On Efficient Storage of Sparse Matrices

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Outline

- Introduction and background
- Sparse matrix storage schemes: Compressed Row, Jagged Diagonal
- Performance Issues
- Concluding remarks and future directions

Challenges in Large-scale Numerical Computing

High Performance Computing Challenges

- Climate Models e.g. Community Climate System Model
- High-temperature Superconductor model calculation

Supercomputer Systems

- Superscalar e.g., SGI Altix, IBM Power and Power4
- Parallel vector supercomputers e.g., Earth Simulator, Cray X1

Widening gap between sustained and peak performance!!

Krylov Subspace Methods

Solve for $x \in R^n$

$$Ax = b$$

where $A \in R^{n \times n}$ is large and sparse.

Main computational tasks in a Krylov subspace method (e.g. Conjugate Gradient)

1. **sparse matrix times vector (MVP):** $w = Av$
2. dot product: $c = x^T y$
3. vector update (saxpy): $y = y + \alpha x, \alpha \in R$
4. preconditioning operation

Exploiting Sparsity

Target architecture: Vector supercomputers e.g. The Earth Simulator, CRAY X1

1. **Regular structure:** e.g., banded: Store the diagonals; can be implemented efficiently with excellent performance (flops).
2. **General structure:** Either adapt the diagonal storage scheme or reorder the matrix to obtain a diagonal structure.

Observation:

On vector machines long vectors can improve the performance of MVP calculation significantly

Compressed Row Storage (CRS)

$$\begin{pmatrix} a_{00} & a_{01} & a_{02} & a_{03} & a_{04} \\ a_{10} & a_{11} & 0 & 0 & 0 \\ a_{20} & 0 & a_{22} & 0 & 0 \\ a_{30} & 0 & 0 & a_{33} & 0 \\ a_{40} & 0 & 0 & 0 & a_{44} \end{pmatrix}$$

(a)

$$\begin{pmatrix} a_{00} & a_{01} & a_{02} & a_{03} & a_{04} \\ a_{10} & a_{11} & 0 & 0 & 0 \\ a_{20} & a_{22} & 0 & 0 & 0 \\ a_{30} & a_{33} & 0 & 0 & 0 \\ a_{40} & a_{44} & 0 & 0 & 0 \end{pmatrix}$$

(b)

value	a_{00}	a_{01}	a_{02}	a_{03}	a_{04}	a_{10}	a_{11}	a_{20}	a_{22}	a_{30}	a_{33}	a_{40}	a_{44}
colind	0	1	2	3	4	0	1	0	2	0	3	0	4
rowptr	0	5	7	9	11	13							

(c)

Figure 1: (a) Sparsity pattern of the 6×6 "arrow-head" matrix. (b) The "arrow-head" matrix after CRS compression. (c) Compressed Row Storage (CRS) data structure for the "arrow-head" matrix.

MVP in CRS

```
for (int i = 0; i < m ; i++) {
   upper = rowptr[i+1]; // fetch the upper index
// loop over row i
  for (int j = rowptr[i]; j < upper; j++) {
       b[i] = b[i] + value[j] * v[colind[j]];
   }
}
```

Figure 2: Matrix-vector multiplication in CRS scheme

Most rows contain only few nonzero entries (ρ_i) compared with the matrix dimension – $\rho_i \ll n$ implies shorter vector in the inner for-loop.

Jagged Diagonal Storage(JDS)

$$\begin{pmatrix} a_{00} & 0 & 0 & a_{03} & 0 \\ a_{10} & a_{11} & 0 & 0 & 0 \\ a_{20} & 0 & a_{22} & 0 & 0 \\ a_{30} & a_{31} & a_{32} & a_{33} & a_{34} \\ a_{40} & 0 & 0 & 0 & a_{44} \end{pmatrix} \qquad \begin{pmatrix} a_{00} & a_{03} & 0 & 0 & 0 \\ a_{10} & a_{11} & 0 & 0 & 0 \\ a_{20} & a_{22} & 0 & 0 & 0 \\ a_{30} & a_{31} & a_{32} & a_{33} & a_{34} \\ a_{40} & a_{44} & 0 & 0 & 0 \end{pmatrix}$$

(a) (b)

value	a_{30}	a_{10}	a_{20}	a_{00}	a_{40}	a_{31}	a_{11}	a_{22}	a_{03}	a_{44}	a_{32}	a_{33}	a_{34}
colind	0	0	0	0	0	1	1	2	3	4	2	3	4
jdptr	0	5	10	11	12	13							
perm	3	1	2	0	4								

(c)

Figure 3: (a) Sparsity pattern of the 6 × 6 row permuted “arrow-head” matrix. (b) The row-permuted “arrow-head” matrix after JDS compression. (c) Jagged diagonal storage (JDS) data structure for the “arrow-head” matrix.

