,k}$ can be stored in the memory allocated for $c_{j,i}$ which is getting eliminated. As a consequence the ρ and κ entries corresponding to the fill-in $c_{j,k}$ have to be changed.

$\begin{array}{cccc} l & k & i & j \\ \vdots & \vdots & \ddots & \\ i & & \cdots * & \cdots * & \cdots & i & & \cdots \bigcirc & \cdots \bigcirc & \cdots \\ & \vdots & \vdots & \vdots & \ddots & & \vdots & \vdots & \vdots & \ddots \\ j & & \cdots * & \cdots & \cdots * & \cdots & j & & \cdots + & \cdots & \cdots \otimes & \cdots \end{array}$	$\begin{array}{cccc} l & k & i & j \\ \vdots & \vdots & \ddots & \\ i & & \cdots * & \cdots * & \cdots & i & & \cdots \bigcirc & \cdots \bigcirc & \cdots \\ & \vdots & \vdots & \vdots & \ddots & & \vdots & \vdots & \vdots & \ddots \\ j & & \cdots * & \cdots & \cdots * & \cdots & j & & \cdots + & \cdots & \cdots \otimes & \cdots \end{array}$
(a)	(b)

Fig. 7. (a) before and (b) after the elimination of $c_{j,i}$. The memory allocated for $c_{j,i}$ is reused to store the fill-in $c_{j,k}$.

4.2 Technique 2

Consider in Figure 8 (a) where $j = i + 1$. After the elimination of $c_{j,i}$ the entire row becomes zero. Hence the fill-out in row i can be reused to store the fill-in generated in row j as shown in Figure 8 (b). Consider the CRS of C' in

$$\begin{array}{cccccc|cccccc}
 h & l & k & n & i & j & h & l & k & n & i & j \\
 \vdots & \vdots & \vdots & \vdots & \ddots & & \vdots & \vdots & \vdots & \vdots & \ddots & \\
 i & \cdots & * & \cdots & * & 0 & * & i & \cdots & \otimes & \cdots & \otimes & 0 & \circlearrowleft & i & \cdots & \otimes & j \\
 j & & \cdots & & * & \cdots & * & & \cdots & & * & \cdots & & & & & \otimes & j
 \end{array}$$

Fig. 8. Example for the use of second technique : (a) Before and (b) after the elimination of $c_{j,i}$.

Figure 9 (a) where $c_{6,5}$ has been added to the matrix in Figure 1 (c). Applying above techniques yields 9 fill-out's, 6 fill-in's, and 3 reused fill-out's.

The CRS C' after reverse elimination of all intermediate rows has the following format:

$$\begin{aligned}\alpha &= [\mathbf{0}, \mathbf{0}, \mathbf{0}, \mathbf{0}, c_{7,1}, c_{7,2}, c_{7,3}, \mathbf{0}, \mathbf{0}, c_{8,1}, c_{8,2}, c_{8,3}, \mathbf{0}, c_{9,1}, c_{9,2}, c_{9,3}, \mathbf{0}, \mathbf{0}] \\ \kappa &= [-1, -1, -1, -1, 1, 2, 3, -1, -1, 1, 2, 3, -1, 1, 2, 3, -1, -1] \\ \rho &= [1, 1, 1, -1, -1, -1, 5, 10, 14] \quad .\end{aligned}$$

Figure 9 (b) shows the memory access pattern of reverse elimination mapped onto the extended Jacobian.

5 Numerical Results

We compare runtime and memory consumption of our new CRS-based algorithm (**JacAccOnCRS**) with reverse elimination of all intermediate rows of C' (**JacAccOnEJ**). Both methods try to accumulate the Jacobian of the following function:

