OPTIMALITY-PRESERVING ELIMINATION OF LINEARITIES IN JACOBIAN ACCUMULATION *

UWE NAUMANN † AND JEAN UTKE ‡

Abstract. We consider a mathematical function that is implemented in a high-level programming language such as C or Fortran. This function is assumed to be differentiable in some neighborhood of a set of input arguments. For available local partial derivatives of the arithmetic operators and intrinsic functions provided by the programming language, the Jacobian of the function at the given arguments can be accumulated by using the chain rule. This technique is known as automatic differentiation of numerical programs.

Under the above assumptions the values of the local partial derivatives are well defined for given values of the inputs. A code for accumulating the Jacobian matrix that is based on the chain rule takes these partial derivatives as input and computes the nonzero entries of the Jacobian using only scalar multiplications and additions. The exploitation of the associativity of the chain rule or, equivalently, the algebraic properties of the corresponding field $(\mathbb{R}, *, +)$ – in particular, associativity of the multiplication and distributivity – to minimize the number of multiplications leads to a combinatorial optimization problem that is widely conjectured to be NP-hard. Several heuristics have been developed for its approximate solution. Their efficiency always depends on the total number of partial derivatives.

Linearities in the function lead to constant partial derivatives that do not depend on the input values. We present a specialized constant folding algorithm to decrease the size of the combinatorial problem in order to increase the efficiency of heuristics for its solution. Moreover, we show that this algorithm preserves optimality in the sense that an optimal solution for the reduced problem yields an objective value no worse than that of an optimal solution for the original problem.

Key words. Jacobian accumulation, linearities, constant folding

AMS subject classifications. 90C27, 26B10, 68N99

1. The Problem.

A given vector function

$$\boldsymbol{f}(\boldsymbol{x}) : \mathbb{R}^n \mapsto \mathbb{R}^m$$

is implemented in a numerical program in some higher programming language such as C or Fortran. For the purpose of automatic differentiation (AD) [5], the numerical programs are represented by directed acyclic graphs (DAG) with elemental partial derivatives as edge labels. AD provides a variety of elimination techniques that allow propagation of derivative information. The choice of the technique is subject to the structure of $\boldsymbol{f}$ and application-dependent optimization criteria.

Generally the code for $\boldsymbol{f}$ contains control flow (loops, branches) that does not allow the representation with a single DAG. Locally, for example within a basic block, a representative DAG can be constructed. For the purpose of this paper we assume a scenario where the accumulation of a local Jacobian is beneficial. In practical terms, we may encounter a frequently executed innermost loop body that has an evaluation cost that is relatively high compared to the cost of storing a local Jacobian. We find

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†Software and Tools for Computational Engineering, RWTH Aachen University, D-52056 Aachen, Germany; naumann@stce.rwth-aachen.de

‡Mathematics and Computer Science Division, Argonne National Laboratory, 9700 South Cass Avenue, Argonne, IL 60439–4844, USA; utke@mcs.anl.gov

a highly efficient procedure to calculate the local Jacobians, which are then used in a fashion determined by the context.

The paper is structured as follows. Section 1.1 introduces the main ideas behind AD and how they are used as the context for our work. In Section 1.2 we collect elimination techniques that are used to accumulate the Jacobian based on linearized variants of the computational graph. In Section 1.3 we summarize the problems that motivated our work. Section 2 represents the heart of the paper. We present new algorithms for the optimality-preserving elimination of linearities in Jacobian accumulation by constant folding. An interesting observation is made in the context of *face elimination*. Section 3 concludes the paper with a discussion of how the new algorithms are used in practice.

1.1. The Context. The DAG based combinatorial problem is detailed in Section 1.2. However, for the sake of better understanding of our contribution, we introduce here the relevant AD concepts. Rather than repeating the theoretical basis, we use an example for this purpose. For a formal introduction to the mathematical principles underlying AD, we refer the reader to [5, 13, 4, 2, 3].

Consider the following excerpt from a toy example written in C. Suppose that this section of the code is embedded in a larger computation aiming at the computation of the components of some vector `h` as a function of an input vector `x`.

```
01   h[k]=sin(x[0]*x[1]); k+=1;
02   if (fmod(k,2))
03      h[k]=2*h[k-1];
04   else
05      for (i=0;i<k;i++) {
06          t1=x[0]+x[1];
07          t2=t1*sin(x[0]);
08          x[0]=cos(t1*t2);
09          x[1]=-sqrt(t2);
10      }
11   h[k]+=x[0]*x[1];
```

Line numbers have been added for simpler referencing within the text. The statements in the lines 06–09 form a basic block F_3; see Figure 1.1 on page 4. Note that F_3 is executed `k` times. If `k` is used to iterate through the elements of the potentially very large vector `h`, then it may be worth putting additional effort into the optimization of the derivative code for F_3.

Conceptually, AD is based on a decomposition of the evaluation routine for $\boldsymbol{f}$ into a three-address code[1] of the form

$$v_j = \varphi_j(v_i, v_h) \tag{1.1}$$

for $j = 1, \ldots, q$ and $h, i = 1-n, \ldots, q$, $j > h, i$. The n *independent* variables $x_1, \ldots, x_n$ correspond to $v_{1-n}, \ldots, v_0$. We consider the computation of the first derivative of the *dependent* variables $y_1, \ldots, y_m$ represented by m variables $v_j : j \in 1-n, \ldots, q$ with respect to the independents. The resulting $m \times n$ matrix is known as the *Jacobian matrix* of $\boldsymbol{f}$.

