Optimal Bi-directional Determination of Sparse Jacobian Matrices

Mini Goyal *and* **Shahadat Hossain**
Department of Mathematics and Computer Science
University of Lethbridge, Canada

Second International Workshop on Combinatorial Scientific Computing (CSC05), Toulouse, France

Outline

- The Problem
- Bi-directional Determination
- Optimal Bi-directional Determination
- Integer Linear Programming Model
- Complexity
- Preliminary Experimental Results

Introduction

Let

$$F = \begin{pmatrix} f_1 & f_2 & \dots & f_m \end{pmatrix}^T$$

be a mapping $F : \Re^n \rightarrow \Re^m$. Assume that F is continuously differentiable in the domain of interest and let $F'(x)$ denote the Jacobian matrix of F at x.

Given vectors $s \in \Re^n$ and $w \in \Re^m$, we can compute

$b = F'(x)s$ via one forward pass of automatic differentiation (AD).

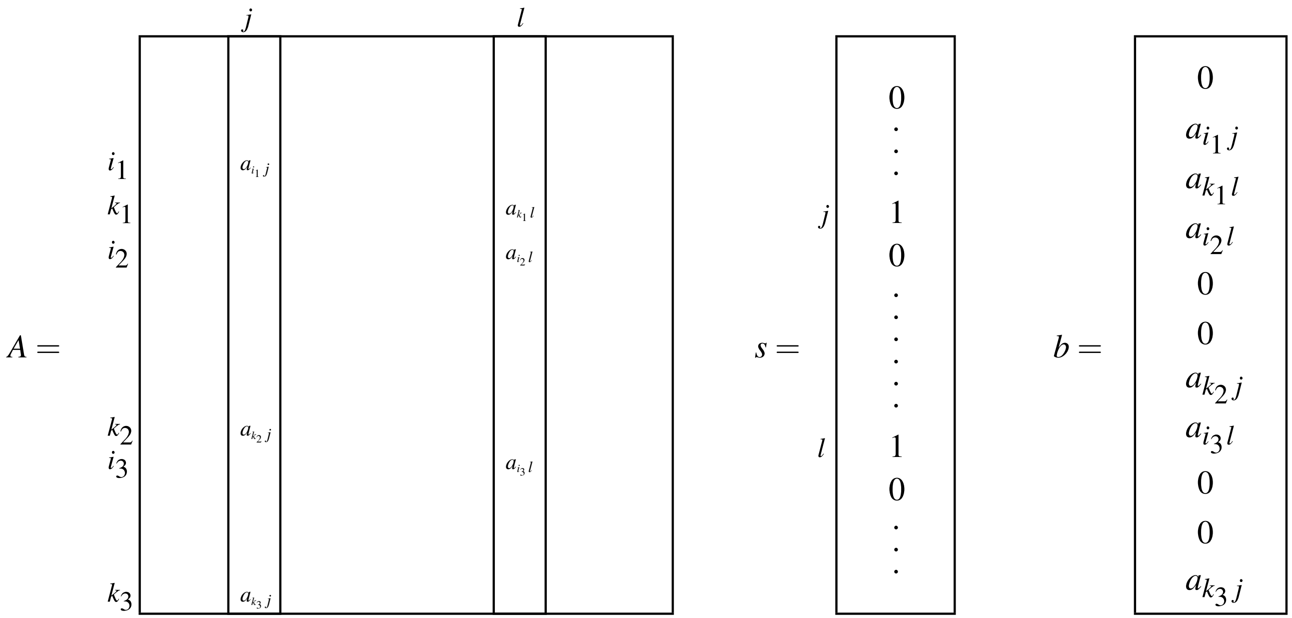
$c^T = w^T F'(x)$ via one reverse pass of AD.

Assumptions

- Jacobian matrix is sparse
- The sparsity pattern of the Jacobian matrix is known a priori and independent of the actual values of x.

Exploiting Sparsity - Curtis, Powell and Reid (1974)

Let $F'(x) \equiv A$,



Columns j and l are *structurally orthogonal* i.e. there does not exist a row index i for which both $a_{ij} \neq 0$ and $a_{il} \neq 0$. Determine the unknowns in columns j and l of matrix A from the product $As = b$ (obtained via one forward pass).

Examples

Partition the columns of A into structurally orthogonal groups of columns,

$$A = \begin{bmatrix} \times & & & & \\ \times & \times & & & \\ \times & & \times & & \\ \times & & & \times & \\ \times & & & & \times \end{bmatrix}, S = \begin{bmatrix} 1 & 0 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \end{bmatrix}$$

Partition the columns of A^T into structurally orthogonal groups of columns,

$$A = \begin{bmatrix} \times & \times & \times & \times & \times \\ & \times & & & \\ & & \times & & \\ & & & \times & \\ & & & & \times \end{bmatrix}, W^T = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 1 & 1 & 1 \end{bmatrix}$$

The Arrowhead Example

$$A = \begin{bmatrix} \times & \times & \times & \times & \times \\ \times & \times & & & \\ \times & & \times & & \\ \times & & & \times & \\ \times & & & & \times \end{bmatrix}$$

We need 5 matrix-vector multiplications either by forward or by reverse AD.

