DATA STRUCTURES

Data Structures. General Observations

➤ The use of a proper data structures is critical to achieving good performance.

✍ Generate a symmetric sparse matrix A in matlab and time the operations of accessing (only) all entries by columns and then by rows. Observations?

➤ Many data structures; sometimes unnecessary variants.

➤ These variants are more useful in the context of iterative methods

➤ Basic linear algebra kernels (e.g., matrix-vector products) depend on data structures.

Some Common Data Structures (from SPARSKIT)

DNS	Dense	**ELL**	Ellpack-Itpack
BND	Linpack Banded	**DIA**	Diagonal
COO	Coordinate	**BSR**	Block Sparse Row
CSR	Compressed Sparse Row	**SSK**	Symmetric Skyline
CSC	Compressed Sparse Column	**NSK**	Nonsymmetric Skyline
MSR	Modified CSR	**JAD**	Jagged Diagonal

- Most common (and important): CSR (/ CSC), COO

The coordinate format (COO)

$$A = \begin{pmatrix} \mathbf{1.} & \mathbf{0.} & \mathbf{0.} & \mathbf{2.} & \mathbf{0.} \\ \mathbf{3.} & \mathbf{4.} & \mathbf{0.} & \mathbf{5.} & \mathbf{0.} \\ \mathbf{6.} & \mathbf{0.} & \mathbf{7.} & \mathbf{8.} & \mathbf{9.} \\ \mathbf{0.} & \mathbf{0.} & \mathbf{10.} & \mathbf{11.} & \mathbf{0.} \\ \mathbf{0.} & \mathbf{0.} & \mathbf{0.} & \mathbf{0.} & \mathbf{12.} \end{pmatrix}$$

AA	JR	JC
12.	5	5
9.	3	5
7.	3	3
5.	2	4
1.	1	1
2.	1	4
11.	4	4
3.	2	1
6.	3	1
4.	2	2
8.	3	4
10.	4	3

- Simplest data structure -
- Often used as 'entry' format in packages
- Variant used in matlab and matrix market
- Also known as 'triplet format'

Compressed Sparse Row (CSR) format

$$A = \begin{pmatrix} 12. & 0. & 0. & 11. & 0. \\ 10. & 9. & 0. & 8. & 0. \\ 7. & 0. & 6. & 5. & 4. \\ 0. & 0. & 3. & 2. & 0. \\ 0. & 0. & 0. & 0. & 1. \end{pmatrix}$$

AA	JA
12	1
11	4
10	1
9	2
8	4
7	1
6	3
5	4
4	5
3	3
2	4
1	5

IA
1
3
6
10
12
13

- IA(j) points to beginning or row j in arrays AA, JA
- Related formats: Compressed Sparse Column format, Modified Sparse Row format (MSR).
- Used predominantly in Fortran & portable codes [e.g. Metis] – what about C?

CSR (CSC) format - C-style

* CSR: Collection of pointers of rows & array of row lengths

```
typedef struct SpaFmt {
/*--------------------------------------------
| C-style CSR format - used internally
| for all matrices in CSR/CSC format
|---------------------------------------------*/
  int n;          /* size of matrix           */
  int *nzcount;  /* length of each row        */
  int **ja;       /* to store column indices  */
  double **ma;    /* to store nonzero entries */
} SparMat;
```

`aa[i][*]` == entries of i-th row (col.);

`ja[i][*]` == col. (row) indices,

`nzcount[i]` == number of nonzero elmts in row (col.) `i`

Data structure used in Csparse [T. Davis' code, U. Florida]

```
typedef struct cs_sparse
{/* matrix in compressed-column or triplet form */
 int nzmax ; /* maximum number of entries */
 int m ;     /* number of rows */
 int n ;     /* number of columns */
 int *p ;    /* column pointers (size n+1) or
                col indices (size nzmax) */
 int *i ;    /* row indices, size nzmax */
 double *x ; /* numerical values, size nzmax */
 int nz ;    /* # of entries in triplet matrix,
                -1 for compressed-col */
} cs ;
```

