SPARSE MATRIX IMPLEMENTATION IN OCTAVE

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ABSTRACT
This paper discusses the implementation of the sparse matrix support with Octave. It addresses the algorithms that have been used, their implementation, including examples of using sparse matrices in scripts and in dynamically linked code. The octave sparse functions are compared with their equivalent functions with Matlab, and benchmark timings are calculated.

1. INTRODUCTION

The size of mathematical problems that can be treated at any particular time is generally limited by the available computing resources. Both the speed of the computer and its available memory place limitations on the problem size.

There are many classes of mathematical problems which give rise to matrices, where a large number of the elements are zero. In this case it makes sense to have a special matrix type to handle this class of problems where only the non-zero elements of the matrix are stored. Not only does this reduce the amount of memory to store the matrix, but it also means that operations on this type of matrix can take advantage of the a-priori knowledge of the positions of the non-zero elements to accelerate their calculations. A matrix type that stores only the non-zero elements is generally called sparse.

This article addresses the implementation of sparse matrices within Octave [1,2], including their storage, creation, fundamental algorithms used, their implementations and the basic operations and functions implemented for sparse matrices. Benchmarking of Octave’s implementation of sparse operations compared to their equivalent in Matlab [3] are given and their implications discussed. Furthermore, the method of using sparse matrices with Octave oct-files is discussed.

In order to motivate this use of sparse matrices, consider the image of an automobile crash simulation as shown in Figure 1. This image is generated based on ideas of DIFFCrash [4] – a software package for the stability analysis of crash simulations. Physical bifurcations in automobile design and numerical instabilities in simulation packages often cause extremely sensitive dependencies of simulation results on even the smallest model changes. Here, a prototypic extension of DIFFCrash uses octave’s sparse matrix functions (and large computers with lots of memory) to produce these results.

2. BASICS

2.1. Storage of Sparse Matrices

It is not strictly speaking necessary for the user to understand how sparse matrices are stored. However, such an understanding will help to get an understanding of the size of sparse matrices. Understanding the storage technique is also necessary for those users wishing to create their own oct-files.

There are many different means of storing sparse matrix data. What all of the methods have in common is that they attempt to reduce the complexity and storage given a-priori knowledge of the particular class of problems that will be solved. A good summary of the available techniques for storing sparse matrix is given by Saad [5]. With full matrices, knowledge of the point of an element of the matrix within the matrix is implied by its position in the computers.
memory. However, this is not the case for sparse matrices, and so the positions of the non-zero elements of the matrix must equally be stored.

An obvious way to do this is by storing the elements of the matrix as triplets, with two elements being their position in the array (rows and column) and the third being the data itself. This is conceptually easy to grasp, but requires more storage than is strictly needed.

The storage technique used within Octave is the compressed column format. In this format the position of each element in a row and the data are stored as previously. However, if we assume that all elements in the same column are stored adjacent in the computers memory, then we only need to store information on the number of non-zero elements in each column, rather than their positions. Thus assuming that the matrix has more non-zero elements than there are columns in the matrix, we win in terms of the amount of memory used.

In fact, the column index contains one more element than the number of columns, with the first element always being zero. The advantage of this is a simplication in the code, in that their is no special case for the first or last columns. A short example, demonstrating this in C is.

```c
for (j = 0; j < nc; j++)
    for (i = cidx (j); i < cidx(j+1); i++)
        printf ("Element (%d,%d) is %d\n",
                ridx(i), j, data(i));
```

A clear understanding might be had by considering an example of how the above applies to an example matrix. Consider the matrix

\[
\begin{bmatrix}
1 & 2 & 0 & 0 \\
0 & 0 & 0 & 3 \\
0 & 0 & 0 & 4
\end{bmatrix}
\]

The non-zero elements of this matrix are

\[
(1, 1) = 1 \\
(1, 2) = 2 \\
(2, 4) = 3 \\
(3, 4) = 4
\]

This will be stored as three vectors `cidx`, `ridx` and `data`, representing the column indexing, row indexing and data respectively. The contents of these three vectors for the above matrix will be

\[
\begin{align*}
\text{cidx} &= [0, 1, 2, 2, 4] \\
\text{ridx} &= [0, 0, 1, 2] \\
\text{data} &= [1, 2, 3, 4]
\end{align*}
\]

Note that this is the representation of these elements with the first row and column assumed to start at zero, while in Octave itself the row and column indexing starts at one. With the above representation, the number of elements in the $i^{th}$ column is given by $cidx(i + 1) - cidx(i)$.