Listing 1.1. f.cpp

```
void f(double* x, int n, int l) {  
    double * h = new double [n];
```

$$\begin{array}{c}
\left[\begin{array}{ccccccccc}
-1 & & & & & & & & \\
0 & -1 & & & & & & & \\
0 & 0 & -1 & & & & & & \\
c_{4,1} & 0 & c_{4,3} & -1 & & & & & \\
c_{5,1} & c_{5,2} & 0 & 0 & -1 & & & & \\
0 & c_{6,2} & c_{6,3} & 0 & c_{6,5} & -1 & & & \\
0 & 0 & 0 & c_{7,4} & 0 & c_{7,6} & -1 & & \\
0 & 0 & 0 & c_{8,4} & c_{8,5} & 0 & 0 & -1 & \\
0 & 0 & 0 & 0 & c_{9,5} & c_{9,6} & 0 & -1 & \\
\end{array} \right] \quad \left(a \right) \\
\left[\begin{array}{ccccccccc}
-1 & -1 & & & & & & & \\
& -1 & & & & & & & \\
\bigcirc & \bigcirc & \bigcirc & 0 & & & & & \\
\bigcirc & \bigcirc & \otimes & \otimes & 0 & & & & \\
\times & & \times & \bigcirc & \bigcirc & -1 & & & \\
\times & \times & \otimes & \bigcirc & & & -1 & & \\
\times & \times & \times & \bigcirc & \bigcirc & & & -1 & \\
\end{array} \right] \quad \left(b \right)
\end{array}$$

Fig. 9. Modified C' (a) and the corresponding memory structure (b) after reverse elimination.

```

for ( i=0; i<1; i++ ){
    if ( i%2==0 ) {
        h[0] = x[n-1]*x[0];
        for ( j=1; j<n; j++ )
            h[j] = x[j-1]*x[j];
    } else {
        x[0] = h[n-1]*h[0];
        for ( j=1; j<n; j++ )
            x[j]=h[j-1]*h[j];
    }
}

```

We set $n = 100$ and $l \in \{10, \dots, 150\}$. Obviously, $C' \in \mathbb{R}^{q \times q}$ where $q = (l+1) \cdot n$. All results have been obtained on an Intel Pentium 4 CPU running at 3.00GHz with 1GB of memory.

JacAccOnCRS performs the following steps:

1. Creation of C' and B by running an overloaded version of F .
2. Fill-in detection by the symbolic algorithm described in Section 2.
3. Allocation CRS and initialization of original non-zero entries.
4. Reverse elimination on C' in CRS format.
5. Extraction of F' from C' in CRS format.

JacAccOnEJ performs the following steps:

1. Creation of C' and B by running an overloaded version of F .
2. Reverse elimination on C' .
3. Extraction of F' from C' .

We observe an overall speedup of roughly five as illustrated in Figure 10. Symbolic reverse elimination on B is about ten times faster than the corresponding procedure on C' . On the given computer architecture we are able to handle problems of sizes $l = 250$ and $l = 1000$ (for $n = 100$) using **JacAccOnEJ** and **JacAccOnCRS**, respectively.

6 Conclusion

Jacobian accumulation on the extended Jacobian can be improved significantly – both in terms of memory requirement and overall runtime – by using static

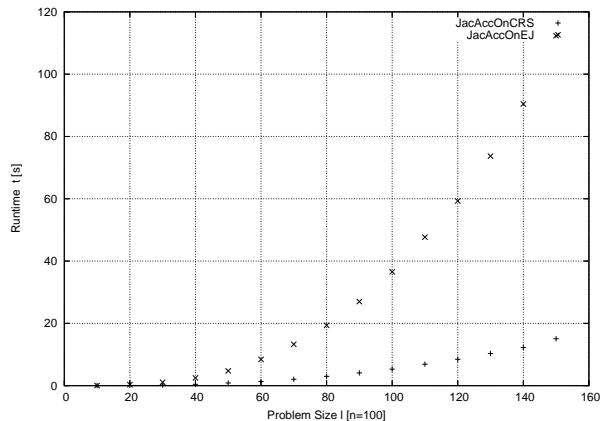


Fig. 10. Runtime of JacAccOnCRS vs. JacAccOnEJ.

sparse storage allocated based on the result of a symbolic elimination algorithm. The use of fill-out for storing potential fill-in is expected to yield even better results. Further in-depth investigation of the combinatorial and memory access problems is necessary to undercut the runtime of classical Jacobian accumulation techniques such as finite difference approximation or forward mode automatic differentiation [8].

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