- Can be used for CSR, CSC, and COO (triplet) storage
- Easy to use from Fortran

The Diagonal (DIA) format

$$\boldsymbol{A} = \begin{pmatrix} \mathbf{1.} & \mathbf{0.} & \mathbf{2.} & \mathbf{0.} & \mathbf{0.} \\ \mathbf{3.} & \mathbf{4.} & \mathbf{0.} & \mathbf{5.} & \mathbf{0.} \\ \mathbf{0.} & \mathbf{6.} & \mathbf{7.} & \mathbf{0.} & \mathbf{8.} \\ \mathbf{0.} & \mathbf{0.} & \mathbf{9.} & \mathbf{10.} & \mathbf{0.} \\ \mathbf{0.} & \mathbf{0.} & \mathbf{0.} & \mathbf{11.} & \mathbf{12.} \end{pmatrix}$$

$$\text{DA} = \boxed{\begin{array}{ccc} * & 1. & 2. \\ 3. & 4. & 5. \\ 6. & 7. & 8. \\ 9. & 10. & * \\ 11 & 12. & * \end{array}} \qquad \text{IOFF} = \boxed{\text{-1} \quad 0 \quad 2}$$

The Ellpack-Itpack format

$$\boldsymbol{A} = \begin{pmatrix} \mathbf{1.} & \mathbf{0.} & \mathbf{2.} & \mathbf{0.} & \mathbf{0.} \\ \mathbf{3.} & \mathbf{4.} & \mathbf{0.} & \mathbf{5.} & \mathbf{0.} \\ \mathbf{0.} & \mathbf{6.} & \mathbf{7.} & \mathbf{0.} & \mathbf{8.} \\ \mathbf{0.} & \mathbf{0.} & \mathbf{9.} & \mathbf{10.} & \mathbf{0.} \\ \mathbf{0.} & \mathbf{0.} & \mathbf{0.} & \mathbf{11.} & \mathbf{12.} \end{pmatrix}$$

$$\mathsf{AC} = \boxed{\begin{array}{ccc} 1. & 2. & 0. \\ 3. & 4. & 5. \\ 6. & 7. & 8. \\ 9. & 10. & 0. \\ 11 & 12. & 0. \end{array}} \qquad \mathsf{JC} = \boxed{\begin{array}{ccc} 1 & 3 & 1 \\ 1 & 2 & 4 \\ 2 & 3 & 5 \\ 3 & 4 & 4 \\ 4 & 5 & 5 \end{array}}$$

Block matrices

$$A = \left(\begin{array}{cc|cc|cc} \mathbf{1.} & \mathbf{2.} & \mathbf{0.} & \mathbf{0.} & \mathbf{3.} & \mathbf{4.} \\ \mathbf{5.} & \mathbf{6.} & \mathbf{0.} & \mathbf{0.} & \mathbf{7.} & \mathbf{8.} \\ \hline \mathbf{0.} & \mathbf{0.} & \mathbf{9.} & \mathbf{10.} & \mathbf{11.} & \mathbf{12.} \\ \mathbf{0.} & \mathbf{0.} & \mathbf{13.} & \mathbf{14.} & \mathbf{15.} & \mathbf{16.} \\ \hline \mathbf{17.} & \mathbf{18.} & \mathbf{0.} & \mathbf{0.} & \mathbf{20.} & \mathbf{21.} \\ \mathbf{22.} & \mathbf{23.} & \mathbf{0.} & \mathbf{0.} & \mathbf{24.} & \mathbf{25.} \end{array}\right)$$

$$\mathsf{AA} = \begin{array}{|cc|cc|cc|} \hline 1. & 3. & 9. & 11. & 17. & 20. \\ 5. & 7. & 15. & 13. & 22. & 24. \\ 2. & 4. & 10. & 12. & 18. & 21. \\ 6. & 8. & 14. & 16. & 23. & 25. \\ \hline \end{array}$$

$$\mathsf{JA} = \boxed{\ 1\ \ 5\ \ 3\ \ 5\ \ 1\ \ 5\ }$$
$$\mathsf{IA} = \boxed{\ 1\ \ 3\ \ 5\ \ 7\ }$$

