Sparse Matrix Data Structures for High Performance Computing

Edmond Chow
School of Computational Science and Engineering
Georgia Institute of Technology

June 29, 2016

Sparse matrix data structures

- Only nonzero elements are stored in sparse matrix data structures, which makes possible the storage of sparse matrices of large dimension.
- Sometimes some zeros are stored (explicit zeros) to maintain block or symmetric sparsity patterns, for example.
- Formats are generally optimized for sparse matrix-vector multiplication (SpMV).
- Conversion cost to an efficient format may be important.

Coordinate format (COO)

Example:

$$\begin{bmatrix} 10 & 11 & \\ & 12 & 13 \\ & & 14 \end{bmatrix}$$

COO format uses three arrays for the above matrix:

rowind	2	1	3	1	2
colind	2	2	3	1	3
a	12	11	14	10	13

with N=3 and NNZ=5.

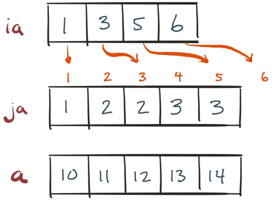
Nonzeros can be in any order in general.

Compressed sparse row format (CSR)

Example:

$$\begin{bmatrix} 10 & 11 & \\ & 12 & 13 \\ & & 14 \end{bmatrix}$$

CSR format uses three arrays for the above matrix:



with N=3.

Rows are stored contiguously in memory. This is useful if row-wise access should be effcient. (Within a row, entries may not be in order.)

A simple variation is compressed sparse row format (CSC).

Data access patterns for SpMV

In straightforward implementations of $y = Ax$ for matrices in COO and CSR formats, the arrays are traversed in order. Memory access of data in these arrays is predictable and efficient.

However, x is accessed in irregular order in general, and may use caches poorly.

Example:

$$\begin{bmatrix} y_1 \\ y_2 \\ y_3 \\ y_4 \\ y_5 \\ y_6 \\ y_7 \\ y_8 \end{bmatrix} = \begin{bmatrix} x & & & & x & & x & \\ & x & & x & & & x & \\ & & x & & x & & & x \\ & x & & x & & x & & \\ x & & x & & x & & & \\ & & & x & & x & & \\ x & x & & & & & x & \\ & & x & & & & & x \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \\ x_5 \\ x_6 \\ x_7 \\ x_8 \end{bmatrix}$$

Data access patterns for SpMV

If "cache size" for x is 3, this SpMV has bad cache behavior:

$$
\begin{bmatrix} y_1 \\ y_2 \\ y_3 \\ y_4 \\ y_5 \\ y_6 \\ y_7 \\ y_8 \end{bmatrix}
=
\begin{bmatrix}
x & & & & x & & x & \\
 & x & & x & & & x & \\
 & & x & & x & & & x \\
 & x & & x & & x & & \\
x & & x & & x & & & \\
 & & & x & & x & & \\
x & x & & & & & x & \\
 & & x & & & & & x
\end{bmatrix}
\begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \\ x_5 \\ x_6 \\ x_7 \\ x_8 \end{bmatrix}
$$

The matrix can be reordered to be banded:

$$
\begin{bmatrix} y_1 \\ y_2 \\ y_3 \\ y_4 \\ y_5 \\ y_6 \\ y_7 \\ y_8 \end{bmatrix}
=
\begin{bmatrix}
x & x & & & & & & \\
x & x & x & & & & & \\
 & x & x & x & & & & \\
 & & x & x & x & & & \\
 & & & x & x & x & & \\
 & & & & x & x & x & \\
 & & & & & x & x & x \\
 & & & & & & x & x
\end{bmatrix}
\begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \\ x_5 \\ x_6 \\ x_7 \\ x_8 \end{bmatrix}
$$

so that it has perfect cache behavior.

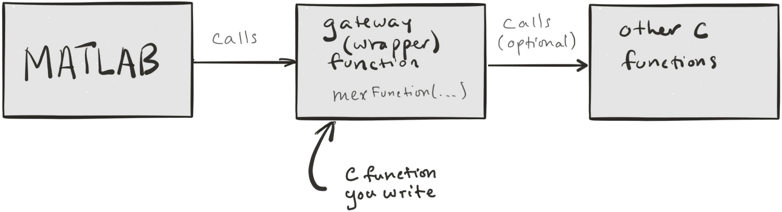
Viewing Matlab's internal sparse matrix data structure

For sparse matrices, Matlab uses compressed sparse column format.

We can use Matlab's **mex** interface to view the raw sparse matrix data structure.