The *elemental* functions φ_j, $j = 1, \ldots, q$, are assumed to have jointly continuous partial derivatives in a neighborhood of the current argument. The values of these

[1] We assume that there are at most binary arithmetic operators and intrinsic functions. The generalization is trivial.

partials can be computed in parallel with the function itself for given values of the independent variables. Consequently, the *forward mode* of AD propagates directional derivatives as

$$\dot{v}_j = \frac{\partial \varphi_j}{\partial v_h}(v_i, v_h) * \dot{v}_h + \frac{\partial \varphi_j}{\partial v_i}(v_i, v_h) * \dot{v}_i \quad \text{for } j = 1, \ldots, q. \tag{1.2}$$

In *reverse mode* we compute adjoints of the variables on the right-hand side in (1.1) as a function of local partial derivatives and the adjoint of the variable on the left-hand side:

$$\begin{aligned} \bar{v}_i &= \bar{v}_j * \frac{\partial \varphi_j}{\partial v_i}(v_i, v_h) \\ \bar{v}_h &= \bar{v}_j * \frac{\partial \varphi_j}{\partial v_h}(v_i, v_h) \end{aligned} \quad \text{for } j = q, \ldots, 1-n. \tag{1.3}$$

Equations (1.2) and (1.3) can be used to accumulate the Jacobian of $\boldsymbol{f}$ at a computational complexity that is proportional to n and m, respectively. One simply lets $\dot{\boldsymbol{x}}$ or $\bar{\boldsymbol{y}}$ range over the Cartesian basis vectors in $\mathbb{R}^n$ or $\mathbb{R}^m$. Basic blocks can be considered as vector functions themselves. Forward and reverse mode AD, or, as we will see below, local combinations of the two, can be applied to compute the local Jacobians. If $\boldsymbol{y} = \boldsymbol{f}(\boldsymbol{x})$ is computed by a sequence of basic blocks $F_1, \ldots, F_l$ and assuming the availability of the local Jacobians $F'_1, \ldots, F'_l$, then equations (1.2) and (1.3) can be generalized as follows:

$$\dot{y}_j = F'_j \dot{x}_j \quad \text{for } j = 1, \ldots, l \tag{1.4}$$

and

$$\bar{x}_j = (F'_j)^T \bar{y}_j \quad \text{for } j = l, \ldots, 1 \quad , \tag{1.5}$$

where $x_j = (x_i^j \in V : i = 1, \ldots, n_j)$ and $y_j = (y_i^j \in V : i = 1, \ldots, m_j)$ are the inputs and outputs of F_j, respectively.

The control-flow graph of the example is shown in Figure 1.1 (a). Assuming that code for accumulating the local Jacobians $F'_1, \ldots, F'_4$ of the basic blocks $F_1, \ldots, F_4$ is available (some aspects of how to generate such code automatically and how to optimize it is the subject of this paper), the forward and reverse modes of AD compute products of the Jacobian and its transposed with a vector, respectively. In Figure 1.1 (b) products of the local Jacobians F'_i with the directions $\dot{x}_i$ in the input space of each basic block F_i, $i = 1, \ldots, 4$, are propagated forward in the direction of the flow of control. The direction is reversed in reverse mode. Products of the transposed Jacobians $(F'_i)^T$ with adjoint vectors in the respective output spaces are propagated reverse to the direction of the flow of control. In Figure 1.1 (c) we have switched the orientation of the edges to illustrate this fact.

To finish this introductory example, we make the following important point: Thanks to the associativity of the chain rule it is possible to *preaccumulate* derivative information of certain parts of the code and use this information in the propagation of directional derivatives (in forward mode) or adjoints (in reverse mode). Occasionally it is worthwhile to put additional effort into the optimization of this preaccumulation code. In this paper we discuss various issues arising from the optimization of Jacobian code in the context of automatic source transformation techniques.

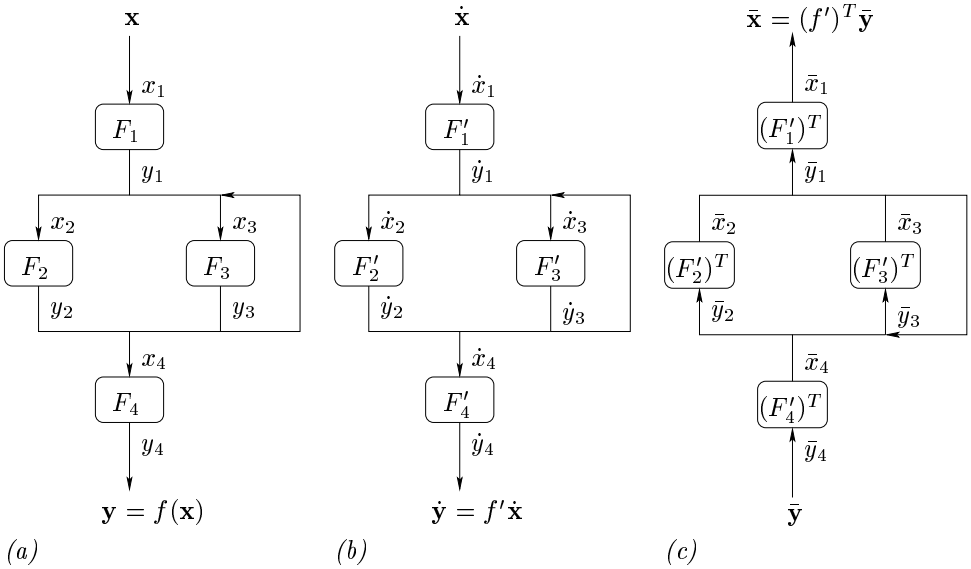

FIG. 1.1. *Control flow graph of (a) original code, (b) tangent linear model, (c) adjoint model*

1.2. Elimination Methods. Let $\boldsymbol{f}$ represent a basis block that is subject to preaccumulation as outlined in the previous section. The DAG $G = (V, E)$ is induced by the code for $\boldsymbol{f}$ [1]. We use a numbering scheme with n independent vertices $x_1 = v_{1-n}, \ldots, x_n = v_0 \in X$, p intermediate vertices $v_1, \ldots, v_p \in Z$, m dependent vertices $y_1 = v_{p+1}, \ldots, y_m = v_{p+m} \in Y$, representing the corresponding independent, intermediate, and dependent variables. For notational simplicity and without loss of generality we assume that the dependent variables are mutually independent. This situation can always be reached by introducing auxiliary assignments. Consequently, $V = X \cup Z \cup Y$. The numbering is subject to the dependence relation $\prec$, where $v_i \prec v_j$ (and $v_h \prec v_j$ as in (1.1)), and $v_i \prec v_j \Rightarrow i < j$. In Figure 1.2 (a) we show