➤ Columns of AA hold 2 x 2 blocks. JA(k) = col. index of (1,1) entries of k-th block. FORTRAN: declare as AA(2,2,6)

- Can also store the blocks row-wise in AA.

$$AA = \begin{array}{|cccc|} \hline 1. & 5. & 2. & 6. \\ 3. & 7. & 4. & 8. \\ \hline 9. & 15. & 10. & 14. \\ 11. & 13. & 12. & 16. \\ \hline 17. & 22. & 18. & 23. \\ 20. & 24. & 21. & 25. \\ \hline \end{array} \qquad \begin{array}{l} JA = \boxed{\;1\;\;5\;\;3\;\;5\;\;1\;\;5\;} \\ IA = \boxed{\;1\;\;3\;\;5\;\;7\;} \end{array}$$

- In other words $\boldsymbol{AA}$ is simply transposed

- What are the advantages and disadvantages of each scheme?

- Block formats are important in many applications..

- Also valuable: block structure with variable block size.

Sparse matrices – data structure in C

- Recall:

```
typedef struct SpaFmt {
/*---------------------------------------------
| C-style CSR format - used internally
| for all matrices in CSR format
|---------------------------------------------*/
  int n;
  int *nzcount;  /* length of each row */
  int **ja;      /*  to store column indices  */
  double **ma;   /*  to store nonzero entries */
} CsMat, *csptr;
```

- Can store rows of a matrix (CSR)
- or its columns (CSC)
- How to perform the operation $y = A * x$ in each case?

Matvec – row version

```
void matvec( csptr mata, double *x, double *y )
{
   int i, k, *ki;
   double *kr;
   for (i=0; i<mata->n; i++) {
      y[i] = 0.0;
      kr = mata->ma[i];
      ki = mata->ja[i];
      for (k=0; k<mata->nzcount[i]; k++)
         y[i] += kr[k] * x[ki[k]];
   }
}
```

➤ Uses sparse dot products (sparse SDOTS)

✍ Operation count

Matvec – Column version

```
void matvecC( csptr mata, double *x, double *y )
{
  int n = mata->n, i, k, *ki;
  double *kr;
  for (i=0; i<n; i++)
    y[i] = 0.0;
  for (i=0; i<n; i++) {
    kr = mata->ma[i];
    ki = mata->ja[i];
    for (k=0; k<mata->nzcount[i]; k++)
      y[ki[k]] += kr[k] * x[i];
  }
}
```

- Uses sparse vector combinations (sparse SAXPY)

✍ Operation count

Matvec – row version - FORTRAN

```
      subroutine amux (n, x, y, a, ja, ia)
      real*8  x(*), y(*), a(*), t
      integer n, ja(*), ia(*), i, k
c----- row loop
      do 100 i = 1,n
c----- inner product of row i with vector x
         t = 0.0d0
         do 99 k=ia(i), ia(i+1)-1
            t = t + a(k)*x(ja(k))
  99     continue
         y(i) = t
 100  continue
      return
      end
```

Matvec – column version - FORTRAN

```
      subroutine atmux (n, x, y, a, ja, ia)
      real*8 x(*), y(*), a(*)
      integer n, ia(*), ja(*)
      integer i, k
c----- set y to zero
      do 1 i=1,n
         y(i) = 0.0
 1    continue
c----- column loop
      do 100 i = 1,n
c----- sparse saxpy
         do 99 k=ia(i), ia(i+1)-1
            y(ja(k)) = y(ja(k)) + x(i)*a(k)
  99     continue
 100  continue
c
      return
      end
```

Sparse matrices in matlab

- ✍ Generate a tridiagonal matrix T
- ✍ Convert T to sparse format
- ✍ See how you can generate this sparse matrix directly using `sparse`
- ✍ See how you can use `spconvert` to achieve the same result
- ✍ What can you observe about the way the triplets of a sparse matrix are ordered?
- ✍ Important for performance: `spalloc`. See the difference between

`A = sparse(m,n)`   and   `A = spalloc(m,n,nzmax)`