Although Octave uses a compressed column format, it should be noted that compressed row formats are equally possible. However, in the context of mixed operations between mixed sparse and dense matrices, it makes sense that the elements of the sparse matrices are in the same order as the dense matrices. Octave stores dense matrices in column major ordering, and so sparse matrices are equally stored in this manner.

A further constraint on the sparse matrix storage used by Octave is that all elements in the rows are stored in increasing order of their row index, which makes certain operations faster. However, it imposes the need to sort the elements on the creation of sparse matrices. Having unordered elements is potentially an advantage in that it makes operations such as concatenating two sparse matrices together easier and faster, however it adds complexity and speed problems elsewhere.

### 2.2. Creating Sparse Matrices

There are several means to create sparse matrices

- **Returned from a function**: There are many functions that directly return sparse matrices. These include `speye`, `sprand`, `spdiags`, etc.
• **Constructed from matrices or vectors:** The function `sparse` allows a sparse matrix to be constructed from three vectors representing the row, column and data. Alternatively, the function `spconvert` uses a three column matrix format to allow easy importation of data from elsewhere.

• **Created and then filled:** The function `sparse` or `sprand` can be used to create an empty matrix that is then filled by the user.

• **From a user binary program:** The user can directly create the sparse matrix within an `oct-file`.

There are several functions that return specific sparse matrices. For example the sparse identity matrix is often needed. It therefore has its own function to create it as `speye(n)` or `speye(r,c)`, which creates an `n`-by-`n` or `r`-by-`c` sparse identity matrix.

Another typical sparse matrix that is often needed is a random distribution of random elements. The functions `sprand` and `sprandn` perform this for uniform and normal random distributions of elements. They have exactly the same calling convention, where `sprand(r,c,d)`, creates an `r`-by-`c` sparse matrix with a density of filled elements of `d`.

Other functions of interest that directly creates a sparse matrix, are `spdiags` or its generalization `spdiags`, that can take the definition of the diagonals of the matrix and create the sparse matrix that corresponds to this. For example

```
s = spdiag(sparse(randn(1,n)), -1);
```

creates a sparse `(n+1)`-by-`(n+1)` sparse matrix with a single diagonal defined.

The recommended way for the user to create a sparse matrix, is to create two vectors containing the row and column index of the data and a third vector of the same size containing the data to be stored. For example

```
function x = foo (r, j)
    idx = randperm (r);
    x = (zeros(r-2,1); rand(2,1)) (idx);
endfunction

ri = [];
cci = [];
d = [];

for j=1:c
    dtmp = foo (r, j);
    idx = find (dtmp != 0.);
    ri = [ri; idx];
    cci = [cci; j*ones(length(idx),1)];
    d = [d; dtmp(idx)];
endfor
s = sparse (ri, cci, d, r, c);
```

creates an `r`-by-`c` sparse matrix with a random distribution of 2 elements per row. The elements of the vectors do not need to be sorted in any particular order as Octave will sort them prior to storing the data. However, pre-sorting the data will make the creation of the sparse matrix faster.

The function `spconvert` takes a three or four column real matrix. The first two columns represent the row and column index, respectively, and the third and four columns, the real and imaginary parts of the sparse matrix. The matrix can contain zero elements and the elements can be sorted in any order. Adding zero elements is a convenient way to define the size of the sparse matrix. For example

```
s = spconvert([[1 2 3 4; 1 3 4 4; 1 2 3 0]'])
```

Compressed Column Sparse (rows=4, ...
```
cols=4, nnz=3)
```
```
(1 , 1) -> 1
(2 , 3) -> 2
(3 , 4) -> 3
```

An example of creating and filling a matrix might be

```
k = 5;
nz = r * k;
s = spalloc (r, c, nz)
for j = 1:c
    idx = randperm (r);
    s(:, j) = [zeros(r-k, 1); ...
               rand(k, 1)] (idx);
endfor
```

It should be noted, that due to the way that the Octave assignment functions are written that the assignment will reallocate the memory used by the sparse matrix at each iteration of the above loop. Therefore the `spalloc` function ignores the `nz` argument and does not preassign the memory for the matrix. Therefore, code using the above structure should be vectorized to minimize the number of assignments and reduce the number of memory allocations.