Bi-directional Determination of Sparse Jacobian Matrices

Obtain vectors $s_1, s_2, ..., s_{p_c}$ and $w_1, w_2, ..., w_{p_r}$ such that matrix-vector products

$$b_i = As_i, i = 1, 2, ..., p_c \text{ or } B = AS$$

and the vector-matrix product

$$c_j^T = w_j^T A, j = 1, 2, ..., p_r \text{ or } C^T = W^T A$$

determine the $m \times n$ matrix A uniquely.

Computing the Arrowhead Matrix

$$A = \begin{bmatrix} \times & \times & \times & \times & \times \\ \times & \times & & & \\ \times & & \times & & \\ \times & & & \times & \\ \times & & & & \times \end{bmatrix}, S = \begin{bmatrix} 1 & 0 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \end{bmatrix}, W^T = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 \end{bmatrix}$$

Two forward passes and one reverse pass are sufficient to determine A.

If the seed matrices S and W are such that the nonzero entries of A can be read-off from the products $AS = B$ and $W^T A = C^T$ than we have *direct determination*

Efficient Bi-directional Determination of Sparse Jacobian Matrices

Obtain vectors $s_1, s_2, ..., s_{p_c}$ and $w_1, w_2, ..., w_{p_r}$ such that matrix-vector products $B = AS$ and the vector-matrix product $C^T = W^T A$ determine the $m \times n$ matrix A uniquely and $p_r + p_c$ is minimized.

A *p-coloring* of graph $G = (V, E)$ is a function $\phi : V \rightarrow \{1, ..., p\}$ such that $\phi(v_i) \neq \phi(v_j)$ if $\{v_i, v_j\} \in E$.

Let $A \in \Re^{m \times n}$. Define $G_b(A) = (U \cup V, E)$ where U corresponds the set of column vertices and V corresponds the set of row vertices and for $u_j \in U$ and $v_i \in V$, $\{v_i, u_j\} \in E$ if $a_{ij} \neq 0$.

A Graph Coloring Formulation

Bi-directional p-coloring: A mapping $\phi : \{U \cup V\} \rightarrow \{1, 2, ..., p\}$ is called a *bi-directional p-coloring* of bipartite graph $G_b = (U \cup V, E)$ if the following conditions apply:

1. ϕ is p-coloring.
2. The set of colors used on vertices in U and V are disjoint, i.e. for $u_j \in U$ and $v_i \in V$ $\phi(u_j) \neq \phi(v_i)$.
3. Every path of length 3 in $G_b(A)$ uses at least 3 different colors.

The *bi-chromatic number*, χ_b, of $G_b(A)$ is the smallest p for which $G_b(A)$ has a bi-directional p-coloring.

Example

Given a sparse matrix A, obtain a bi-directional p-coloring of $G_b(A)$ such that $p = p_r + p_c$ is minimized.

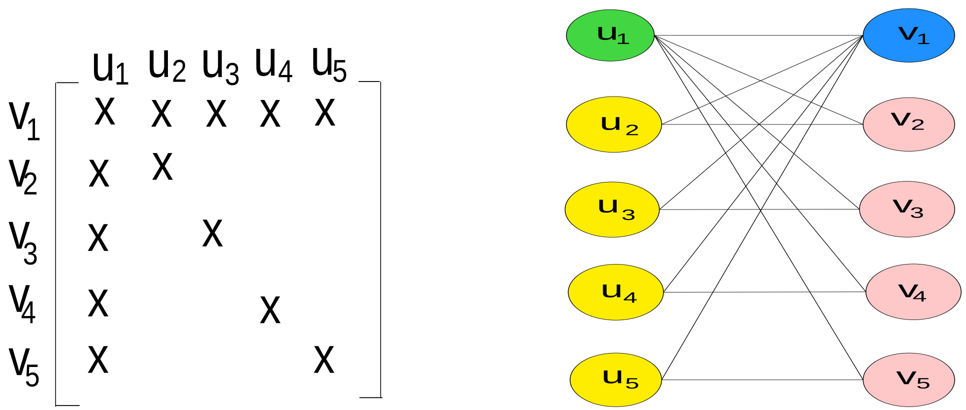


Figure 1: Optimal bi-directional p-coloring of the arrowhead example

Bi-directional Determination of Sparse Jacobian Matrices

- Bi-coloring is NP-hard.
- Heuristic methods
  - Hossain and Steihaug [1998], Coleman and Verma [1998], Gebremedhin, Manne and Pothen [2004]
- Exact methods
  - Let
    ρ_{max} : maximum number of nonzeros in any row,
    κ_{max} : maximum number of nonzeros in any column.
    A lower bound on the number of matrix-vector (or vector-matrix) products in one dimensional determination of A is $\min(\kappa_{max}, \rho_{max})$.
  - Find a good lower bound on the number of matrix-vector (vector-matrix) products in bi-directional determination.

Optimal Bidirectional Determination - An Integer Linear Programming Formulation (ILP)

Variables used in the ILP formulation of bi-directional p-coloring follows.