MVP in JDS

```
for (int j = 0; j < rho_max ; j++) {
 upper = jdptr[j+1]; // fetch the upper index
 // loop over jagged diagonal j
 for (int i = jdptr[j]; i < upper; i++) {
  col = colind[i];
  b[i] = b[i] + value[i] * v[col];
  }
 }
```

Figure 4: Matrix-vector multiplication in JDS scheme

- **Needs an *m*-vector to store the original row order.**
- **Extra work to restore the correct order in the result .**

Transposed Jagged Diagonal Storage (TJDS)

$$\begin{pmatrix} a_{00} & a_{01} & a_{02} & a_{03} & a_{04} \\ a_{10} & a_{11} & a_{22} & a_{33} & a_{44} \\ a_{20} & 0 & 0 & 0 & 0 \\ a_{30} & 0 & 0 & 0 & 0 \\ a_{40} & 0 & 0 & 0 & 0 \end{pmatrix}$$

(a)

value	a_{00}	a_{01}	a_{02}	a_{03}	a_{04}	a_{10}	a_{11}	a_{22}	a_{33}	a_{44}	a_{20}	a_{30}	a_{40}
rowind	0	0	0	0	0	1	1	2	3	4	2	3	4
tjdptr	0	5	10	11	12	13							

(b)

Figure 5: (a) The “arrow-head” matrix after the columns have been compressed. (b) Transposed jagged diagonal storage (TJDS) data structure for the “arrow-head” matrix.

MVP in TJDS

```
for (int i = 0; i < col-max ; i++) {
 upper = tjdptr[i+1]; // fetch the upper index
 ind = 0; //index to iterate over v’s elements
 // loop over jagged diagonal j
 for (int j = tjdptr[i]; j < upper; j++) {
  row = rowind[j];
  b[row] = b[row] + value[j] * v[ind];
  ind++;
  }
 }
```

