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Optimal Direct Determination of Sparse Jacobian Matrices *

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Abstract

It is well known that a sparse Jacobian matrix can be determined with fewer function evaluations or automatic differentiation *passes* than the number of independent variables of the underlying function. In this paper we show that by grouping together rows into blocks one can reduce this number further. We propose a graph coloring technique for row partitioned Jacobian matrices to efficiently determine the nonzero entries using a direct method. We characterize *optimal direct determination* and derive results on the optimality of any direct determination technique based on column computation. The computational results from coloring experiments on Harwell-Boeing test matrix collection demonstrate that our row partitioned direct determination approach can yields considerable savings in function evaluations or AD passes over methods based on the Curtis, Powell, and Reid technique.

Keywords: Jacobian matrix, graph coloring, row partitioning

1 Introduction

Computation or estimation of the Jacobian matrix $J \equiv \left\{ \frac{\partial f_i}{\partial x_j} \right\}$ of a mapping $f : \mathbf{R}^n \to \mathbf{R}^m$ is an important subproblem in many numerical procedures. Mathematical derivatives can be approximated or calculated by a variety of techniques including automatic (or algorithmic) differentiation (AD) [12], finite differencing (FD) [7], and computational divided differencing (CDD) (or algorithmic differencing) [24].

We assume that the Jacobian matrices have a fixed sparsity pattern in the domain of interest. Further, we compute the whole column of J even if only a few components are

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needed. A computer subroutine implementing a function will evaluate the common subexpressions only once rather than reevaluating the same subexpression in different components of the vector $f(x)$.

Automatic differentiation techniques can be employed as an alternative to FD to approximate J. Unlike FD, AD techniques yield derivative values free of truncation errors. AD views computer programs evaluating a mathematical function as a "giant" mapping composed of elementary mathematical functions and arithmetic operations. Applying the Chain rule the evaluation program can be augmented to accumulate the "elementary" partial derivatives so that the function and its derivatives at chosen input are computed. An excellent introduction to AD techniques can be found in ([12]).

The notational conventions used in this paper are introduced below. Additional notations will be described as needed. If an uppercase letter is used to denote a matrix (e.g., A), then the (i,j) entry is denoted by $A(i,j)$ or by corresponding lowercase letter a_{ij}. We also use colon notation [10] to specify a submatrix of a matrix. For $A \in R^{m\times n}$, $A(i,:)$ and $A(:,j)$ denotes the ith row and the jth column respectively. For a vector of column indices v, $A(:,v)$ denotes the submatrix consisting of columns whose indices are contained in v. For a vector of row indices u, $A(u,:)$ denotes the submatrix consisting of rows whose indices are contained in u. A vector is specified using only one dimension. For example, the ith element of $v \in R^n$ is written $v(i)$. The transpose operator is denoted by $(\cdot)^T$. A blank or "0" represents a zero entry and any other symbol in a matrix denotes a nonzero entry.

Both AD and FD allow the estimates of the nonzero entries of J to be obtained as matrix-vector products. For a sparse matrix with known sparsity pattern or if the sparsity can be determined easily [13] substantial savings in the computational cost (i.e. the number of matrix-vector products) can be achieved.

A group of columns in which no two columns have nonzero elements in the same row position is known as *structurally orthogonal*. If columns j and k are structurally orthogonal, then for each row index i at most one of $J(i,j)$ and $J(i,k)$ can be nonzero. In general $\sum_j J(i,j) = J(i,k)$ for some k (k will depend on i) where the sum is taken over a group of structurally orthogonal columns. An estimate of the nonzero elements in the group can be obtained in

$$\left.\frac{\partial f(x+ts)}{\partial t}\right|_{t=0} = f'(x)s \approx As = \frac{1}{\varepsilon}[f(x+\varepsilon s) - f(x)] \equiv b$$

with a forward difference (one extra function evaluation) where b is the finite difference approximation and $s = \sum_j e_j$. With forward automatic differentiation the unknowns elements in the group are obtained as the product $b = f'(x)s$ accurate up to the round-off error resulting from the finite machine precision.

A *Graph* $G = (V,E)$ is a set V of *vertices* and a set E of *edges*. An edge $e \in E$ is denoted by an unordered pair $\{u,v\}$ which connects vertices u and v, $u,v \in V$. A graph G is said to be a *complete* graph or *clique* if there is an edge between every pair of distinct vertices. In this paper multiple edges between a pair of vertices are considered as a single edge. A *p-coloring* of the vertices of G is a function $\Phi : V \to \{1,2,\cdots,p\}$ such that $\{u,v\} \in E$ implies $\Phi(u) \neq \Phi(v)$. *The chromatic number* $\chi(G)$ of G is the smallest p for which it has a *p-coloring*. An *optimal coloring* is a *p-coloring* with $p = \chi(G)$. Given an $m \times n$ matrix A, the *intersection graph* of the columns of A is denoted by $G(A) = (V,E)$ where corresponding to $A(:,j), j = 1,2,\ldots,n$, there is a vertex $v_j \in V$ and $\{v_j, v_l\} \in E$ if and only if $A(:,j)$ and $A(:,l), l \neq j$ have nonzero elements in the same row position.

The matrix determination problem can be conveniently modelled by graphs [4, 22] and such graph models often reveal valuable properties that can be utilized in finding efficient solutions. It has been observed that finding a partition of the columns of A in groups of structurally orthogonal columns is equivalent to coloring the vertices of the intersection graph $G(A)$. A combined approach where sparsity is exploited more effectively by a bidirectional partitioning scheme has been proposed in [6, 15]. These techniques use the forward and reverse modes of AD to compute the product AV and W^TA for matrices V

and W. On the other hand, the aforementioned partitioning schemes have been found to be "unsatisfactory" on certain sparsity patterns [4, 14]. Furthermore, it is not clear what constitutes an optimal partition in these direct methods. This paper describes an optimal direct determination procedure for determining Jacobian matrices. The main contributions of this paper are summarized below.

1. **Characterization of the determination of sparse Jacobian matrices based on matrix-vector products**:
   We view the Jacobian matrix determination problem as a matrix problem and apply combinatorial and graph theoretic techniques as tools for analyzing and designing algorithms for efficient determination. Consequently, we propose a uniform characterization of all direct methods that uses matrix-vector products to obtain the nonzero estimates. This is not an entirely new idea. However, to the best of our knowledge we are unaware of any published literature that provides a precise definition of direct methods and characterization of their optimality. Sections 2 and 3 present the main results of this work - an uniform theoretical framework expressed in the language of linear algebra for all direct methods including the CPR-based methods.