The above problem can be avoided in `oct-files`. However, the construction of a sparse matrix from an `oct-file` is much more complex than can be discussed in this brief introduction, and you are referred to section 6 to have a full description of the techniques involved.

### 2.3. Sparse Functions in Octave

An important consideration in the use of the sparse functions of Octave is that many of the internal functions of Octave, such as `diag`, cannot accept sparse matrices as an input. The sparse implementation in Octave therefore uses the `dispatch` function to overload the normal Octave functions with equivalent functions that work with sparse matrices. However, at any time the sparse matrix specific version of the function can be used by explicitly calling its function name.
The table below lists all of the sparse functions of Octave together (with possible future extensions that are currently unimplemented, listed last). Note that in this specific sparse forms of the functions are typically the same as the general versions with a sp prefix. In the table below, and the rest of this article the specific sparse versions of the functions are used.

- Generate sparse matrices: spalloc, spdiags, speye, sprand, sprandn, (sprandsym)
- Sparse matrix conversion: full, sparse, spconvert, spfind
- Manipulate sparse matrices issparse, nnz, nonzeros, nzmax, spfun, spzeros, spy,
- Graph Theory: etree, etreeplot, gplot, treeplot, (treelayout)
- Sparse matrix reordering: ecolamd, colamd, colperm, csymamd, symamd, randperm, (dnpermc, symrcm)
- Linear algebra: matrix_type, spchol, spcholinv, spchol2inv, spdet, spinv, spkron, splchol, splu, (condest, eig, normest, sprank, svds, spaugment, spq)
- Iterative techniques: luinc, (bicg, bicgstab, cholinc, cgs, gmres, lsqr, minres, pcg, pcr, qmr, symmlq)
- Miscellaneous: spparms, symbfact, sptests, spprod, spcsumsum, spsum, spxmsq, spmin, spmax, spatan2, spdiag

In addition all of the standard Octave mapper functions (ie. basic math functions that take a single argument) such as abs, etc can accept sparse matrices. The reader is referred to the documentation supplied with these functions within Octave itself for further details.

2.4. Sparse Return Types

The two basic reasons to use sparse matrices are to reduce the memory usage and to not have to do calculations on zero elements. The two are closely related and the computation time might be proportional to the number of non-zero elements or a power of the number of non-zero elements depending on the operator or function involved.

Therefore, there is a certain density of non-zero elements of a matrix where it no longer makes sense to store it as a sparse matrix, but rather as a full matrix. For this reason operators and functions that have a high probability of returning a full matrix will always return one. For example adding a scalar constant to a sparse matrix will almost always make it a full matrix, and so the example

\[ \text{speye}(3) + 0 \]
\[ \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \]

returns a full matrix as can be seen. Additionally all sparse functions test the amount of memory occupied by the sparse matrix to see if the amount of storage used is larger than the amount used by the full equivalent. Therefore speye(2) * 1 will return a full matrix as the memory used is smaller for the full version than the sparse version.

As all of the mixed operators and functions between full and sparse matrices exist, in general this does not cause any problems. However, one area where it does cause a problem is where a sparse matrix is promoted to a full matrix, where subsequent operations would re-sparsify the matrix. Such cases are rare, but can be artificially created, for example (flipr(speye(3)) + speye(3)) - speye(3) gives a full matrix when it should give a sparse one. In general, where such cases occur, they impose only a small memory penalty.