Figure 6: Matrix-vector multiplication in TJDS scheme

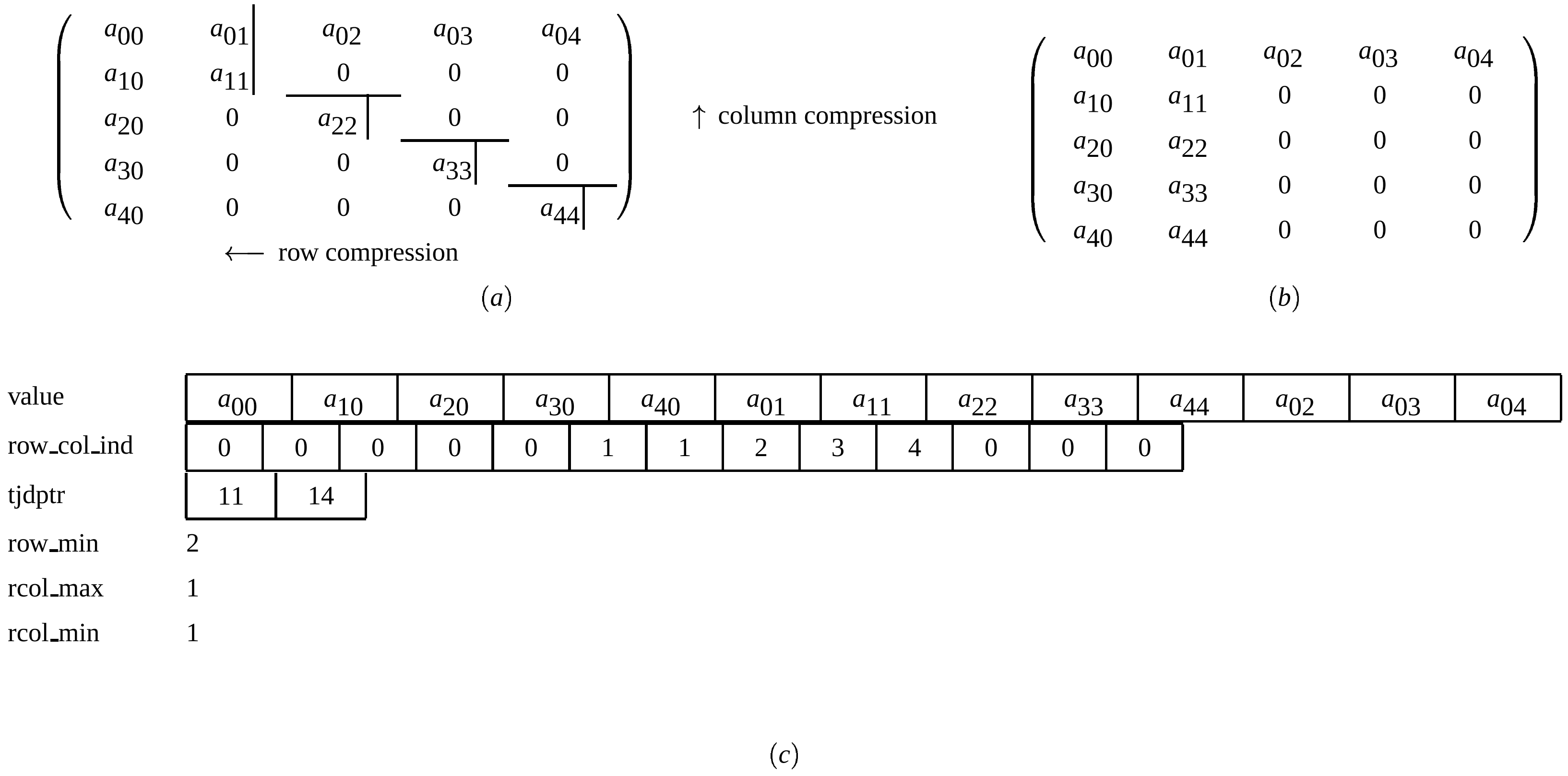
No need for a permutation vector in TJDS scheme

Bi Jagged Diagonal Storage (Bi-JDS) – New Sparse Matrix Storage Scheme

1. JDS and TJDS are suitable for MVP calculation on vector machines.
2. The number of nonzero entries in each row may vary considerably for general sparse matrices e.g. the arrow-head matrix under JDS or TJDS is stored as many short jagged diagonals.

The **Bi-JDS scheme** partitions a sparse matrix into two segments and compresses the matrix in both column and row directions.

Bi-JDS Data Structure



$$\begin{pmatrix} a_{00} & a_{01} & a_{02} & a_{03} & a_{04} \\ a_{10} & a_{11} & 0 & 0 & 0 \\ a_{20} & 0 & a_{22} & 0 & 0 \\ a_{30} & 0 & 0 & a_{33} & 0 \\ a_{40} & 0 & 0 & 0 & a_{44} \end{pmatrix}$$

↑ column compression

⟵ row compression

(a)

$$\begin{pmatrix} a_{00} & a_{01} & a_{02} & a_{03} & a_{04} \\ a_{10} & a_{11} & 0 & 0 & 0 \\ a_{20} & a_{22} & 0 & 0 & 0 \\ a_{30} & a_{33} & 0 & 0 & 0 \\ a_{40} & a_{44} & 0 & 0 & 0 \end{pmatrix}$$

(b)

value	a_{00}	a_{10}	a_{20}	a_{30}	a_{40}	a_{01}	a_{11}	a_{22}	a_{33}	a_{44}	a_{02}	a_{03}	a_{04}
row_col_ind	0	0	0	0	0	1	1	2	3	4	0	0	0
tjdptr	11	14											

row_min 2

rcol_max 1

rcol_min 1

(c)

Figure 7: (a) Bi-JDS partition of the 6 × 6 “arrow-head” matrix. (b) The “arrow-head” matrix after column and row compression. (c) Bi-jagged diagonal (Bi-JDS) data structure for the “arrow-head” matrix