2. **Graph coloring techniques to obtain the optimal partition**:
   The test results from our column segments approach applied on a number of Harwell-Boeing test problems provides the clearest evidence that the CPR-based direct methods are not optimal on practical problems. Further, the Eisenstat example which has been frequently used in the literature as a counter example to the claim of optimality of CPR-based methods can now be optimally partitioned using the techniques presented in this paper.

The presentation of the paper is structured as follows. In section 2 we propose a partitioning scheme based on structurally orthogonal column segments to determine sparse Jacobian matrices. The characterization of direct determination of Jacobian matrices presented in this section is based on familiar matrix-vector products. Section 3 presents a graph coloring formulation of the partitioning problem and shows that the coloring problem is unlikely to be solved efficiently. Several complexity results concerning the colorability of the column-segment graph is given. The section ends with the conditions for optimality of direct determination methods. Section 4 contains results from coloring experiments with test matrices in Harwell-Boeing collection. Finally, the paper is concluded in section 5 with a discussion on topics for further studies.

2 Direct Determination and Row Partitioning

In this section we formulate the Jacobian matrix determination problem as a partitioning problem and provide a precise characterization of direct determination. The column segment partitioning technique for efficient determination of sparse Jacobian matrices is given next. We assume that the sparsity pattern of the Jacobian matrices in the domain interest is known a priori.

The Jacobian Matrix Determination Problem:

Obtain vectors $s_1, \cdots, s_p$ such that the matrix-vector products

$$b_i \equiv As_i,\ i = 1, \cdots, p \text{ or } B \equiv AS$$

determine the $m \times n$ matrix A uniquely. Matrix S is the *seed matrix*.

Denote by ρ_i the number of nonzero elements in row i of A and let $v \in R^{\rho_i}$ contain the column indices of (unknown) nonzero elements in row i of A. Let $S \in R^{n \times p}$ be any (seed) matrix. Compute

$$B = AS.$$

Let

$$A(i,v) = \begin{pmatrix} \alpha_1 & \cdots & \alpha_{\rho_i} \end{pmatrix} = \alpha^T, \alpha \in R^{\rho_i},$$
$$B(i,:) = \begin{pmatrix} \beta_1 & \cdots & \beta_p \end{pmatrix} = \beta^T, \beta \in R^p,$$

and

$$\hat{S}_i^{\,T} = S(v,:).$$

Then

$$\hat{S}_i \alpha = \beta \tag{1}$$

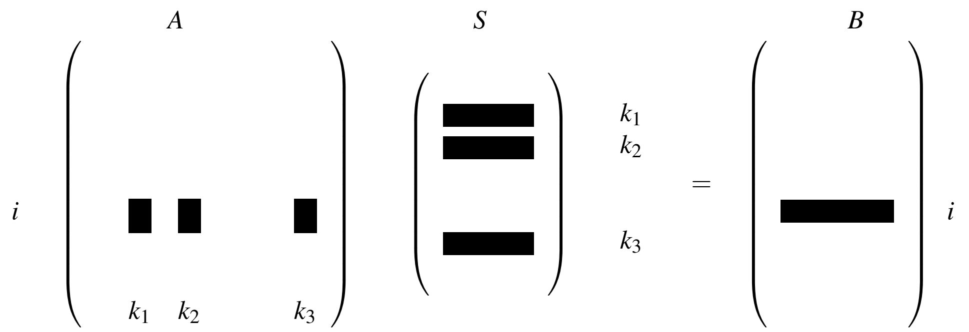

Figure 1: Determination of the unknown entries with column indices k_1, k_2, and k_3 in row i of A.

In Figure 1 row i (with $\rho_i = 3$ nonzero entries) of the matrix A are to be determined. The vector

$$v = \begin{pmatrix} k_1 & k_2 & k_3 \end{pmatrix}$$

contains the column indices of the unknown elements

$$A(i,v) = \alpha^T, \ \alpha \in R^{\rho_i}$$

in row i that are to be solved for from

$$\hat{S}\alpha = \beta$$

where $\hat{S} \equiv S(v,:)$ and $\beta = B(i,:)$ are known quantities. The darkened boxes in Figure 1 constitute the reduced linear system (1).

Definition 2.1 If for every $1 \leq k \leq \rho_i$ there is an index $1 \leq k' \leq p$ such that $\alpha_k = \beta_{k'}$ then we say that row i of A is determined *directly*. We have *direct determination* of A if each row of A can be determined directly.

Let u be a vector containing indices such that $u(k) = k', \ k = 1, \cdots, \rho_i$ for k' as given in Definition 2.1. Then $\alpha = \beta(u)$ so that the nonzero elements in row $i, i = 1, \cdots, m$ can be read off the vector β since the sparsity pattern of A is available. Definition 2.1 leads to the following observations regarding the reduced system:

1. If $\rho_i = p$, then $\hat{S}_i$ is a permutation matrix (permuted identity matrix).

2. If $\rho_i < p$, then $\hat{S}_i(u,:)$ is a permutation matrix.

3. If $\overline{u}$ contains the indices not in u, then $\beta(\overline{u}) = 0$ if the seed matrix is constructed from structurally orthogonal columns of A.

An important implication of observation 3 is that, in general, matrix B need not be the "compressed" Jacobian matrix as defined in ([1, 4, 7]). Therefore a precise definition of "direct methods" is necessary. The following example

$$A = \begin{pmatrix} a_{11} & 0 & 0 & a_{14} & 0 & 0 \\ 0 & a_{22} & 0 & 0 & a_{25} & 0 \\ 0 & 0 & a_{33} & 0 & 0 & a_{36} \\ a_{41} & a_{42} & a_{43} & 0 & 0 & 0 \\ a_{51} & 0 & 0 & 0 & a_{55} & a_{56} \\ 0 & a_{62} & 0 & a_{64} & 0 & a_{66} \\ 0 & 0 & a_{73} & a_{74} & a_{75} & 0 \end{pmatrix}$$

due to Stanley Eisenstat has appeared in the literature on Jacobian matrix computation illustrating that the CPR-based direct methods may fail to find an optimal direct determination. The CPR seed matrix for this example is the identity matrix I_6. It has been common to say that the best way to estimate or compute this example is using 5 matrix-vector product (see [4, 22]) with