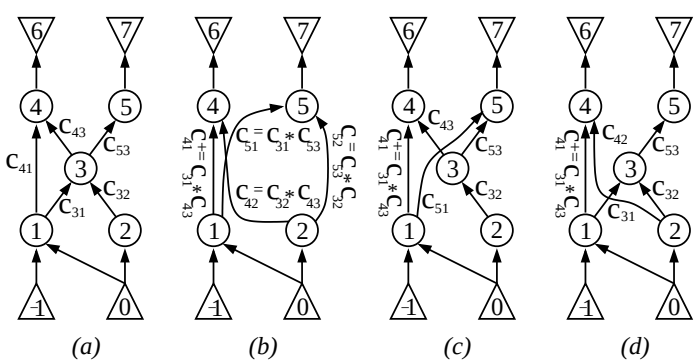

FIG. 1.2. *(a) Computational graph G for (1.6), (b) vertex elimination $G - 3$, (c) edge-front elimination $G - (1, 3)$, (d) edge-back elimination $G - (3, 4)$*

the DAG for F_3 from the previous section. It represents a decomposition of the code into a sequence assignments of the results of the elemental operations φ to unique

intermediate variables, for example,

$$\begin{aligned} v_1 &= v_{-1} + v_0;\ v_2 = \sin(v_0);\ v_3 = v_1 + v_2;\ v_4 = v_1 * v_3; \\ v_5 &= \sqrt{v_3};\ v_6 = \cos(v_4);\ v_7 = -v_5 \quad . \end{aligned} \tag{1.6}$$

This representation is also referred to as the *code list*. The intrinsics and operators provided by the underlying programming language constitute the possible elemental operations. Edges $(i,j) \in E$ are labeled with partial derivatives $c_{ji} = \frac{\partial \varphi_j}{\partial v_i} \in \mathbf{R}$ of the elemental operations associated with vertex j with respect to the corresponding arguments. For instance, in the example we have $c_{64} = -\sin(v_4)$. All edge labels form the matrix

$$\boldsymbol{C}(\boldsymbol{x}) : \mathbf{R}^n \mapsto \mathbf{R}^{(p+m)\times(n+p)} \quad .$$

The computation of the Jacobian $\boldsymbol{f}'(\boldsymbol{x})$ can be interpreted as an elimination sequence in $\boldsymbol{C}$:

$$\sigma : \mathbf{R}^{(p+m)\times(n+p)} \mapsto \mathbf{R}^{m\times n} \quad .$$

Equivalently, σ transforms G into a bipartite graph $\sigma(G)$ whose edge labels are the nonzero elements of $\boldsymbol{f}'$. Alternatively, Gaussian elimination can be applied to the *extended Jacobian* $\boldsymbol{C} - \boldsymbol{I}$, where $\boldsymbol{I}$ is the identity as shown, for example, in [5].

The graph-based elimination steps are categorized in vertex, edge, and face eliminations. In G a vertex $j \in V$ is eliminated by connecting its predecessors with its successors [7]. An edge (i,k) with $i \prec j$ and $j \prec k$ is labeled with $c_{ki} + c_{kj} \cdot c_{ji}$ if it existed before the elimination of j. We say that *absorption* takes place. Otherwise, (i,k) is generated as *fill-in* and labeled with $c_{kj} \cdot c_{ji}$ The vertex j is removed from G together with all incident edges. Figure 1.2 (b) shows the result of eliminating vertex 3 from the graph in Figure 1.2 (a).

An edge (i,j) is *front eliminated* by connecting i with all successors of j, followed by removing (i,j) [10]. The corresponding structural modifications of the c-graph in Figure 1.2 (a) are shown in Figure 1.2 (c) for front elimination of $(1,3)$. The new edge labels are given as well. Edge-front elimination eventually leads to intermediate vertices in G becoming *isolated*; that is, these vertices no longer have predecessors. Isolated vertices are simply removed from G together with all incident edges.

Back elimination of an edge $(i,j) \in E$ results in connecting all predecessors of i with j [10]. The edge (i,j) itself is removed from G. The back elimination of $(3,4)$ from the graph in Figure 1.2 (a) is illustrated in Figure 1.2 (d). Again, vertices can become isolated as a result of edge-back elimination because they no longer have successors. Such vertices are removed from G.

Numerically the elimination is the application of the chain rule, that is, a sequence of *fused-multiply-add* (fma) operations

$$c_{ki} = c_{ji} * c_{kj}\ \ (+c_{ki}) \quad \leftarrow \text{optional} \tag{1.7}$$

where the additions take place in the case of absorption or fill-in is created as described above.

Aside from special cases a single vertex or edge elimination will result in more than one fma. *Face elimination* was introduced as the elimination operation with the finest granularity of exactly one multiplication[2] per elimination step.

[2] Additions are not necessarily directly coupled.

Vertex and edge elimination steps have an interpretation in terms of vertices and edges of G, whereas face elimination is performed on the corresponding directed line graph $\mathcal{G}$. Following [9], we define the directed line graph $\mathcal{G} = (\mathcal{V}, \mathcal{E})$ corresponding to $G = (V, E)$ as follows:

$$\mathcal{V} = \{ \textcircled{i,j} : (i,j) \in E\} \cup \{ \textcircled{\oplus,j} : v_j \in X\} \cup \{ \textcircled{i,\ominus} : v_i \in Y\}$$

and

$$\begin{aligned}\mathcal{E} = \{(&\textcircled{i,j}, \textcircled{j,k}) : (i,j),(j,k) \in E\}\\ \cup \{(&\textcircled{\oplus,j}, \textcircled{j,k}) : v_j \in X \wedge (j,k) \in E\}\\ \cup \{(&\textcircled{i,j}, \textcircled{j,\ominus}) : v_j \in Y \wedge (i,j) \in E\} \quad .\end{aligned}$$

That is, we add a source vertex $\oplus$ and a sink vertex $\ominus$ to G connecting all independents to $\oplus$ and all dependents to $\ominus$. $\mathcal{G}$ has a vertex $v \in \mathcal{V}$ for each edge in the extended G, and $\mathcal{G}$ has an edge $e \in \mathcal{E}$ for each pair of adjacent edges in G. Figure 1.3 gives an example of constructing the directed line graph in (b) from the graph in (a). All intermediate vertices $\textcircled{i,j} \in \mathcal{V}$ inherit the labels c_{ji}. In order to formalize face elimination, it is advantageous to move away from the double-index notation and use one that is based on a topological enumeration of the edges in G. Hence, $\mathcal{G} = (\mathcal{V}, \mathcal{E})$ becomes a DAG with $\mathcal{V} \subset I\!N$ and $\mathcal{E} \subset I\!N \times I\!N$ and certain special properties. The set of all predecessors of $j \in \mathcal{V}$ is denoted as P_j. Similarly, S_j denotes the set of its successors in $\mathcal{G}$. A vertex $j \in \mathcal{V}$ is called *isolated* if either $P_j = \emptyset$ or $S_j = \emptyset$. Face elimination is defined in [9] between two incident intermediate vertices i and j in $\mathcal{G}$ as follows:

1. If there exists a vertex $k \in \mathcal{V}$ such that $P_k = P_i$ and $S_k = S_j$, then set $c_k = c_k + c_j c_i$ *(absorption)*; else $\mathcal{V} = \mathcal{V} \cup \{k'\}$ with a new vertex k' such that $P_{k'} = P_i$ and $S_{k'} = S_j$ *(fill-in)* and labeled with $c_{k'} = c_j c_i$.
2. Remove (i,j) from $\mathcal{E}$.
3. Remove $i \in \mathcal{V}$ if it is isolated. Otherwise, if there exists a vertex $i' \in \mathcal{V}$ such that $P_{i'} = P_i$ and $S_{i'} = S_i$, then
   - set $c_i = c_i + c_{i'}$ *(merge)*;
   - remove i'.
4. Repeat Step 3 for $j \in \mathcal{V}$.