There is however one known case where this behavior of Octave’s sparse matrices will cause a problem. That is in the handling of the spdiag function. Whether spdiag returns a sparse or full matrix depends on the type of its input arguments. So

\[ a = \text{diag}(\text{sparse}([1,2,3]), -1); \]

should return a sparse matrix. To ensure this actually happens, the sparse function, and other functions based on it like speye, always returns a sparse matrix, even if the memory used will be larger than its full representation.

2.5. Finding out Information about Sparse Matrices

There are a number of functions that allow information concerning sparse matrices to be obtained. The most basic of these is issparse that identifies whether a particular Octave object is in fact a sparse matrix.

Another very basic function is nnz that returns the number of non-zero entries there are in a sparse matrix, while the function nzmax returns the amount of storage allocated to the sparse matrix. Note that Octave tends to crop unused memory at the first opportunity for sparse objects. There are some cases of user created sparse objects where the value returned by nzmax will not be the same as nnz, but in general they will give the same result. The function spstats returns some basic statistics on the columns of a sparse matrix including the number of elements, the mean and the variance of each column.

When solving linear equations involving sparse matrices Octave determines the means to solve the equation based on the type of the matrix as discussed in section. Octave probes the matrix type when the div (/) or ldiv (\) operator is first used with the matrix and then caches the type. However the matrix type function can be used to determine
the type of the sparse matrix prior to use of the div or ldiv operators. For example

```matlab
a = tril(sprandn(1024, 1024, 0.02), -1) + speye(1024);
matrix_type(a);
ans = Lower
```

show that Octave correctly determines the matrix type for lower triangular matrices. `matrix_type` can also be used to force the type of a matrix to be a particular type. For example

```matlab
a = matrix_type(tril(sprandn(1024, ..., 1024, 0.02), -1) + speye(1024), 'Lower');
```

This allows the cost of determining the matrix type to be avoided. However, incorrectly defining the matrix type will result in incorrect results from solutions of linear equations, and so it is entirely the responsibility of the user to correctly identify the matrix type.

There are several graphical means of finding out information about sparse matrices. The first is the `spy` command, which displays the structure of the non-zero elements of the matrix, as can be seen in Figure 4. More advanced graphical information can be obtained with the `treeplot`, `etreeplot` and `gplot` commands.

One use of sparse matrices is in graph theory, where the interconnections between nodes is represented as an adjacency matrix [6]. That is, if the $i$-th node in a graph is connected to the $j$-th node. Then the $ij$-th node (and in the case of undirected graphs the $ji$-th node) of the sparse adjacency matrix is non-zero. If each node is then associated with a set of co-ordinates, then the `gplot` command can be used to graphically display the interconnections between nodes.

As a trivial example of the use of `gplot`, consider the example

```matlab
A = sparse([2,6,1,3,2,4,3,5,4,6,1,5], [1,1,2,2,3,3,4,4,5,5,6,6],1,6,6);
xy = [0,4,8,6,4,2;5,0,5,7,5,7]';
gplot(A,xy)
```

which creates an adjacency matrix $A$ where node 1 is connected to nodes 2 and 6, node 2 with nodes 1 and 3, etc. The co-ordinates of the nodes is given in the $n$-by-2 matrix $xy$. The output of the `gplot` command can be seen in Figure 2.

The dependences between the nodes of a Cholesky factorization can be calculated in linear time without explicitly needing to calculate the Cholesky factorization by the `etree` command. This command returns the elimination tree of the matrix and can be displayed graphically by the command `treeplot(etree(A))` if $A$ is symmetric or `treeplot(etree(A+A'))` otherwise.

2.6. Mathematical Considerations

The attempt has been made to make sparse matrices behave in exactly the same manner as their full counterparts. However, there are certain differences between full and sparse behavior and with the sparse implementations in other software tools.

Firstly, the `/` and `^` operators must be used with care. Consider what the examples

```matlab
s = speye(4);
a1 = s.^2;
a2 = s.^s;
a3 = s.^-2;
a4 = s./2;
a5 = 2./s;
a6 = s./s;
```

will give. The first example of $s$ raised to the power of 2 causes no problems. However $s$ raised element-wise to itself involves a a large number of terms $0.\times 0$ which is 1. Therefore $s.\times s$ is a full matrix. Likewise $s.\times -2$ involves terms like $0.\times -2$ which is infinity, and so $s.\times -2$ is equally a full matrix.