- 0-1 variable w_j denotes whether $(w_j = 1)$ or not $(w_j = 0)$ color j, $1 \leq j \leq p_U$ has been assigned to some vertex $u \in U$.
- 0-1 variable w_j denotes whether $(w_j = 1)$ or not $(w_j = 0)$ color j, $p_U + 1 \leq j \leq p_U + p_V$ has been assigned to some vertex $v \in V$.
- 0-1 variable $x_{i,j}$ denotes whether $(x_{i,j} = 1)$ or not $(x_{i,j} = 0)$ vertex i, $1 \leq i \leq n$ has been assigned color $j, 1 \leq j \leq p_U$.
- 0-1 variable $x_{i,j}$ denotes whether $(x_{i,j} = 1)$ or not $(x_{i,j} = 0)$ vertex i, $n+1 \leq i \leq m+n$ has been assigned color $j, p_U + 1 \leq j \leq p_U + p_V$.

An ILP Model for Optimal Bi-directional Determination

$$\text{minimize} \quad \sum_{j=1}^{p_U+p_V} w_j \tag{1}$$

$$\sum_{j=1}^{p_U} x_{i,j} = 1, \text{ for } i \in U \tag{2}$$

$$\sum_{j=p_U+1}^{p_U+p_V} x_{i,j} = 1, \text{ for } i \in V \tag{3}$$

$$x_{i,j} + x_{l,j'} + x_{i',j} + x_{l',j'} \leq (w_j + w_{j'} + 1) \tag{4}$$

(for every path $v_i - u_l - v_{i'} - u_{l'}$ of length 3)

$$
\begin{aligned}
w_j &\leq \sum_{i \in U} x_{i,j} && \text{for } j = 1, \ldots, p_U && (5)\\
w_j &\leq \sum_{i \in V} x_{i,j} && \text{for } j = p_U + 1, \ldots, p_U + p_V && (6)\\
\sum_{i \in U} x_{i,j} &\leq n w_j && \text{for } j = 1, \ldots, p_U && (7)\\
\sum_{i \in V} x_{i,j} &\leq m w_j && \text{for } j = p_U + 1, \ldots, p_U + p_V && (8)\\
w_{j+1} &\leq w_j && \text{for } j = 1, \ldots, p_U - 1 && (9)\\
w_{j+1} &\leq w_j && \text{for } j = p_U + 1, \ldots, p_U + p_V - 1 && (10)\\
w_j &\in \{0, 1\}, && \text{for } 1 \leq j \leq p_U + p_V && (11)\\
x_{i,j} &\in \{0, 1\}, && \text{for } i \in U \cup V, 1 \leq j \leq p_U + p_V && (12)
\end{aligned}
$$

Null Color Elimination

Null Color: Consider a p-coloring problem with colors $1 \ldots p$ for a graph $G(V,E)$. Assuming that G can be optimally colored with $p-1$ colors, consider a solution where color i is not used: $(n_1, n_2, \ldots, n_{i-1}, n_i(=0), n_{i+1}, \ldots, n_p)$, where n_i denotes the number of vertices colored with color i. The color i for which $n_i = 0$ is known as the *null color*.

Example, the assignment (1,0,2,3) is equivalent to (1,3,2,0), (0,1,2,3), (1,2,0,3).

The constraints (9) and (10) ensures that in a feasible solution, the null colors will not be present.

Complexity

Number of variables:

$$(n+1)p_U + (m+1)p_V$$

Number of 3-paths:

$$\text{num3paths} = \sum_{i=1}^{m} (\rho_i - 1) \left[\sum_{j:a_{ij} \neq 0} (\kappa_j - 1) \right]$$

Number of constraints:

$$(\text{num3paths} * p_U * p_V) + (m+n) + 2(p_U + p_V) + (p_U + p_V - 2)$$

Experimental Results

Matrix	Statistics		One-directional*		Bi-directional					
	ρ_{max}	κ_{max}	*DSM*	*Exact*	Direct Cover			Exact		
					RG	CG	TG	RG	CG	TG
ibm32	8	7	8	8	0(1)	8(0)	8(1)	1(1)	6(0)	7(1)
ash219	2	9	4	4	0(1)	5(0)	5(1)	0(1)	4(0)	4(1)
ash331	2	12	6	6	0(1)	6(0)	6(1)	0(1)	6(0)	6(1)
ash608	2	12	6	6	0(1)	7(0)	7(1)	0(1)	6(0)	6(1)
impcol-a	8	5	8	8	6(0)	0(1)	6(1)	6(0)	0(1)	6(1)
impcol-c	8	8	8	8	1(1)	4(0)	5(1)	1(1)	3(0)	4(1)

* column partitioning
RG : total number of row groups
CG : total number of column groups
TG : RG + CG
ρ_{max}: maximum number of nonzeros in any row
κ_{max}: maximum number of nonzeros in any column

Conclusion

- Formulation of optimal bi-directional determination.
- Large problems are difficult solve:
  - Memory constraints
  - Symmetry
- More elaborate numerical tests are needed.