In Figure 1.3 (c) we show the elimination of $(i,j) \in \mathcal{E}$, where $i = \textcircled{1,3}$ and $j = \textcircled{3,4}$.

A complete face elimination sequence σ_f yields a tripartite directed line graph $\sigma_f(\mathcal{G})$ that can be back transformed into the bipartite graph representing the Jacobian $\boldsymbol{f}'$.

In [9] it was shown that vertex and edge eliminations can be interpreted as groups of face eliminations and that face elimination sequences can undercut the number of multiplications of an optimal vertex or edge elimination sequence. We note that any G can be transformed into the corresponding $\mathcal{G}$ but that a back transformation generally is not possible once face elimination steps have been applied. Therefore, face eliminations cannot precede vertex and edge eliminations.

In a source transformation context the operations (1.7) are expressed as actual code, the Jacobian accumulation code `jac`. The latter is based on (1.1) augmented

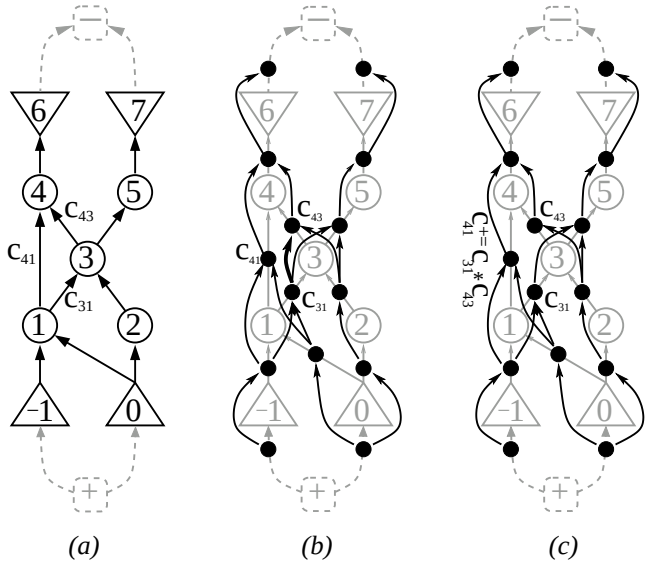

FIG. 1.3. *(a) G extended, (b) $\mathcal{G}$ overlaid, (c) face elimination*

with statements that compute the c_{ji} for all $i \prec j$. For (1.6) we get[3]

$$
\begin{aligned}
&v_1 = v_{-1} + v_0;\ c_{1,-1} = 1;\ c_{1,0} = 1;\\
&v_2 = \sin(v_0);\ c_{2,0} = \cos(v_0);\\
&v_3 = v_1 + v_2;\ c_{3,1} = 1;\ c_{3,2} = 1;\\
&v_4 = v_1 * v_3;\ c_{4,1} = v_3;\ c_{4,3} = v_1;\\
&v_5 = \sqrt{v_3};\ c_{5,3} = (2\sqrt{v_3})^{-1};\\
&v_6 = \cos(v_4);\ c_{6,4} = -\sin(v_4);\\
&v_7 = -v_5;\ c_{7,5} = -1; \quad .
\end{aligned}
$$

As most of the intermediate variables are used only once, their creation and assignment should be avoided by the source transformation tool. However, they are helpful for illustrative purposes as `jac` can be written in terms of these auxiliary variables. For example, forward vertex elimination, that is, the elimination sequence (1,2,3,4,5) in G (Figure 1.2), leads to the following Jacobian accumulation code:

$$
\begin{aligned}
1:&\quad c_{3,-1} = c_{3,1} * c_{1,-1};\ c_{3,0} = c_{3,1} * c_{1,0};\ c_{4,-1} = c_{4,1} * c_{1,-1};\ c_{4,0} = c_{4,1} * c_{1,0};\\
2:&\quad c_{3,0} \mathrel{+}= c_{3,2} * c_{2,0};\\
3:&\quad c_{4,-1} \mathrel{+}= c_{4,3} * c_{3,-1};\ c_{4,0} \mathrel{+}= c_{4,3} * c_{3,0};\ c_{5,-1} = c_{5,3} * c_{3,-1};\ c_{5,0} = c_{5,3} * c_{3,0};\\
4:&\quad c_{6,-1} = c_{6,4} * c_{4,-1};\ c_{6,0} = c_{6,4} * c_{4,0};\\
5:&\quad c_{7,-1} = c_{7,5} * c_{5,-1};\ c_{7,0} = c_{7,5} * c_{5,0} \quad .
\end{aligned}
$$

For convenience we use the increment operation += known from C. A practical mea-

[3]For better readability we write the indices of the c_{ji} with commas.

sure for the cost of computing $\boldsymbol{f}' = \sigma(\boldsymbol{C}(\boldsymbol{x}))$ is the count of multiplications $\#_*$ of edge labels. The cost of the forward vertex elimination sequence[4] above is 13. In Section 3 we discuss other options for measures.

1.3. Constant Elimination Operations. The edge label multiplications can be categorized into *trivial*, *constant*, and *variable* multiplications ($*_t$, $*_c$, $*_v$) based on the type of operands as shown in Figure 1.4. For a repeated Jacobian computation (that is, computations for distinct $\boldsymbol{x}$), only the $*_v$ have to be re-executed. The $*_t$ can be transformed into toggling the sign, and $*_c$ can be executed at compile time in *constant propagation* fashion. Therefore we take only $\#_{*_v}$ as our cost measure.