MVP with Bi-JDS

```
//The jagged diagonals are full-length; so jptr array is not needed.
for (int j = 0; j < rho_min ; j++) {
 ind = 0;
 for (i = m*j; i < m*(j+1); i++) {
    col = row_colind[i];
    b[ind] = b[ind] + value[i]*v[col];
    ind++;
    }
 }
 // Now update the product with the contribution from transposed jagged diagonals.
 k = 0;
 for (int i = 0; i < rcol_max; i++){
    ind=minrow+1;
    for (int indtjd=tjdptr[i]; indtjd < tjdptrr[i+1]; indtjd++){
        row = row_colind[k];
        b[row] = b[row] + val[indtjd]*v[ind];
        ind=ind+1;
        k=k+1;
    }
 }
```

Storage Requirements

$$\begin{array}{ll} \text{memory}_{\text{JDS}}: & 2nnz(A)+\rho_{max}+1+m \\ \text{memory}_{\text{TJDS}}: & 2nnz(A)+\kappa_{max}+1 \\ \text{memory}_{\text{BiJDS}}: & 2nnz(A)+n_{\text{tjd}}+1 \end{array}$$

where

$n_{\text{tjd}} = (\kappa_{max} - \kappa_{min})$

ρ_{max} = maximum number of nonzero entries in any row of A,

κ_{max} = maximum number of nonzero entries in any column of A, and

κ_{min} = minimum number of nonzero entries in any column of A.

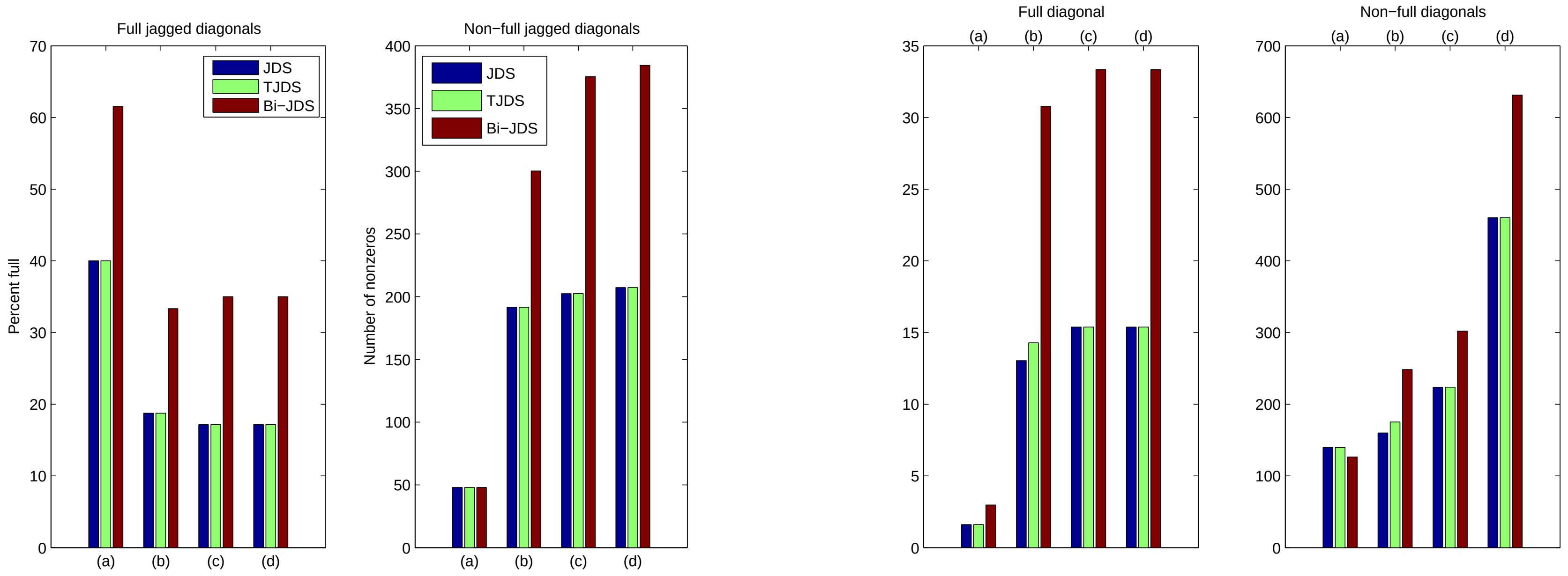
Computational Experiments

Table 1: The Harwell-Boeing Test Problems Info.