$$S = \begin{pmatrix} 1 & 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 1 & 0 \\ 1 & 0 & 0 & 0 & 1 \\ 0 & 1 & 1 & 0 & 0 \\ 0 & 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 & 1 \end{pmatrix}$$

and computing

$$B = AS = \begin{pmatrix} a_{11} & a_{14} & a_{11}+a_{14} & 0 & 0 \\ a_{22} & a_{25} & 0 & a_{22}+a_{25} & 0 \\ a_{33} & a_{36} & 0 & 0 & a_{33}+a_{36} \\ a_{41}+a_{42}+a_{43} & 0 & a_{41} & a_{42} & a_{43} \\ a_{51} & a_{55}+a_{56} & a_{51} & a_{55} & a_{56} \\ a_{62} & a_{64}+a_{66} & a_{64} & a_{62} & a_{66} \\ a_{73} & a_{74}+a_{75} & a_{74} & a_{75} & a_{73} \end{pmatrix}$$

using AD forward mode or FD. It can be verified that for each nonzero element in A there is a linear equation from which the element is recovered without any further arithmetic operation. For example the nonzero elements in row 5 is determined in the the reduced linear system

$$\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} \alpha_1 \\ \alpha_2 \\ \alpha_3 \end{pmatrix} = \begin{pmatrix} \beta_1 \\ \beta_2 \\ \beta_3 \\ \beta_4 \\ \beta_5 \end{pmatrix} \equiv \begin{pmatrix} a_{51} \\ a_{55}+a_{56} \\ a_{51} \\ a_{55} \\ a_{56} \end{pmatrix}$$

yielding

$$\begin{pmatrix} \alpha_1 \\ \alpha_2 \\ \alpha_3 \end{pmatrix} = \begin{pmatrix} a_{51} \\ a_{55} \\ a_{56} \end{pmatrix}$$

Essentially, the determination of nonzero elements in the example corresponds to the first three rows being determined independent of the remaining rows as shown below. Partitioning the rows of A into blocks A_1 and A_2 as in Figure 2 matrix A is determined in two steps - first determine A_1 using 2 matrix-vector products whence the estimates for A_2 are ignored. Then use 3 additional matrix-vector products to determine A_2 and ignore A_1 estimates. This method of estimation by independent blocks of rows has also been considered in [11] as partial argument separability or column splitting. However, as we demonstrate here, this is

$$
\begin{array}{l}
A_1\left\{\vphantom{\begin{array}{c}a\\a\\a\end{array}}\right.\\
A_2\left\{\vphantom{\begin{array}{c}a\\a\\a\\a\end{array}}\right.
\end{array}
\quad
\left(\begin{array}{cccccc}
a_{11} & 0 & 0 & a_{14} & 0 & 0\\
0 & a_{22} & 0 & 0 & a_{25} & 0\\
0 & 0 & a_{33} & 0 & 0 & a_{36}\\
\hline
a_{41} & a_{42} & a_{43} & 0 & 0 & 0\\
a_{51} & 0 & 0 & 0 & a_{55} & a_{56}\\
0 & a_{62} & 0 & a_{64} & 0 & a_{66}\\
0 & 0 & a_{73} & a_{74} & a_{75} & 0
\end{array}\right)
\Longrightarrow
\left(\begin{array}{c} A_1 \\ \hline A_2 \end{array}\right)
\Longrightarrow
\left(\begin{array}{c} A_1 \\ \hline \times \end{array}\right),
\quad
\left(\begin{array}{c} \times \\ \hline A_2 \end{array}\right)
$$

Figure 2: Determine A_1 and A_2 separately

not the best way to determine the matrix. The following seed matrix with only 4 columns yields direct determination of A. Let

$$
S = \begin{pmatrix}
0 & 0 & 1 & 1\\
0 & 1 & 0 & 1\\
1 & 0 & 0 & 1\\
1 & 1 & 0 & 0\\
1 & 0 & 1 & 0\\
0 & 1 & 1 & 0
\end{pmatrix}.
$$

Then,

$$
B = AS = \begin{pmatrix}
a_{14} & a_{14} & a_{11} & a_{11}\\
a_{25} & a_{22} & a_{25} & a_{22}\\
a_{33} & a_{36} & a_{36} & a_{33}\\
a_{43} & a_{42} & a_{41} & a_{43}+a_{41}+a_{42}\\
a_{55} & a_{56} & a_{51}+a_{55}+a_{56} & a_{51}\\
a_{64} & a_{62}+a_{64}+a_{66} & a_{66} & a_{62}\\
a_{73}+a_{74}+a_{75} & a_{74} & a_{75} & a_{73}
\end{pmatrix}.
$$

Figure 3: Optimal determination of Eisenstat example matrix

The reduced system for row 5 is

$$
\begin{pmatrix}
0 & 1 & 0\\
0 & 0 & 1\\
1 & 1 & 1\\
1 & 0 & 0
\end{pmatrix}
\begin{pmatrix}\alpha_1\\ \alpha_2\\ \alpha_3\end{pmatrix}
=
\begin{pmatrix}\beta_1\\ \beta_2\\ \beta_3\\ \beta_4\end{pmatrix}
\equiv
\begin{pmatrix} a_{55}\\ a_{56}\\ a_{51}+a_{55}+a_{56}\\ a_{51}\end{pmatrix}
$$

yielding

$$
\begin{pmatrix}\alpha_2\\ \alpha_3\\ \alpha_1\end{pmatrix}
=
\begin{pmatrix} a_{55}\\ a_{56}\\ a_{51}\end{pmatrix}.
$$

Again, it is a straight-forward exercise to check that the remaining rows of A can be determined directly.

The proposal of Newsam and Ramsdell [22] entails the estimation of the nonzero elements as groups of "isolated" elements. Given matrix A, the nonzero element $A(i,j)$ is said to be *isolated* from the nonzero element $A(p,q)$ if and only if $A(i,q) = A(p,j) = 0$ or $j = q$. Our next result shows that direct determination yields element isolation.

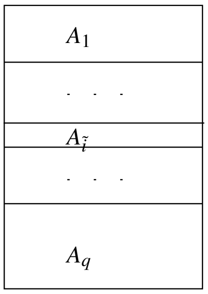

Figure 4: Row q-partition of A where $A_{\tilde{i}}$ denotes $A(w_{\tilde{i}},:)$

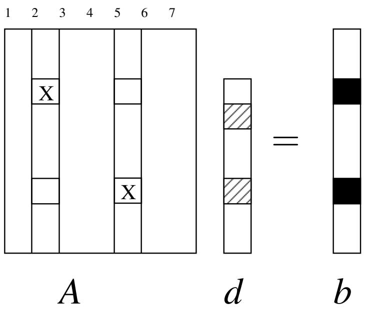

Figure 5: If the elements marked $\square$ are zero, then the elements marked $\boxed{\text{X}}$ are "isolated" and can be determined in one matrix-vector product $Ad = b$.