Mex files – calling C codes from Matlab

- C codes are usually more efficient than Matlab programs.
- Some types of algorithms are easier to to write in C than in Matlab.
- You may want to use Matlab to call functions in an existing C library.



Mex gateway function

```
void mexFunction(int nlhs, mxArray *plhs[],
                 int nrhs, const mxArray *prhs[]);
```

`nlhs` – number of objects to return

`plhs` – array of objects to be returned

`nrhs` – number of inputs

`prhs` – array of input objects

Example: `a = add_mex(b,c);`

```
nlhs = 1        nrhs = 2
plhs = [a]      prhs = [b, c]
```

Compile mex program: `mex add_mex.c` from Matlab prompt.
Compile with `-largeArrayDims` flag if sparse matrices are used.

add_mex.c

```c
#include <stdio.h>
#include "mex.h"

// Usage: a = add_mex(b,c), where a,b,c are scalars

void mexFunction(int nlhs, mxArray *plhs[],
                 int nrhs, const mxArray *prhs[])
{
    printf("sizeof nlhs: %d\n", nlhs);
    printf("sizeof nrhs: %d\n", nrhs);

    double b = *mxGetPr(prhs[0]);
    double c = *mxGetPr(prhs[1]);

    printf("b: %f\n", b);
    printf("c: %f\n", c);

    double a = b+c;

    plhs[0] = mxCreateDoubleScalar(a);
}
```

dump_matrix_mex.c

```c
// Usage: dump_matrix_mex(A) where A is a sparse matrix.
// Matlab sparse matrices are CSC format with 0-based indexing.

void mexFunction(int nlhs, mxArray *plhs[],
                 int nrhs, const mxArray *prhs[])
{
    int n;
    const mwIndex *ia, *ja;
    const double *a;

    n  = mxGetM (prhs[0]);
    ia = mxGetJc(prhs[0]); // column pointers
    ja = mxGetIr(prhs[0]); // row indices
    a  = mxGetPr(prhs[0]); // values

    int i, j;
    for (i=0; i<n; i++)
        for (j=ia[i]; j<ia[i+1]; j++)
            printf("%5d %5d   %f\n", ja[j]+1, i+1, a[j]);
}
```

matvec_mex.c

```c
static void Matvec(int n, const mwIndex *ia, const mwIndex *ja,
                   const double *a, const double *x, double *y)
{
    int i, j;
    double t;

    for (i=0; i<n; i++) {
        t = 0.;
        for (j=ia[i]; j<ia[i+1]; j++)
            t += a[j]*x[ja[j]];
        y[i] = t;
    }
}

// Usage: y = matvec_mex(a, x);
void mexFunction(int nlhs, mxArray *plhs[],
                 int nrhs, const mxArray *prhs[])
{
    int n = mxGetN(prhs[0]);
    plhs[0] = mxCreateDoubleMatrix(n, 1, mxREAL); // solution vector

    Matvec(n, mxGetJc(prhs[0]), mxGetIr(prhs[0]), mxGetPr(prhs[0]),
        mxGetPr(prhs[1]), mxGetPr(plhs[0]));
}
```

Advanced sparse matrix data structures

Reference:
M. Kreutzer, G. Hager, G. Wellein, H. Fehske, and A. R. Bishop: A unified sparse matrix data format for modern processors with wide SIMD units, 2014.

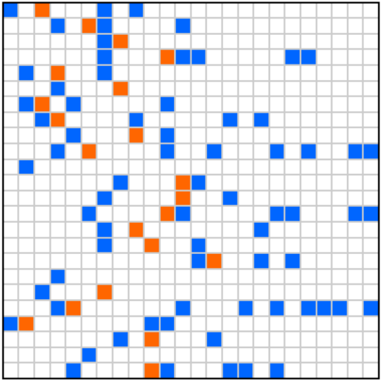
Some figures below are taken from the above reference.