For the `/` operator $s./2$ has no problems, but $2./s$ involves a large number of infinity terms as well and is equally a full matrix. The case of $s./s$ involves terms like $0./0$ which is a NaN and so this is equally a full matrix with the zero elements of $s$ filled with NaN values. The above behavior is consistent with full matrices, but is not consistent with sparse implementations in Matlab [7]. If the user re-
quires the same behavior as in Matlab then for example for the case of \( 2 ./ s \) then appropriate code is

```matlab
function z = f(x), z = 2 ./ x; end function
spfun (@f, s);
```

and the other examples above can be implemented similarly.

A particular problem of sparse matrices comes about due to the fact that as the zeros are not stored, the sign-bit of these zeros is equally not stored. In certain cases the sign-bit of zero is important [8]. For example

```matlab
a = 0 ./ [-1, 1; 1, -1];
b = 1 ./ a
-Inf     Inf
Inf    -Inf
```

```matlab
c = 1 ./ sparse (a)
Inf     Inf
Inf     Inf
Inf     Inf
```

To correct this behavior would mean that zero elements with a negative sign-bit would need to be stored in the matrix to ensure that their sign-bit was respected. This is not done at this time, for reasons of efficiency, and so the user is warned that calculations where the sign-bit of zero is important must not be done using sparse matrices.

In general any function or operator used on a sparse matrix will result in a sparse matrix with the same or a larger number of non-zero elements than the original matrix. This is particularly true for the important case of sparse matrix factorizations. The usual way to address this is to reorder the matrix, such that its factorization is sparser than the factorization of the original matrix. That is the factorization of \( LU = PSQ \) has sparser terms \( L \) and \( U \) than the equivalent factorization \( LU = S \).

Several functions are available to reorder depending on the type of the matrix to be factorized. If the matrix is symmetric positive-definite, then `symamd` or `csymamd` should be used. Otherwise `colamd` or `ecolamd` should be used. For completeness the reordering functions `colperm` and `randperm` are also available.

As an example, consider the ball model which is given as an example in the EIDORS project [9, 10], as shown in Figure 3. The structure of the original matrix derived from this problem can be seen with the command `spy(A)`, as seen in Figure 4.

The standard LU factorization of this matrix, with row pivoting can be obtained by the same command that would be used for a full matrix. This can be visualized with the command `[l, u, p] = lu(A); spy(l+u);` as seen in Figure 5. The original matrix had 17825 non-zero terms, while this LU factorization has 531544 non-zero terms, which is a significant level of fill in of the factorization and represents a large overhead in working with this matrix.

The appropriate sparsity preserving permutation of the original matrix is given by `colamd` and the factorization us-
Fig. 5. Structure of the un-permuted LU factorization of EIDORS ball problem

Fig. 6. Structure of the permuted LU factorization of EIDORS ball problem

ing this reordering can be visualized using the command \( q = \text{colamd}(A); [l, u, p] = \text{lu}(A(:,q)); \text{spy}(l+u) \). This gives 212044 non-zero terms which is a significant improvement.

Furthermore, the underlying factorization software updates its estimate of the optimal sparsity preserving reordering of the matrix during the factorization, so can return an even sparser factorization. In the case of the LU factorization this might be obtained with a fourth return argument as \([l, u, p, q] = \text{lu}(A); \text{spy}(l+u)\). This factorization has 143491 non-zero terms, and its structure can be seen in Figure 6.

Finally, Octave implicitly reorders the matrix when using the \( \text{div} \) and \( \text{ldiv} \) operators, and so no the user does not need to explicitly reorder the matrix to maximize performance.

### 3. LINEAR ALGEBRA ON SPARSE MATRICES

Octave includes a polymorphic solver for sparse matrices, where the exact solver used to factorize the matrix, depends on the properties of the sparse matrix itself. Generally, the cost of determining the matrix type is small relative to the cost of factorizing the matrix itself, but in any case the matrix type is cached once it is calculated, so that it is not re-determined each time it is used in a linear equation.