Theorem 1 *Direct determination implies that all nonzero elements determined in a matrix-vector product are isolated elements.*

Proof. Let a_{ij} and a_{kl} be two arbitrary nonzero elements of A that are determined directly in $AS(:,\check{p})$ for some $\check{p} \in \{1,2,\ldots,p\}$. If $j = l$, then a_{ij} and a_{kl} are isolated. Since a_{ij} and a_{kl} are determined directly, $i \neq k$. Also, a_{ij} determined directly implies $a_{ij} = e_i^T AS(:,\check{p})$ and hence $a_{il} = 0$. Similarly, we conclude that $a_{kj} = 0$. But then the elements a_{ij} and a_{kl} are isolated as required. $\square$

In Figure 2 matrix A is directly determined from the product $B = AS$. The unknown elements that are determined from product $B(:,j) = AS(:,j)$ are isolated. For example, in column 1 of B all entries except the last one are isolated. Formalizing the partitioning of rows leads to the concept of column segments.

2.1 Column Segment Seed

Let Π be a partition of $\{1,2,\ldots,m\}$ yielding $w_1, w_2, \ldots, w_q$ where $w_{\tilde{i}}$ contains the row indices that constitute block $\tilde{i}$ and $A(w_{\tilde{i}},:) \in R^{m_{\tilde{i}} \times n}$, $\tilde{i} = 1,2,\ldots,q$.

Definition 2.2 A segment of column j in block $\tilde{i}$ of A denoted by $A(w_{\tilde{i}},j), \tilde{i} = 1,2,\ldots,q$ is called a *column segment.*

Figure 4 shows a row q-partitioned A where vector $w_{\tilde{i}}$ contains the row indices that constitute block $A_{\tilde{i}}$. Note that the rows can be permuted so that they are consecutive in the blocks resulting from Π.

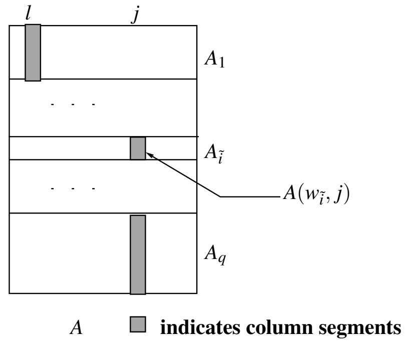

Figure 6: Segment of column j in block $A_{\tilde{i}}$ is denoted by $A(w_{\tilde{i}}, j)$

Definition 2.3

- `(Same Column)`

  Column segments $A(w_{\tilde{i}}, j)$ and $A(w_{\tilde{k}}, j)$ are structurally orthogonal

- `(Same Row Block)`

  Column segments $A(w_{\tilde{i}}, j)$ and $A(w_{\tilde{i}}, l)$ are structurally orthogonal if they do not have nonzero entries in the same row position.

- `(Different)`

  Column segments $A(w_{\tilde{i}}, j)$ and $A(w_{\tilde{k}}, l)$, $\tilde{i} \neq \tilde{k}$ and $j \neq l$ are structurally orthogonal if

  - $A(w_{\tilde{i}}, j)$ and $A(w_{\tilde{i}}, l)$ are structurally orthogonal and
  - $A(w_{\tilde{k}}, j)$ and $A(w_{\tilde{k}}, l)$ are structurally orthogonal

An *orthogonal partition of column segments* is a mapping

$$\kappa : \{\tilde{i}, j\} \rightarrow \{1, 2, \ldots, p\} \text{ for } \tilde{i} = 1, 2, \ldots, q \text{ and } j = 1, 2, \ldots, n$$

where column segments in each group are structurally orthogonal.

Theorem 2 *Let κ be any orthogonal partition of the column segments in p groups. Then there exists a $n \times p$ seed matrix S that yields direct determination.*

Proof. Define column $j, 1 \leq j \leq p$ in the $n \times p$ seed matrix

$$S(:, j) = \sum_{\{k : \kappa(\tilde{i}, k) = j, 1 \leq \tilde{i} \leq q\}} e_k.$$

It suffices to show that for any row i of A, $\hat{S}_i$ contains a $\rho_i \times \rho_i$ permutation matrix as a submatrix. Assume that row i of A is included in block $A(w_{\tilde{i}}, :)$. Let v_i be a vector containing the column indices of the nonzero entries of row i. Then $\hat{S}_i^T = S(v_i, :)$ (so that the number of rows in $\hat{S}_i^T$ is ρ_i). Also $\kappa(\tilde{i}, v_i(k')) \neq \kappa(\tilde{i}, v_i(k''))$ since the column segments $A(w_{\tilde{i}}, v_i(k'))$ and $A(w_{\tilde{i}}, v_i(k''))$ are not structurally orthogonal for $1 \leq k', k'' \leq \rho_i$. For each nonzero entry $A(i, v_i(k'))$, $1 \leq k' \leq \rho_i$ we have $S(v_i(k'), \kappa(\tilde{i}, v_i(k'))) = 1$. We claim that all other entries in column $v_i(k')$ of $S(v_i, :)$ are identical 0. If not then let $S(v_i(k''), \kappa(\tilde{i}, v_i(k'))) = 1$ for some index k''. But then $A(w_{\tilde{i}}, v_i(k'))$ and $A(w_{\tilde{i}}, v_i(k''))$ are structurally orthogonal - a contradiction. Therefore $S(v_i, \kappa(\tilde{i}, v_i(k')))$ is a unit coordinate vector of length ρ_i. Also since κ is a function the unit coordinate vectors corresponding to ρ_i nonzero entries $A(i, v_i)$ are unique and hence constitute a $\rho_i \times \rho_i$ permutation matrix. $\square$

The "seed matrix" construct provides a convenient way to express the sparsity exploiting "compression" in Jacobian matrix calculation. The definition of direct methods of this this paper allows for seed matrices that are more efficient than the CPR compression. The seed matrices for the Eisenstat example demonstrate that directly determined elements are isolated. In the next section we show that the converse is also true and hence establish that element isolation characterizes direct determination.

