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)

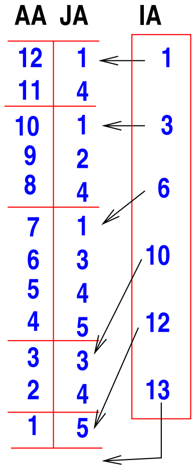
$$A = \begin{pmatrix} 1. & 0. & 0. & 2. & 0. \\ 3. & 4. & 0. & 5. & 0. \\ 6. & 0. & 7. & 8. & 9. \\ 0. & 0. & 10. & 11. & 0. \\ 0. & 0. & 0. & 0. & 12. \end{pmatrix}$$

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

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



➤ 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

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

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

The Ellpack-Itpack format

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

AC =

1.	2.	0.
3.	4.	5.
6.	7.	8.
9.	10.	0.
11	12.	0.

JC =

1	3	1
1	2	4
2	3	5
3	4	4
4	5	5

Block matrices

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

AA =

1.	3.	9.	11.	17.	20.
5.	7.	15.	13.	22.	24.
2.	4.	10.	12.	18.	21.
6.	8.	14.	16.	23.	25.

JA = | 1 5 3 5 1 5 |

IA = | 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 =

1.	5.	2.	6.
3.	7.	4.	8.
9.	15.	10.	14.
11.	13.	12.	16.
17.	22.	18.	23.
20.	24.	21.	25.

JA = | 1 5 3 5 1 5 |

IA = | 1 3 5 7 |

➤ In other words 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)`