No known algorithm produces an optimal elimination sequence for a general DAG with polynomial complexity. To approximate an optimal $\hat{\sigma}_f(\mathcal{G})$ such that

$$\#_{*_v}(\hat{\sigma}_f(\mathcal{G})) = \min_{\sigma_f(\mathcal{G})} \{\#_{*_v}(\sigma_f)\} \quad ,$$

we can use heuristics [12].

	c_{ji} \ c_{kj}	trivial	constant	variable
trivial:	$c_{ji} \equiv \pm 1$	$*_t$	$*_t$	$*_t$
constant:	$c_{ji} \equiv const$	$*_t$	$*_c$	$*_v$
variable:	$c_{ji} = c_{ji}(\boldsymbol{x})$	$*_t$	$*_v$	$*_v$

FIG. 1.4. *Multiplications* $c_{ji} * c_{kj}$

One can argue that code optimization via constant propagation and constant folding algorithms built into compilers is already capable of optimizing $*_t$ and $*_c$ away. Therefore, an AD source transformation tool would not necessarily have to be concerned with the explicit removal of the nonvariable multiplications. However, we need to be concerned with the cost of the heuristic approximation of $\hat{\sigma}$, which makes any reduction of the initial problem size by constant folding desirable, even though the approximation time is absorbed into compile time, not run time. For sufficiently large problems this cost is a critical hurdle, as is particularly evident for face elimination. The directed line graph $\mathcal{G}$ is a much larger data structure than G, which translates into a vast search space for any face elimination heuristic. A heuristic that is aware of the edge label categories and maintains those correctly for fill-ins and updates is even more complex and costly. Therefore, a viable heuristic may not distinguish label categories, and one can easily construct cases where $\#_*(\sigma_1) = \#_*(\sigma_2)$ but $\#_{*_v}(\sigma_1) < \#_{*_v}(\sigma_2)$. Constant folding can shrink the size of G (and $\mathcal{G}$) significantly for codes with large linear portions. We concentrate on the following issues:

1. Reduction of the problem size through constant folding in G
2. Constant folding and preservation of optimality
3. Implementation

2. Linearities and Constant Folding. The search spaces for the various elimination techniques can be expressed as metagraphs $M(G)$ with vertices representing

[4]Note that the cost of computing the Jacobian by the classical forward and reverse modes is $n * |E|$ and $m * |E|$, respectively. For (1.6) we have $n = m = 2$ and $|E| = 10$. Forward (resp. reverse) vertex elimination is equivalent to the *sparse* forward (resp. reverse) mode of AD [5].

G at different elimination stages. $M(G)$ is a DAG. Each edge indicates an elimination step labeled with its cost. An elimination sequence σ is a path in $M(G)$ from the minimal vertex representing G to the maximal vertex that represents the bipartite $\sigma(G)$. An optimal sequence is a path with the minimal sum of metagraph edge labels; see Figure 2.1. For edge elimination all edges (i, j) in G' determine the number of

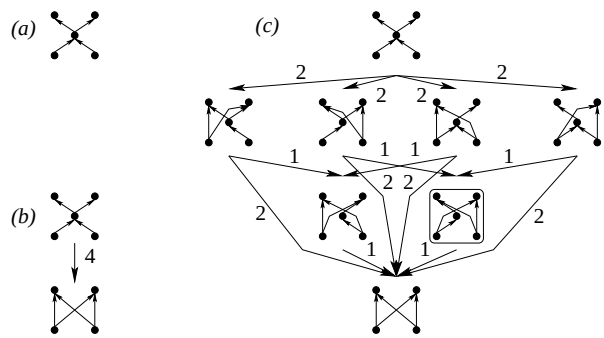

FIG. 2.1. *(a) G, (b) vertex elimination metagraph, (c) edge elimination metagraph*

out-edges of each vertex G' in the metagraph by

$$2|\{(i,j) : i,j \in Z\}| \; + \; |\{(i,j) : i \in X, j \in Z\}| + \; |\{(i,j) : i \in Z, j \in Y\}| \quad .$$

The number of edges in G is a reasonable indicator for the size of the metagraph, that is, the search space.

As a starting point we consider a transformation of $G = (V, E)$ using a sequence σ_{e_c} of constant edge eliminations,[5] that is, $\#_{*_v}(\sigma_{e_c}(G)) = 0$. This yields $G' = (V', E') = \sigma_{e_c}(G)$ such that $|E'| \leq |E|$, which reduces the search space. The resulting graph G' implies a metagraph $M(G')$, which is a subgraph of $M(G)$ with G' as minimal vertex. We have to ensure that $M(G')$ still contains a path with the minimal sum of metagraph edge labels. In other words, an *optimality preserving* σ_{e_c} satisfies $\#_{*_v}(\hat{\sigma}_f(\mathcal{G}')) \not> \#_{*_v}(\hat{\sigma}_f(\mathcal{G}))$.

2.1. Single Expression Use Graphs. Similarly to Section 1.2 we denote the set of direct successors of a vertex v_i by $S_i = \{v_j | (i,j) \in E\}$; the set of direct predecessors of v_j is denoted by $P_j = \{v_i | (i,j) \in E\}$. G has the single expression use (seu) property if $|S_i| = 1 \; \forall v_i \in Z$. This is true, for instance, for any set of right-hand sides of assignments that can be computed independently from each other. For such G there exists a polynomial algorithm that constructs an optimal elimination sequence $\hat{\sigma}_f$ first introduced in [11].

ALGORITHM 1 (optimal seu elimination). *For a given seu graph G perform vertex elimination steps in the following order, $\forall v_i, i = 1, \ldots, p$:*

(1) Determine a minimal $v_i - X$ separating set $\underline{P_i}$.

(2) If $|\underline{P_i}| < |P_i|$ perform vertex elimination of all vertices $\{v_j : v_j \prec v_i \wedge v_k \prec v_j \forall v_k \in \underline{P_i}\}$ reverse ordered by index j.

After these steps have been performed for all v_i,

(3) perform vertex elimination of all remaining vertices reverse ordered by index j.

[5] View a vertex elimination as a group of edge eliminations.