3 The coloring problem

In this section the matrix partitioning problem of section 2 is modelled as a graph coloring problem. This section presents one of the main results of this paper, namely, a precise characterization of optimal direct methods for the determination of Jacobian matrices. The use of graph techniques for analyzing the matrix determination problem for symmetric and nonsymmetric matrices are reported in [3, 4, 6, 15, 19, 22].

Definition 3.1 Given matrix A and row q-partition Π, the *column-segment graph* associated with A under partition Π is a graph $G_\Pi(A) = (V,E)$ where the vertex $v_{\tilde{i}j} \in V$ corresponds to the column segment $A(w_{\tilde{i}}, j)$ not identically 0, and $\{v_{\tilde{i}j}, v_{\tilde{k}l}\} \in E$ $1 \leq \tilde{i}, \tilde{k} \leq q, 1 \leq j,l \leq n$ if and only if column segments $A(w_{\tilde{i}}, j)$ and $A(w_{\tilde{k}}, l)$ are not structurally orthogonal.

The problem of determining Jacobian matrices using column segments can be stated as the following graph problem.

Theorem 3 *Φ is a coloring of $G_\Pi(A)$ if and only if Φ induces a orthogonal partition κ of the column segments of A.*

Proof. Let Π be a row $q-$partition of A. Vertices corresponding to a group of structurally orthogonal column segments can be colored with the same color since there cannot be any edge among them. On the other hand, given a p-coloring of $G_\Pi(A)$ the column segments corresponding to a particular color are structurally orthogonal. Hence the coloring induces an orthogonal partition of the column segments. □

A polynomial time algorithm for solving the coloring problem of Theorem 3 can also solve the partitioning problem efficiently. We next show that this coloring problem is no easier than the general graph coloring problem ([21]). The constructions we use in the proofs are similar to the one used in [22]. The following technical lemma shows that given an arbitrary graph which G is p-colorable we can define a new graph $\overline{G}$ which is also p-colorable. Then $\overline{G}$ is shown to be isomorphic to $G_\Pi(A)$ for some matrix A and a row q-partition Π.

Let $|\cdot|$ denote the number of elements contained in a set.

Lemma 1 *Given a graph $G = (V,E)$, and positive integers $1 \leq p \leq |V| = n$ and $1 \leq q$ there is a graph $\overline{G} = (\overline{V}, \overline{E})$ such that $\overline{G}$ is p-colorable if and only if G is p-colorable.*

Proof. The construction of $\overline{G}$ can be described as follows:

1. the vertex set $\overline{V} = \bigcup_{i=1}^{n}(V_i \bigcup U_i \bigcup \{v_{iq}\})$ consists of :

   (a) the "replication vertices" $V_i = \{v_{i1}, v_{i2}, \ldots, v_{i(q-1)}\}$

   (b) the "clique vertices" $U_i = \{u_{i1}, u_{i2}, \ldots, u_{i(p-1)}\}$

   (c) the "connector vertex" = v_{iq}

   defined for each vertex $v_i \in V$ and

2. the edge set $\overline{E} = E' \bigcup E'' \bigcup E'''$ is defined as

   (a) the "clique edges" $E' = \bigcup_{i=1}^{n} E'_i$ where $E'_i = \{\{u_{ik}, u_{il}\} | 1 \leq k,l \leq (p-1), k \neq l\}$,

(b) the "enforcement edges" $E'' = \bigcup_{i=1}^{n} E_i''$ where

$$E_i'' = \{\{v_{ik}, u_{il}\} | 1 \le k \le q, 1 \le l \le (p-1)\} \text{ and,}$$

(c) the "cross edges" $E''' = \bigcup_{i=1}^{n} E_i'''$ where

$$E_i''' = \big\{\{v_{ik}, v_{jl}\} | \{v_i, v_j\} \in E, \text{for some fixed } k \in \{1,2,\ldots,q\} \text{ and for all } 1 \le l \le q.\big\}$$

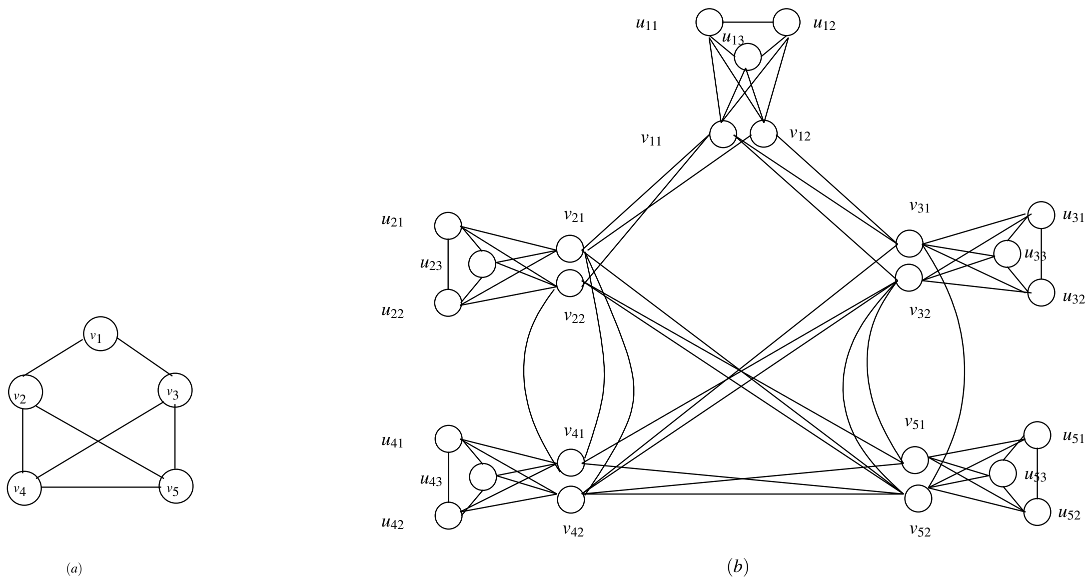

Figure 7: (a) Graph $G = (V,E)$ (b) Graph $\overline{G} = (\overline{V}, \overline{E})$ as in Theorem 1 with $p = 4$ and $q = 2$.