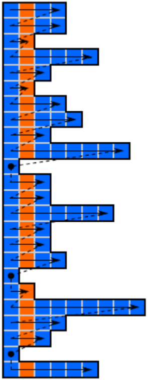
Advanced sparse matrix data structures

Computational considerations:

- SpMV is generally viewed as being limited by memory bandwidth
- On accelerators and coprocessors, memory bandwith may not be the limiting factor
- SIMD (single instruction, multiple data) must be used to increase the flop rate
- It is desirable to use long loops (rather than short loops) to reduce overheads
- Efficient use of SIMD may result in bandwidth being saturated when using a smaller number of cores (saving energy)

CSR format





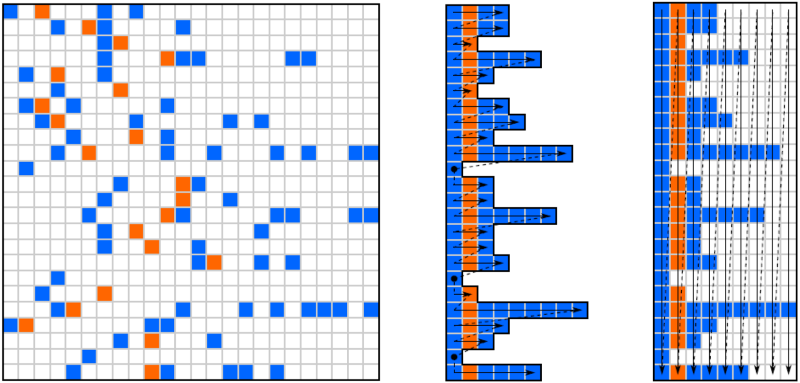
SpMV code using CSR format (SIMD illustration)

```c
for(i = 0; i < N; ++i) {
  for(j = rpt[i]; j < rpt[i+1]; ++j) {
      y[i] += val[j] * x[col[j]];
  }
}
```

```c
1 for(i = 0; i < N; ++i)
2 {
3   tmp0 = tmp1 = tmp2 = tmp3 = 0.;
4   for(j = rpt[i]; j < rpt[i+1]; j+=4)
5   {
6     tmp0 += val[j+0] * x[col[j+0]];
7     tmp1 += val[j+1] * x[col[j+1]];
8     tmp2 += val[j+2] * x[col[j+2]];
9     tmp3 += val[j+3] * x[col[j+3]];
10  }
11  y[i] += tmp0+tmp1+tmp2+tmp3;
12  // remainder loop
13  for(j = j-4; j < rpt[i+1]; j++)
14    y[i] += val[j] * x[col[j]];
15 }
```

If rows are short, then SIMD is not effectively utilized, and “overhead” of the remainder loop and the reduction (line 11) is relatively large.

ELLPACK format



ELLPACK format:

- Entries are stored in a dense array in column major order, resulting in long columns, good for efficient computation.
- Explicit zeros are stored if necessary (zero padding).
- Little zero padding if all rows are about the same length.
- Not efficient if have short and long rows.

Potential solutions for the zero-padding problem

Potential solutions for the zero-padding problem

- Hybrid format (ELL+COO) used on GPUs

Potential solutions for the zero-padding problem

- Hybrid format (ELL+COO) used on GPUs
- Jagged diagonal (JDS) format used on old vector supercomputers

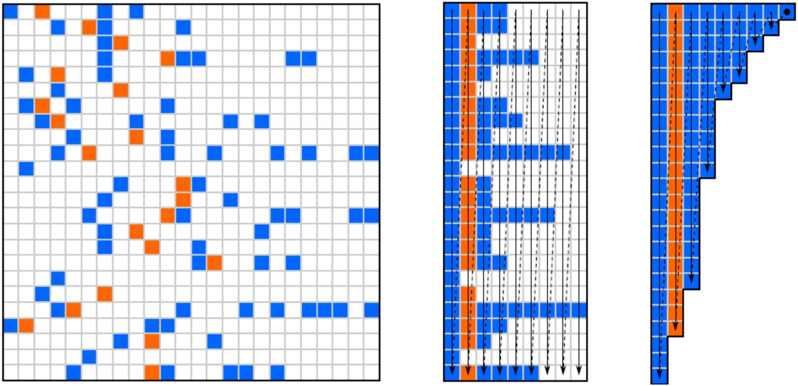
Potential solutions for the zero-padding problem

- Hybrid format (ELL+COO) used on GPUs
- Jagged diagonal (JDS) format used on old vector supercomputers
- Sliced ELLPACK (SELL) format

Potential solutions for the zero-padding problem

- Hybrid format (ELL+COO) used on GPUs
- Jagged diagonal (JDS) format used on old vector supercomputers
- Sliced ELLPACK (SELL) format
- A combination of SELL and JDS: SELL-C-σ