If G is a tree, then this algorithm yields the reverse mode of AD. Because of the seu property there is no advantage to be gained from face elimination over edge or vertex elimination; that is, $\hat{\sigma}_f$ can be written as $\hat{\sigma}_e$. The construction of $\hat{\sigma}_e$ relies on

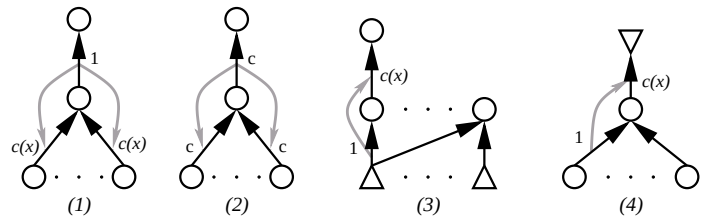

FIG. 2.2. *Four steps in Algorithm 2; labels* c *are constant, and* $c(x)$ *are variable*

attaining the lower bound of operations required for each $v \in Z$ defined by the size of the smallest $v - X$ separating vertex sets. The following algorithm creates a σ_{e_c} that reduces (steps 1-3) or maintains (step 4) the edge count; see also Figure 2.2.

ALGORITHM 2 (seu constant folding). *For a given G create σ_{e_c} with the following steps:*

(1) Back eliminate all trivial edges.
(2) Back eliminate (j,k) if (j,k) and (i,j) are constant $\forall i \in P_j$.
(3) Front eliminate all trivial edges (i,j) if $|P_j| = 1$
(4) Front eliminate all trivial edges (i,j) if $S_j \subseteq Y$.

One can easily see that none of the steps suggested here increases the minimal separating vertex set size and therefore σ_{e_c} is optimality preserving. Note that this may

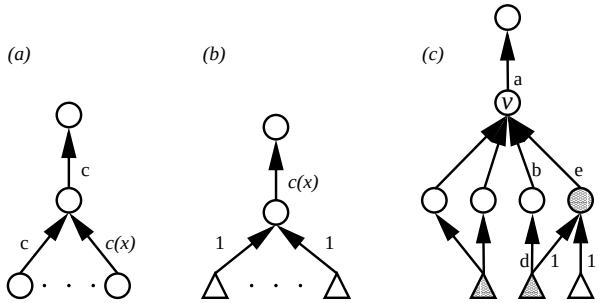

FIG. 2.3. *(a) and (b) situations not covered by Algorithm 2, (c) choosing a $v - X$ separating set*

leave trivial and constant edges in G' that cannot be eliminated with any of the steps given in this algorithm; see Figure 2.3 (a,b). While step 4 does not reduce the edge count, it is the result of considering the possibility of executing elimination steps that necessarily have to be part of the optimal elimination sequence. The application of the constant folding to seu graphs is a theoretical exercise as the optimal solution is constructed and does not require a search space reduction. However, Figure 2.3 (c) illustrates a case not covered by the purely structural information used in the construction of the optimal elimination sequence. Considering step 1 in Algorithm 1 there is a choice in picking a minimal separating set that may lead to a suboptimal elimination sequence. The $v - X$ separating set indicated by the gray filled vertices in Figure 2.3 (c) yields

$$t_1 = b * d; t_2 = a * c; t_3 = a * t_1; t_4 = 1 * t_2; t_5 = t_2 + t_4; t_6 = 1 * t_2$$

as part of the computation, whereas picking all independents as separating set yields

$$t_1 = b * d; t_2 = 1 * c; t_3 = 1 * c + t_1; t_4 = a * t_3; t_5 = a * t_2 \quad .$$

If, however, a, b, d are all constant and c is not, we have two versus one constant multiplications. Fortunately, an addition of minimal vertices is the only case exhibiting such a problem, and it can be overcome simply by choosing the $\underline{P_i}$ such that it leaves the elimination of the vertex in question for step 3.

2.2. Directed Acyclic Graphs. We already pointed to the lack of an algorithm that exactly determines $\hat{\sigma}(G)$ with polynomial complexity. Algorithm 2 was motivated by the construction of $\hat{\sigma}_f$ in Algorithm 1 and the condition $|E'| \leq |E|$. The latter is the actual motivation here as the implied search space reduction permits computationally more expensive heuristics. Between seu graphs on the one side and generic DAGs on the other side there are currently no other, more generic structural properties of DAGs known to imply anything about the optimal elimination sequences. Therefore, a plausible starting point for generic DAGs is to require the seu property for subgraphs. We hypothesize that we preserve optimality through affecting the respective elimination subsequences only.

ALGORITHM 3 (DAG constant folding). *For a given G do the following steps in order:*

(1) If $\forall i \in P_j \wedge k \in S_j$: c_{ji}, c_{kj} are constant, then eliminate[6] *j if $|S_j| = 1$ or $|P_j| = 1$.*

(2a) Back eliminate all trivial edges (i, j) if $|S_i| = 1$.

(2b) Front eliminate all trivial edges (i, j) if $|P_j| = 1$.

We already mentioned the potential of face elimination in the corresponding directed line graph to undercut the operations count of vertex and edge eliminations. Therefore, we have to prove optimality preservation in terms of face elimination sequences.

PROPOSITION 1. *Back elimination of trivial edges with $|S_i| = 1$ (step 2a) preserves optimality.*

Proof. Assume $c_{ji} = 1$, and consider an optimal face elimination sequence σ for $\mathcal{G}$. We can construct σ' for $\mathcal{G}'$ the directed line graph for $G' = G - (i, j)$ with an iteration over σ. In each step k we construct a subsequence σ'_k and a remainder σ_{k+1}. Let r denote the vertex (i, j) in $\mathcal{G}$.

initialize: $k := 1 \quad \sigma_1 := \sigma \quad \mathcal{G}'_1 := \mathcal{G}' \quad \mathcal{G}_1 := \mathcal{G}$

while $\sigma_k \neq \emptyset$ split $\sigma_k = (X, (p, q), \sigma_{k+1})$,

where (p, q) is the first face in σ_k with p or $q \in P_r \cup S_r$

$\sigma'_k := X$

if $q \neq r \wedge p \neq r$ then $\sigma'_k := \sigma'_k \cup (p, q)$ (*)

$\mathcal{G}'_{k+1} := \sigma'_k(\mathcal{G}'_k)$

$\mathcal{G}_{k+1} := (X, (p, q))(\mathcal{G}_k)$

There are three scenarios for (*).