Let Φ be a p-coloring of G and consider $v_i \in V$. A p-coloring Φ' for $\overline{G}$ can be obtained by assigning $\Phi'(v_{ik}) = \Phi(v_i), k = 1,2,\cdots,q$ and the clique vertices U_i are colored so that they satisfy

$$\Phi'(u_{il}) \in \{1,2,\cdots,p\} \text{ and } \Phi'(u_{il}) \ne \Phi'(u_{il'}) \ne \Phi(v_i),\ l \ne l' \text{ for } l = 1,2,\cdots,(p-1).$$

Therefore Φ' is a p-coloring.

Conversely, in a p-coloring of $\overline{G}$ the vertices in U_i' must assume $p-1$ colors forcing the vertices in V_i' to use the remaining color. We can use the color of V_i' for vertex $v_i \in V$. To see that this is a p-coloring just observe that for any edge $\{v_i, v_j\} \in E$, v_i and v_j will assume different colors since the vertices in V_i' and V_j' must have different colors. □

To show that Jacobian estimation by a direct method is no easier than the general graph coloring problem it suffices to show that $\overline{G}$ is isomorphic to column segment graph $G_\Pi(A)$ for some Jacobian matrix A. Let $H = (V,E)$ be a graph where $V = \{v_1, v_2, \cdots, v_n\}$ and $E = \{e_1, e_2, \cdots, e_m\}$. Define $\mathcal{H} \in R^{m \times n}$ such that $e_i = \{v_k, v_l\}$ implies

$$\mathcal{H}(i,k) \ne 0, \mathcal{H}(i,l) \ne 0 \text{ and for } j \ne k \ne l\ \mathcal{H}(i,j) = 0.$$

Then it can be shown that H is isomorphic to $G(\mathcal{H})$.

The techniques used in the following result is very similar to the NP-completeness result in [22] where it is shown for $q = m$.

Theorem 4 *Given a graph $H = (V,E)$ and positive integers $p \le n$ and $q \le m$ there exists a mapping $f : R^{np} \to R^{m+n}$ such that for a row q-partition Π of $f'(x)$, $G_\Pi(f'(x))$ is isomorphic to $\overline{H}$.*

Proof. As outlined in the discussion following Lemma 1 we define matrix $\mathcal{H} \in R^{m\times n}$ such that the column intersection graph $G(\mathcal{H})$ is isomorphic to H. Let

$$A = \begin{pmatrix} \mathcal{H} & \mathbf{0} \\ D & \mathcal{C} \end{pmatrix} \tag{2}$$

where D is a $n \times n$ diagonal matrix with nonzero entries on the diagonal, $\mathcal{C}(i,:)$ has the pattern

$$\begin{array}{cccccccc} & & (i-1)(p-1)+1 & \dots & i(p-1) & & & \\ & & \downarrow & \dots & \downarrow & & & \\ (& \dots\ 0 & \times & \dots & \times & 0 & \dots &) \end{array}$$

for $i = 1,2,\dots,n$, and $\mathbf{0}$ is an $m \times n$ matrix of all zero entries. Figure 8 depicts the sparsity pattern of matrices $\mathcal{H}$ and $\mathcal{C}$ when $p = 4$. The nonzero entry in row i of matrix D together with 3 nonzero elements in the same row of $\mathcal{C}$ constitutes a clique on the corresponding vertices in $G(A)$.

$$\mathcal{H} = \begin{pmatrix} \times & \times & 0 & 0 & 0 \\ \times & 0 & \times & 0 & 0 \\ 0 & \times & 0 & \times & 0 \\ 0 & \times & 0 & 0 & \times \\ 0 & 0 & \times & \times & 0 \\ 0 & 0 & \times & 0 & \times \\ 0 & 0 & 0 & \times & \times \end{pmatrix} \mathcal{C} = \begin{pmatrix} \times & \times & \times & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \times & \times & \times & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \times & \times & \times & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \times & \times & \times & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \times & \times & \times \end{pmatrix}$$

Figure 8: Sparsity structure of matrices $\mathcal{H}$ and $\mathcal{C}$ used in Theorem 4

It is not difficult to construct a mapping $f : R^{np} \to R^{m+n}$ such that its Jacobian matrix at x has the same sparsity pattern as matrix A. Let Π be a row q-partition of A in which the last block $A(w_q,:)$ contains all of $\begin{pmatrix} D & \mathcal{C} \end{pmatrix}$. Then the graphs $\overline{H}$ and $G_\Pi(A)$ will have the same number of vertices which can be easily verified. To establish the edge correspondence we identify the 'clique", the "replication", and the "connector" vertices of $\overline{H}$ with the corresponding vertices in $G_\Pi(A)$. Clearly, the "clique" vertices U_i of $\overline{H}$ correspond to column segments $\mathcal{C}(:,(i-1)(p-1)+1 : i(p-1))$. With a row q-partition column i of A yields q column segments which correspond to the $q-1$ "replication" vertices V_i and the "connector" vertex v_{iq}. It is straightforward to identify the "enforcement" and "clique" edges of $\overline{H}$ with corresponding edges in $G_\Pi(A)$. To establish correspondence with "cross" edges of $\overline{H}$ consider column segments $A(w_{\tilde{l}}, j)$ and $A(w_{\tilde{l}}, k)$ $j \neq k$. If they are not structurally orthogonal then $\{v_i, v_j\}$ is an edge in H so that $\{v_{j\tilde{l}}, v_{k\tilde{l}}\}$ $\tilde{l} = 1,2,\cdots,q$ are the "cross" edges in $\overline{H}$. The column segments not structurally orthogonal also implies that in $G_\Pi(A)$ the vertex corresponding to $A(w_{\tilde{l}}, j)$ is connected by an edge to vertices corresponding to $A(w_{\tilde{l}}, k')$ $k' = 1,2,\dots,q$ which are precisely the "cross" edges of $\overline{H}$. □

Theorems 3 and 4 give the following result.

Theorem 5 *Given a matrix A finding a minimum coloring for $G_\Pi(A)$ is NP-hard.*

Graph $\overline{G} = (\overline{V}, \overline{E})$ illustrated in Figure 7 is isomorphic to the column segment graph $G_\Pi(A)$ where Π is a row 2-partition in which first three rows of A constitute the first row block and the remaining rows constitute the second block.

A *refinement* of row q-partition Π yields a row q'-partition Π' where the row blocks of Π are subdivided further so that $q \leq q'$.