Nr.	Name	m	n	nnz	ρ_{max}	ρ_{min}	κ_{max}	κ_{min}
a.	can144	144	144	720	15	6	15	6
b.	can838	838	838	5424	32	6	32	6
c.	can1054	1054	1054	6625	35	6	35	6
d.	can1072	1072	1072	6758	35	6	35	6
e.	add20	2395	2395	17319	124	2	124	2
f.	bfw398a	398	398	3678	23	3	21	3
g.	bfw398b	398	398	2910	13	2	13	2
h.	bfw782a	782	782	5982	13	2	13	2

Computational Experiments

Figure 8: Properties of the jagged diagonals in sparse storage schemes.

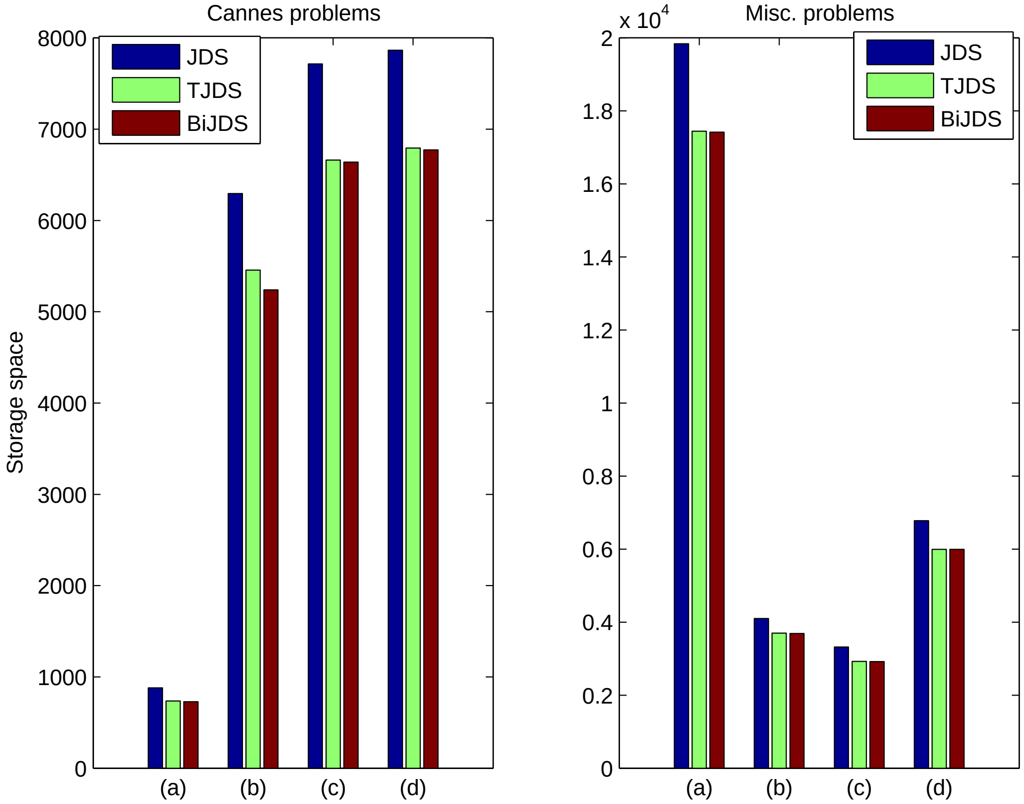


(i) Cannes problems

(ii) Misc. problems

Computational Experiments

Figure 9: Estimate of storage requirements in sparse storage schemes.



Concluding Remarks

1. The BiJDS scheme produces more full-length jagged diagonals as well as longer non-full jagged diagonals compared with JDS or TJDS scheme.
2. The BiJDS scheme is also space efficient and does not need to store the permutation order of the rows of the matrix.
3. Can be combined with blocking strategy to reduce indirect memory access.
4. Extensive numerical tests on practical problems.