1. If $q \in S_r$ ($p \neq r$ is implied), then P_p and S_q are identical between $\mathcal{G}_k$ and $\mathcal{G}'_k$. That means the potential fill-ins are identical $\mathcal{F}_{\mathcal{G}_k}(p, q) = \mathcal{F}_{\mathcal{G}'_k}(p, q) = (\{v\}, \{(v, t) | t \in S_q\} \cup \{(s, v) | s \in P_p\})$; see Figure 2.4. Therefore, this case does not induce any further distinction between σ and σ'.
2. If $q \in P_r$, then there may be a fill-in $\mathcal{F}_{\mathcal{G}_k}(p, q) = (\{v\}, \{(v, r)\} \cup \{(s, v) | s \in P_p\})$, which differs from $\mathcal{F}_{\mathcal{G}'_k}(p, q) = (\{v\}, \{(v, t) | t \in S_r\} \cup \{(s, v) | s \in P_p\})$.

[6] interpreted as edge-front or edge-back elimination, respectively

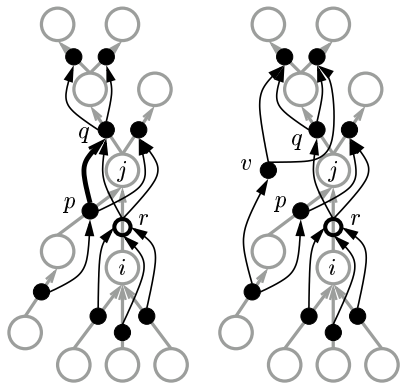

FIG. 2.4. *Scenario 1: a subgraph of $\mathcal{G}$ overlaid over the corresponding subgraph of G before (left) and after (right) face elimination of (p, q)*

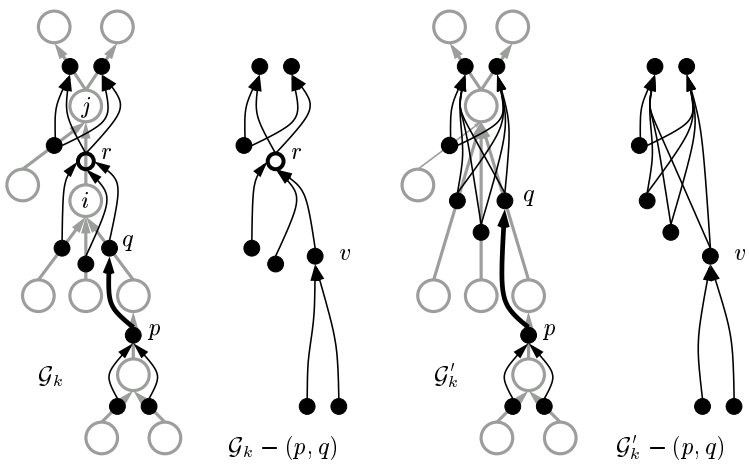

FIG. 2.5. *Scenario 2: face elimination before (left pair) and after (right pair) constant folding*

A subsequent elimination of (v, r) will be skipped according to the condition in (*). This coincides with the fact that the resulting edges are identical to the (v, t) that have already been created in $\mathcal{G}'_{k+1}$; see Figure 2.5. The sets $\{(s, v) | s \in P_q\}$ are identical, and subsequent eliminations of the (s, v) fall under (*).

3. The scenario of $p \in S_r$ is symmetric to $q \in P_r$.

The condition in (*) excludes some elimination steps (p, q). For the entire elimination sequence $\sigma' = \bigcup_k \sigma'_k$ we therefore have $|\sigma'| \not< |\sigma|$. □

The proof for the respective statement for $|P_j| = 1$ (step 2b) follows from symmetry.

PROPOSITION 2. *Vertex elimination of j with (i, j) and (j, k) constant for all $i \in P_j$ and $k \in S_j$ and $(|S_j| = 1 \vee |P_j| = 1)$ preserves optimality (step 1)*

Proof. Assume the case with $|S_j| = 1$. We follow the same argument as the proof for Proposition 1 where we skip all elimination steps (p, q) for which $p = (j, k)$ or $q = (j, k)$. $|P_j] = 1$ follows from symmetry. □

All steps in Algorithm 3 reduce the edge count. Similarly to Algorithm 2 trivial and

constant edges are left in the graph, and we can look for further reductions by adding the following steps to Algorithm 3:

(3a) Back eliminate all trivial edges (i, j) if $|P_i| = 1$.

(3b) Front eliminate all trivial edges (i, j) if $|S_j| = 1$.

This implies $|P_j| > 1$ and $|S_i| > 1$. Otherwise we would have used steps 2a or 2b, respectively.

PROPOSITION 3. *Front eliminate all trivial edges with $|S_j| = 1$ preserves optimality (step 3b).*

Proof. Again we use the same approach of skipping all elimination steps (p, q)

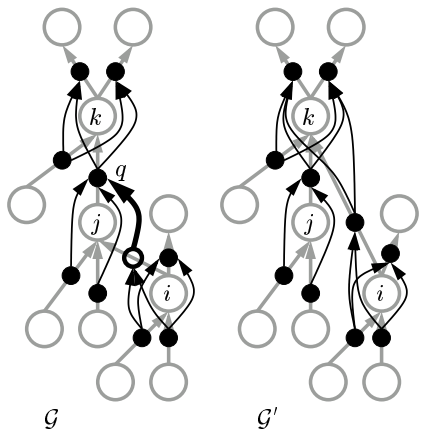

FIG. 2.6. *Trivial labels $c_{ji} = \pm 1$*

with $p = (i, j)$ or $q = (i, j)$; see Figure 2.6. □

Note that there is no reduction in the edge count unless $(i, k) \in G, S_j = \{k\}$, that is, we have absorption. In either case optimality is preserved. There are, however, two issues. First, even with absorption we have to account for the extra addition $c_{ki} = c_{ki} + c_{kj}$ when either c_{kj} or c_{ki} or both are variable; see also Section 3. Second, without absorption we duplicate the potentially variable label c_{kj} by removing the trivial label c_{ji}. This is contrary to the idea of preserving scarcity mentioned in Section 3. The proof for step 3a follows from symmetry.

Similar to steps 3a/3b we can also extend for constant labels with the following two steps:

(4a) Back eliminate (i, j) if $|P_j| = 1, P_i = \{h\}$ and $(h, i), (i, j)$ constant.

(4b) Front eliminate (i, j) if $|S_i| = 1, S_j = \{k\}$ and $(i, j), (j, k)$ constant.

Considering step 4b we observe that in case of absorption there will be no extra addition as long as (i, k) is constant. Even without absorption these steps preserve scarcity as there is no variable fill-in.