Theorem 6 *For a row q'-partition Π' resulting from any refinement of row q-partition Π*

$$\chi(G_{\Pi'}(A)) \leq \chi(G_\Pi(A)).$$

Proof. Let Φ be a coloring of $G_\Pi(A)$. To establish the theorem it suffices to show that Φ induces a coloring of $G_{\Pi'}(A)$. Consider column segment $A(w_{\tilde{i}}, j)$ under Π and the corresponding vertex $v_{\tilde{i}j}$. We claim that setting $\Phi(v_{\tilde{i}'j}) = \Phi(v_{\tilde{i}j})$ where $\tilde{i}'$ are the block indices under Π' obtained from $A(w_{\tilde{i}}, j)$ for $\tilde{i} = 1,2,\ldots,q$ and $j = 1,2,\ldots,n$ yields a coloring for $G_{\Pi'}(A)$.

For vertices $v_{\tilde{i}'j}$ and $v_{\tilde{k}'l}$ corresponding to column segments $A(w_{\tilde{i}'}, j)$ and $A(w_{\tilde{k}'}, l)$, $\Phi(v_{\tilde{i}'j}) = \Phi(v_{\tilde{k}'l})$ if and only if $\Phi(v_{\tilde{i}j}) = \Phi(v_{\tilde{k}l})$ implying that Φ is a coloring for $G_{\Pi'}(A)$. This completes the proof. □

The *element isolation graph* associated with $A \in R^{m\times n}$ is denoted $G_I = (V,E)$ where

$$V = \{A(i,j) \neq 0 : 1 \leq i \leq m, 1 \leq j \leq n\}$$

and

$$E = \{\{A(i,j),\, A(p,q)\} \mid A(i,j) \text{ is not isolated from } A(p,q)\}.$$

The following result is a direct consequence of the definition of the two graphs.

Lemma 2 *Given a $m \times n$ matrix A and a row m-partition Π_m, $\chi(G_{\Pi_m}(A)) = \chi(G_I(A))$.*

let Π_m and Π_1 denote the row m-partition and row 1-partition respectively. The following inequalities follow from Theorem 6.

Corollary 1 $\chi(G_{\Pi_m}(A)) \leq \chi(G_{\Pi'}(A)) \leq \chi(G_\Pi(A)) \leq \chi(G_{\Pi_1}(A)) = \chi(G(A))$

The knowledge of "optimality" of derivative estimation methods is useful in obtaining complexity estimates. The classification scheme for the determination of sparse Hessian matrices given in [19] is similar to what we propose in this paper for Jacobian matrix determination. However, our characterization of direct methods are based on the computation of matrix-vector products in the language of vectors and matrices. With these methods no extra recovery cost (e.g., arithmetic operations) is incurred in determining the unknown elements from their FD or AD estimates. Ignoring symmetry, the methods outlined in [4, 5, 7, 11, 19, 23, 25] are all examples of direct methods.

Theorem 2 estimates a group of isolated elements with one matrix-vector product. Our next results characterize direct methods.

Theorem 7 *Direct determination A in p matrix-vector product is equivalent to a partition of A in p groups of isolated elements.*

Proof. By Theorem 1 direct determination implies that elements determined in each column of $B = AS$ are are isolated. If we have element isolation, then using theorem 2 we can construct seed matrix S with p columns which gives direct determination. □

Theorem 8 *The minimal number of matrix-vector multiply in any direct determination method is $p = \chi(G_I(A))$.*

Proof. Consider the element isolation graph $\chi(G_I(A))$ of matrix A. The nonzero elements (column segments) that are directly determined in the product

$$ASe_k = Be_k, k = 1,2,\ldots,q$$

are structurally orthogonal. Hence the vertices in $\chi(G_I(A))$ corresponding to those directly determined nonzero elements can be given color k. Since all the nonzero elements must be determined directly all vertices in $\chi(G_I(A))$ will receive a color. By Lemma 2 and corollary 1 $p = \chi(G_I(A))$ is minimal. □

4 Numerical Experiments

In this section we provide some coloring results from numerical testing of our row-partitioned Jacobian matrix determination. More detailed numerical testing can be found in [18]. The coloring algorithms backtrack-DSATUR [2] and Chaff [9] are used on matrices from Harwell-Boeing test collection [8].

The main idea of backtrack-DSATUR is to choose, at each search step, an uncolored vertex that defines a new subproblem. This is done for each feasible color for the vertex. The algorithm chooses a vertex with maximal saturation degree (i.e., a vertex which is connected to the largest number of colored vertices). Once all possibilities are explored at the current vertex the algorithm backtracks to the most recently colored vertex for new subproblems that have not been explored. Ties are broken randomly.

The propositional satisfiability problem is concerned with the determination of whether or not there is a truth assignment to the propositional variables appearing in a Boolean formula for which the formula evaluates to true. Van Gelder [9] proposes a "circuit-based" encoding scheme for representing coloring instances as Boolean formulas. The coloring is reconstructed from the solution computed by the satisfiability solver *Chaff* [20].

Table 1 summarizes the coloring results. The backtrack-DSATUR requires fewer colors on $G_\Pi(A)$ than on $G(A)$. However, not all the test problems considered here are solved by this algorithm. In the experiments we use the m-block row partition $\Pi_m \equiv \Pi$. On the other hand, the satisfiability solver returned with a coloring on all the test instances.

Table 1: Exact coloring test results for SMTAPE collection using coloring routines: backtrack-DSATUR and Chaff.

Matrix	$G_\Pi(A),\ q=1$			$G_\Pi(A),\ q=m$		
	Nodes	*Edges*	$\chi(G_\Pi(A))$	*Nodes*	*Edges*	$\chi(G_\Pi(A))$
ash219	85	219	4	438	2205	4
abb313	176	3206	10	1557	65390	(10)9
ash331	104	331	6	662	4185	4
will199	199	960	7	701	7065	7
ash608	188	608	6	1216	7844	4
ash958	292	958	6	1916	12506	(5)4

In Table 1 we report the following information. "Nodes" denotes the number of nodes, "Edges" denotes the number of edges, and $\chi(\cdot)$ denotes the chromatic number of $G(A)$ and $G_\Pi(A)$.

Out of 6 examples we have investigated, 4 of them have shown a reduction in chromatic number from $G(A)$ to $G_\Pi(A)$. The coloring routine based on backtrack-DSATUR does not terminate on examples "ash958" and "abb313'. Best coloring achieved in these case are indicated in $(\cdot)$. On these examples, size of the largest clique cannot be confirmed by the coloring routine . It is interesting to note that whenever the coloring routine terminated it terminated quickly. Coloring on $G_\Pi(A)$ shown are the results obtained in [9]. The problem "abb313" took 316 seconds to be solved and all the remaining instances were solved within 2 seconds.