Linear equations are solved using the following selection tree

1. If the matrix is not square go to 9.
2. If the matrix is diagonal, solve directly and go to 9
3. If the matrix is a permuted diagonal, solve directly taking into account the permutations. Go to 9
4. If the matrix is banded and if the band density is less than that given by \textit{spparms ("bandden")}, continue, else go to 5.
   a. If the matrix is tridiagonal and the right-hand side is not sparse continue, else go to 4b.
      i. If the matrix is hermitian, with a positive real diagonal, attempt Cholesky factorization using \textit{Lapack xPTSV}.
      ii. If the above failed, or the matrix is not hermitian, use Gaussian elimination with pivoting using \textit{Lapack xGTSV}, and go to 9.
   b. If the matrix is hermitian with a positive real diagonal, attempt a Cholesky factorization using \textit{Lapack xPBTRF}.
   c. If the above failed or the matrix is not hermitian with a positive real diagonal use Gaussian elimination with Gaussian elimination with pivoting using \textit{Lapack xGBTRF}, and go to 9.
5. If the matrix is upper or lower triangular perform a sparse forward or backward substitution, and go to 9.
6. If the matrix is a upper triangular matrix with column permutations or lower triangular matrix with row permutations, perform a sparse forward or backward substitution, and go to 9.

7. If the matrix is hermitian with a real positive diagonal, attempt a sparse Cholesky factorization using CHOLMOD [11].

8. If the sparse Cholesky factorization failed or the matrix is not hermitian, perform LU factorization using UMFPACK [12].

9. If the matrix is not square, or any of the previous solvers flags a singular or near singular matrix, find a minimum norm solution.

The band density is defined as the number of non-zero values in the band divided by the number of values in the band. The banded matrix solvers can be entirely disabled by using `spparms` to set `bandden` to 1 (i.e. `spparms('bandden','1')`).

The QR solver factorizes the problem with a Dulmage-Mendelsohn [13] to separate the problem into blocks that can be treated as over-determined, multiple well determined blocks, and a final over-determined block. For matrices with blocks of strongly connected nodes this is a big win as LU decomposition can be used for many blocks. It also significantly improves the chance of finding a solution to ill-conditioned problems rather than just returning a vector of NaN’s.

All of the solvers above, can calculate an estimate of the condition number. This can be used to detect numerical stability problems in the solution and force a minimum norm solution to be used. However, for narrow banded, triangular or diagonal matrices, the cost of calculating the condition number is significant, and can in fact exceed the cost of factoring the matrix. Therefore the condition number is not calculated in these cases, and octave relies on simpler techniques to detect singular matrices or the underlying LAPACK code in the case of banded matrices.

The user can force the type of the matrix with the `matrix_type` function. This overcomes the cost of discovering the type of the matrix. However, it should be noted incorrectly identifying the type of the matrix will lead to unpredictable results, and so `matrix_type` should be used with care.

4. BENCHMARKING OF OCTAVE SPARSE MATRIX IMPLEMENTATION

It is a truism that all benchmarks should be treated with care. The speed of a software package is determined by a large number of factors, including the particular problem treated and the configuration of the machine on which the benchmarks were run. Therefore the benchmarks presented here should be treated as indicative of the speed a user might expect.

That being said we attempt to examine the speed of several fundamental operators for use with sparse matrices. These being the addition (+), multiplication (*) and left-devision (\) operators. The basic test code used to perform these tests is given by

```matlab
n = 0;
while (time < tmin || n < nrun)
    clear a, b;
    a = sprand(order, order, density);
    t = cputime();
    b = a OP a;
    time = time + cputime() - t;
    n = n + 1;
end
```

where `nrun` was 5, `tmin` was 1 second and `OP` was either +, or *. The left-division operator poses particular problems for benchmarking that will be discussed later.

Although the `cputime` function only has a resolution of 0.01 seconds, running the command multiple times and limited by the minimum run time of `tmin` seconds allows this precision to be extended. Running the above code for various matrix orders and densities results in the summary of execution times as seen in Table II.