2.3. Constant Face Elimination. The suggested Algorithm 3 even with the extension steps 3 and 4 does not preeliminate all constant or trivial labels from G. Since we already pointed to the advantage face elimination may yield over vertex and edge elimination, we should consider the possibility of preeliminating constant faces. The search space represented by $M(\mathcal{G})$, the metagraph for the directed line graph, is vastly larger than the $M(G)$ for vertex or edge elimination. Still, the edge count in G, that is, the number of intermediate vertices in $\mathcal{G}$ is a reasonable, although crude, indicator for the search space size.

Any elimination of an (i, j) in $\mathcal{G}$ where $|S_i| = 1$ or $|P_j| = 1$ leads to the removal of i or j, respectively. It can be written as an edge elimination and would therefore already be covered by Algorithm 3. We consider scenarios that cannot be interpreted as edge eliminations. The least amount of structural change is therefore the removal of an edge in $\mathcal{G}$ by face elimination with absorption. That is, we look at (i, j) with constant labels on i and j and $\exists k$ with $P_k = P_i$ and $S_k = S_j$ and k has a constant label as well. Consider the example in Figure 1.3. If both c_{31} and c_{43} are constant and none of the other edge labels are, then the previously introduced algorithm would not fold these two constants. One might expect that, similarly to the DAG, it was safe to preeliminate this face in the directed line graph because the result is absorbed in c_{41} and we basically just remove an edge from $\mathcal{G}$ at no cost. Somewhat surprising it turns out that such an edge removal may actually increase elimination cost, as the example in Figure 2.7 illustrates. The original graph has an optimal elimination sequence of

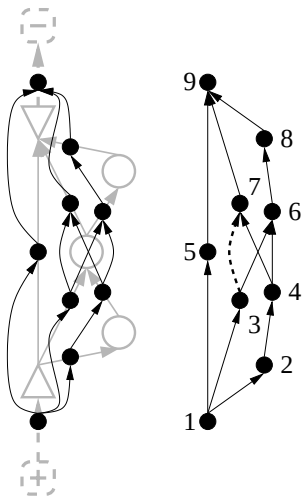

FIG. 2.7. *Removing* $(3, 7)$ *by constant face elimination*

length 3, for instance, $((2, 4), (6, 8), (3, 7))$. Now we assume that both 3 and 7 have constant labels, and we eliminate $(3, 7)$ and absorb into 5, thereby just removing $(3, 7)$. One can perform an exhaustive search and see that there is no complete elimination sequence in the resulting graph $\mathcal{G} - (3, 7)$ with a length ≤ 3.

An attempt to prove the preservation of optimality of a face elimination step that modifies $\mathcal{G}$ to $\mathcal{G}'$ would assume an optimal elimination sequence for $\mathcal{G}$ and then try to show that this elimination sequence contains a subsequence that is complete for $\mathcal{G}'$. This requires that all fill-in generated in $\mathcal{G}'$ is a subset of the fill-in generated in $\mathcal{G}$. With the current rule for merging of vertices in the face elimination definition, this is not necessarily the case once a single edge is removed. Edge and vertex eliminations and the conditions and predecessor and successor sets group edge eliminations in a way that eliminates this issue, as shown in the respective proofs for constant folding steps.

3. Conclusion: Practical Use and Further Observations. Constant folding as presented here is implemented in the OpenAD[7] framework of the Adjoint

[7] `www-unix.mcs.anl.gov/~ utke/OpenAD`

Compiler Technology & Standards (ACTS) project. We mentioned in Section 1 that heuristics may be unaware of the label categories, as is the case with the face elimination heuristics currently used in OpenAD. The target application of OpenAD within the ACTS project is the MIT general circulation model. Since large portions of the model code are linear, one has a convincing case for using constant folding on G and creating a directed line graph only for the nonlinear core.

The choice of the number of multiplications as an optimality measure ignoring additions and memory access appears rather arbitrary when considering the raw execution time of a given Jacobian computation. We are well aware of the impact of data locality, pipelined operations, and so forth, since minimizing the execution time is the ultimate goal. OpenAD contains heuristics that address these practical aspects. For theoretical investigations it is certainly possible to count the individual multiplications and additions separately, as well as memory reads and writes. Additions occur optionally in conjunction with multiplications for vertex and edge elimination. For face elimination, however, one can easily construct cases where a single elimination step entails more than one addition. This is due to the current face elimination merge rule, where the elimination of a face enables the merging of up to two additional vertex pairs in $\mathcal{G}$. Most results on face elimination optimality ignore these additions altogether. It has been conjectured, however, that there is always an optimal elimination sequence that completely avoids additions through merging. This is subject of ongoing research. We also mentioned the issue of extra additions possibly introduced by steps 3 and 4 of Algorithm 3. In practice there is a principal dominance of the execution time of a multiplication over an addition which makes ignoring additions plausible. For data read and write operations there is no such generic statement and their execution times are highly hardware and context dependent. Including these timings would make general assumptions and optimality statements impossible. Moreover, the generated elimination code `jac` is itself subject to subsequent compiler optimization. Therefore, we consider the suggested optimality measure sufficient for this compiler and hardware-independent optimization.

In Algorithm 3, step 3, we mentioned the issue of scarcity preservation. There are functions $\boldsymbol{f}$ that have a dense $\boldsymbol{f}'$ but have graph representations with far fewer edges than the final bipartite graph. In [8, 6] the term *scarcity* was introduced to denote this difference. Scarcity-preserving eliminations have the narrower objective of reducing or maintaining the number of edges with nontrivial labels. Despite the similarity to the objective of constant folding, there are some differences. With constant folding we eventually want to minimize operations for the computation of the Jacobian, whereas scarcity-preserving eliminations minimize the operations for repeated Jacobian vector products. A σ considered here for constant folding is complete, whereas a scarcity-preserving σ will generally be an incomplete elimination sequence. Moreover, the set of scarcity-preserving graph modifications suggested in [8, 6] contains a rerouting operation that can be interpreted as an inverse face elimination. This prevents an easy integration of both objectives. However, one can exploit the idea of cutting an elimination sequence short if there is an intermediate directed line graph representation with fewer vertices than the final tripartite directed line graph. Therefore, we note that the proposed constant folding steps 1, 2a/2b and 4a/4b in Algorithm 3 preserve scarcity as well. Steps 3a/3b preserve scarcity only for absorbed fill-in and if the absorbing label is variable. We can modify the heuristics to represent label categories in the directed line graph to enable a scarcity-preserving face elimination. The investigation of such a modified optimization criterion is the subject of ongoing

research.

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