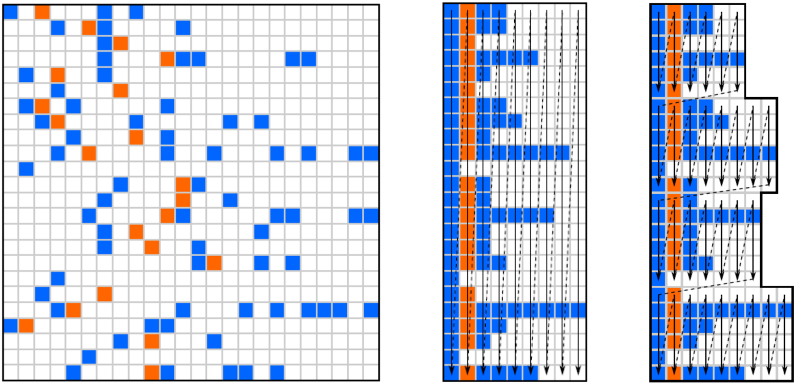
Jagged diagonal format



JDS format sorts the rows by length.

A disadvantage of JDS format is that access to x (in $y = Ax$) may be irregular, leading to poor cache usage.

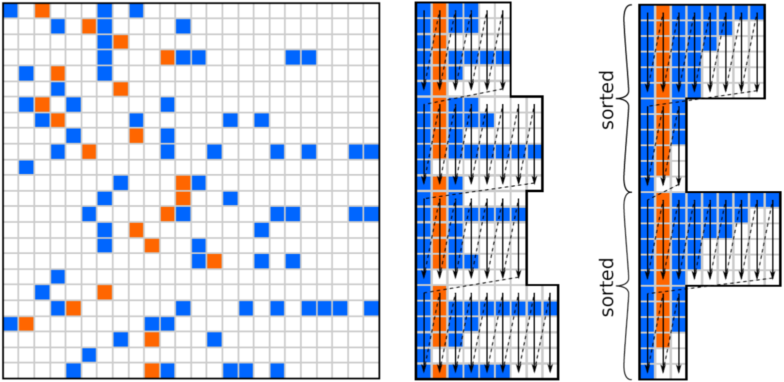
Sliced ELLPACK format



Dense matrix is “sliced” row-wise into chunks.

Avoids problem of irregular access of *x* since the given ordering can be used in the SpMV computation.

SELL-C-σ format

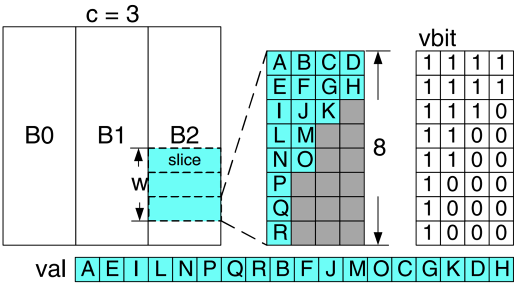


C = chunk size (like in SELL); 6 in above example.
σ = sorting window size; 12 in above example. This parameter helps preserve locality in accesses in x (e.g., if the matrix is banded).

Block formats

A more explicit way to ensure locality in accesses to x is to partition the matrix by block columns.

The ELLPACK Sparse Block (ESB) format uses both partitioning by block rows (like Sliced ELLPACK) and by block columns (for x locality), giving sparse blocks that are stored in an ELLPACK-like format.



In this figure, $c = 3$ block columns are used. Rows are sorted within windows of size w. Instead of column lengths, bit vectors

Some references

- Jagged diagonal format: Saad, Krylov subspace methods on supercomputers, 1989.
- Hybrid ELL+COO format: Bell and Garland, Implementing sparse matrix-vector multiplication on throughput-oriented processors, 2009.
- Sliced ELLPACK format: Monakov, Lokhmotov, and Avetisyan, Automatically tuning sparse matrix-vector multiplication for GPU architectures, 2010.
- ELLPACK Sparse Block (ESB) format: Liu, Smelyanskiy, Chow, and Dubey, Efficient sparse matrix-vector multiplication on x86-based many-core processors, 2013.
- SELL-C-σ format: Kreutzer, Hager, Wellein, Fehske, and Bishop, A unified sparse matrix data format for modern processors with wide SIMD units, 2014.

Exercise

The jagged diagonal format uses the following variables and arrays:

n	– number of rows in matrix
p	– (array) mapping between original row number and sorted row number
m	– number of columns (max number of nonzeros in any row)
len	– (array) length of each column
a	– array of values
col	– corresponding array of column indices

1. For the Laplacian matrix on a 4×4 grid and 5-point stencil in natural ordering (as we have used in class), what is the JDS format (i.e., the contents of the above variables and arrays)?
2. Write code or pseudocode for multiplying a sparse matrix in JDS format by a dense vector, i.e., $y = Ax$.