5 Concluding Remarks

This paper presents a column segment partitioning technique for computing sparse Jacobian matrices efficiently. The partitioning problem has been modelled as a special graph coloring problem which is no easier to solve than the general graph coloring. On the other hand, with column segment partitioning a Jacobian matrix can be determined with fewer AD passes.

In view of the example attributed to Stanley Eisenstat it has long been an open question as to what constituted an optimal direct method. The results presented in this paper provide an uniform theoretical framework expressed in the language of linear algebra for all direct methods including the CPR-based methods.

The ideas presented in this paper lead to a number of new research directions that deserve further enquiry. The bi-directional analogue of column segment partition is expected to have lower computational cost. We are currently exploring these ideas.

Indirect methods can be further classified as *substitution* and *elimination* methods [17, 22] . Our substitution proposal in [16] leads to a one-directional substitution problem called "consecutive zeros" problem which in itself is a hard problem. It will be interesting to study the bi-directional substitution and its graph model.

There are no known direct or substitution methods that can be "optimally" solved in polynomial time. On the other hand, the elimination methods need only $\max_i \rho_i$ matrix-vector products and solution of $\rho_i \times \rho_i$ system of linear equations. Consequently, investigation of the complexity hierarchy of the Jacobian matrix determination problems constitutes an open topic for further study. For example, it would be useful if we knew the point at which the matrix determination problem becomes computationally solvable from being an intractable [21] problem.

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References

[1] B. M. Averick, J. J. Moré, C. H. Bischof, A. Carle, and A. Griewank. Computing large sparse Jacobian matrices using automatic differentiation. *SIAM J. Sci. Comput.*, 15(2):285–294, 1994.

[2] D. Brélaz. New methods to color the vertices of a graph. *Commun. ACM*, 22(4):251–256, Apr. 1979.

[3] T. F. Coleman and J.-Y. Cai. The cyclic coloring problem and estimation of sparse Hessian matrices. *SIAM J. Alg. Disc. Meth.*, 7(2):221–235, 1986.

[4] T. F. Coleman and J. J. Moré. Estimation of sparse Jacobian matrices and graph coloring problems. *SIAM J. Numer. Anal.*, 20(1):187–209, 1983.

[5] T. F. Coleman and J. J. Moré. Estimation of sparse Hessian matrices and graph coloring problems. *Math. Programming*, 28:243–270, 1984.

[6] T. F. Coleman and A. Verma. The efficient computation of sparse Jacobian matrices using automatic differentiation. *SIAM J. Sci. Comput.*, 19(4):1210–1233, 1998.

[7] A. R. Curtis, M. J. D. Powell, and J. K. Reid. On the estimation of sparse Jacobian matrices. *J. Inst. Math. Appl.*, 13:117–119, 1974.

[8] I. S. Duff, R. G. Grimes, and J. G. Lewis. Users' guide for the Harwell-Boeing sparse matrix collection (Release I). Technical Report tr/pa/92/86, CERFACS, 1992.

[9] A. V. Gelder. Another look at graph coloring via propositional satisfiability, 2002. Computational Symposium on Graph Coloring and Generalizations (COLOR02), Ithaca, NY, 7-8 September 2002.

[10] G. H. Golub and C. F. Van Loan. *Matrix Computations*. Johns Hopkins University Press, 3rd edition, 1996.

[11] A. Griewank. Some bounds on the complexity of gradients, Jacobians, and Hessians. In P. M. Pardalos, editor, *Complexity in Nonlinear Optimization*, pages 128–161. World Scientific Publishers, 1993.

[12] A. Griewank. *Evaluating Derivatives: Principles and Techniques of Algorithmic Differentiation*. Number 19 in Frontiers in Appl. Math. SIAM, Philadelphia, Penn., 2000.

[13] A. Griewank and C. Mitev. Detecting Jacobian sparsity patterns by Bayesian probing. *Math. Prog.*, 93(1):1–25, 2002.

[14] A. S. Hossain. *On the Computation of Sparse Jacobian Matrices and Newton Steps*. PhD thesis, Department of Informatics, University of Bergen, 1998. Technical Report 146.

[15] A. S. Hossain and T. Steihaug. Computing a sparse Jacobian matrix by rows and columns. *Optimization Methods and Software*, 10:33–48, 1998.

[16] S. Hossain and T. Steihaug. Reducing the number of AD passes for computing a sparse Jacobian matrix. In G. Corliss, C. Faure, A. Griewank, L. Hascoët, and U. Naumann, editors, *Automatic Differentiation: From Simulation to Optimization*, Computer and Information Science, chapter 31, pages 263–270. Springer, New York, 2001.

[17] S. Hossain and T. Steihaug. Sparsity Issues in the Computation of Jacobian Matrices. In T. Mora, editor, *Proceedings of the International Symposium on Symbolic and Algebraic Computing (ISSAC)*, pages 123–130, New York, 2002. ACM.

[18] S. Hossain and T. Steihaug. Graph coloring in the estimation of mathematical derivatives, 2003. In Preparation.

[19] S. T. McCormick. Optimal approximation of sparse Hessians and its equivalence to a graph coloring problem. *Math. Programming*, 26:153–171, 1983.

[20] M. W. Moskewicz, C. F. Madigan, Y. Zhao, L. Zhang, and S. Malik. Chaff: Engineering an Efficient SAT Solver. In *Proceedings of the 38th Design Automation Conference (DAC'01)*, 2001.

[21] M.R.Garey and D.S.Johnson. *Computers and Intractibility*. W.H.Freeman, San Francisco, 1979.

[22] G. N. Newsam and J. D. Ramsdell. Estimation of sparse Jacobian matrices. *SIAM J. Alg. Disc. Meth.*, 4(3):404–417, 1983.

[23] M. J. D. Powell and Ph. L. Toint. On the estimation of sparse Hessian matrices. *SIAM J. Numer. Anal.*, 16:1060–1074, 1979.

[24] L. B. Rall and T. W. Reps. Algorithmic differencing. In A. Facius and U. Kulisch, editors, *Perspectives on Enclosure Methods*. Springer-Verlag, Vienna, 2001.

[25] T. Steihaug and A. S. Hossain. Graph coloring and the estimation of sparse Jacobian matrices with segmented columns. Technical Report 72, Department of Informatics, University of Bergen, 1997.