The speeds for the small low density problems in Table II are interesting (cf. Matrix order of 500, with densities lower than 1e-03), as they seem to indicate that there is a small incompressible execution time for both Matlab and Octave. This is probably due to the overhead associated with the parsing of the language and the calling of the underlying function responsible for the operator. On the test machine this time was approximately 200 \(\mu s\) for Octave for both operators, while for Matlab this appears to be 70 and 40 \(\mu s\) for the * and + operators respectively. So in this class of problems Matlab outperforms Octave for both operators. However, when the matrix order or density increases it can be seen that Octave significantly out-performs Matlab for both operators.

When considering the left-division operator, we can not use randomly created matrices. The reason is that the fill-in, or rather the potential to reduce the fill-in with appropriate matrix re-ordering, during matrix factorization is determined by the structure of the matrix imposed by the problem it represents. As random matrices have no structure, factorization of random matrices results in extremely large levels of matrix fill-in, even with matrix re-ordering. Therefore, to benchmark the left-division (\) operator, we have selected a number of test matrices that are publicly available [14], and modify the benchmark code as
Table 1. Benchmark of basic operators on Matlab R14sp2 against Octave 2.9.5, on a Pentium 4M 1.6GHz machine with 1GB of memory.

| Order | Density | Execution Time for Operator (sec) | Matlab | Octave |
|-------|---------|-----------------------------------|--------|--------|
|       |         | +                                 | *      | *      |
| 500   | 1e-02   | 0.00049                           | 0.000250 | 0.00039 | 0.00170 |
| 500   | 1e-03   | 0.00008                           | 0.000009 | 0.00022 | 0.00026 |
| 500   | 1e-04   | 0.00005                           | 0.000007 | 0.00020 | 0.00024 |
| 1000  | 1e-02   | 0.0179                            | 0.02273  | 0.00092 | 0.00990 |
| 1000  | 1e-03   | 0.0021                            | 0.00227  | 0.00029 | 0.00042 |
| 1000  | 1e-04   | 0.0011                            | 0.00113  | 0.00023 | 0.00026 |
| 1000  | 1e-05   | 0.0012                            | 0.00111  | 0.00028 | 0.00023 |
| 2000  | 1e-02   | 0.0714                            | 0.23000  | 0.00412 | 0.07049 |
| 2000  | 1e-03   | 0.0058                            | 0.0165   | 0.00055 | 0.00135 |
| 2000  | 1e-04   | 0.0032                            | 0.0026   | 0.00026 | 0.00033 |
| 2000  | 1e-05   | 0.0019                            | 0.0020   | 0.00022 | 0.00026 |
| 2000  | 1e-06   | 0.0018                            | 0.0018   | 0.00024 | 0.00023 |
| 5000  | 1e-02   | 0.05100                           | 3.63200  | 0.02652 | 0.95326 |
| 5000  | 1e-03   | 0.0526                            | 0.03000  | 0.00257 | 0.01896 |
| 5000  | 1e-04   | 0.0076                            | 0.0083   | 0.00049 | 0.00074 |
| 5000  | 1e-05   | 0.0051                            | 0.0051   | 0.00031 | 0.00043 |
| 5000  | 1e-06   | 0.0048                            | 0.0055   | 0.00028 | 0.00026 |
| 10000 | 1e-02   | 0.22200                           | 24.2700  | 0.10878 | 6.55060 |
| 10000 | 1e-03   | 0.02000                           | 0.30000  | 0.01022 | 0.18597 |
| 10000 | 1e-04   | 0.0021                            | 0.00269  | 0.00120 | 0.00252 |
| 10000 | 1e-05   | 0.0094                            | 0.00949  | 0.00407 | 0.00074 |
| 10000 | 1e-06   | 0.0011                            | 0.00098  | 0.00039 | 0.00055 |
| 20000 | 1e-03   | 0.08286                           | 2.65000  | 0.04374 | 1.71874 |
| 20000 | 1e-04   | 0.00444                           | 0.01923  | 0.00490 | 0.01500 |
| 20000 | 1e-05   | 0.00250                           | 0.00258  | 0.00092 | 0.00149 |
| 20000 | 1e-06   | 0.00189                           | 0.00161  | 0.00058 | 0.00121 |
| 50000 | 1e-04   | 0.05500                           | 0.39400  | 0.02794 | 0.28076 |
| 50000 | 1e-05   | 0.00823                           | 0.00877  | 0.00406 | 0.00767 |
| 50000 | 1e-06   | 0.00543                           | 0.00610  | 0.00154 | 0.00332 |

time = 0;
n = 0;
while (time < tmin || n < nrun)
    clear a, b;
    load test.mat % Get matrix 'a'
    x = ones(order,1);
    t = cputime();
    b = a \ x;
    time = time + cputime() - t;
    n = n + 1;
end
time = time / n;

All the the matrices in the University of Florida Sparse Matrix [14] that met the following criteria were used:

- Has real or complex data available, and not just the structure,
- Has between 10,000 and 1,000,000 non-zero element,
- Has equal number of rows and columns,
- The solution did not require more than 1GB of memory, to avoid issues with memory.

When comparing the benchmarks for the left-division operator it must be considered that the matrices in the collection used represent an arbitrary sampling of the available sparse matrix problems. It is therefore difficult to treat the data in aggregate, and so we present the raw data below so that the reader might compare the benchmark for a particular matrix class that interests them.

The performance of the Matlab and Octave left-division operators is affected by the spparms function. In particular the density of terms in a banded matrix that is needed to force the solver to use the LAPACK banded solvers rather than the generic solvers is determined by the command spparms('bandden',val). The default density of 0.5 was used for both Matlab and Octave.

Five classes of problems were represented in the matrices treated. These are:

- Banded positive definite and factorized with the LAPACK xPBTRF function,
- General banded matrix and factorized with the LAPACK xGBTRF function,
- Positive definite and treated by the Cholesky solvers of Matlab and Octave,
- Sparse LU decomposition with UMFPACK, and
- Singular matrices that were treated via QR decomposition.
Also, it should be noted that the LAPACK solvers, and dense BLAS kernels of the UMFPACK and CHOLMOD solvers were accelerated using the ATLAS [15] versions of the LAPACK and BLAS functions. The exact manner in which the ATLAS library is compiled might have an effect on the performance, and therefore the benchmarks might measure the relative performance of the different versions of ATLAS rather than the performance of Octave and Matlab. To avoid this issue Octave was forced to use the Matlab ATLAS libraries with the use of the Unix LD_PRELOAD command.

For the banded problems both Octave and Matlab perform similarly, with only minor differences, probably due to the fact that the same ATLAS library was used. Matlab is slightly faster for problems with very short run times, probably for similar reasons as for small multiplications and additions.

One class of problems where the speed of Octave significantly exceeds that of Matlab are the positive definite matrices that are not solved with the LAPACK banded solvers (xPTSV or xPBTRF). This is due in large part to the use of CHOLMOD [11] together with the use of METIS [16] for the graph partitioning. As CHOLMOD will become the sparse Cholesky solver in future versions of Matlab, this situation is a temporary advantage for Octave. The worst case for this is the Andrews/Andrews matrix, where Matlab did not complete the solution due to a lack of memory. Once Matlab uses CHOLMOD, it might be expected that in this case as well similar speeds might be expected.

The differences in the problems solved via LU decomposition using UMFPACK are harder to explain. There are a couple of very large discrepancies in the results, with Octave winning in some cases (cf. Hollinger/g7jac100) and Matlab in others (cf Zhao/Zhao2).

Both Octave and Matlab use recent versions of UMFPACK, with Octave using a slightly newer version to allow the use of C99 compatible complex numbers where the real and imaginary parts are stored together. There are however no changes between the versions of UMFPACK used that would explain any performance differences. Octave has a slight advantage when the arguments are complex, due it is use of C99 compatible complex as it is this format that is used internally to UMFPACK. Another possible source of differences is that UMFPACK calls internally a column reordering routine, and Octave uses this functionality. Perhaps Matlab attempts to independently guess an initial column reordering. In any case, in 11 of the cases where UMFPACK was used the speed of Matlab exceeded the speed of Octave, while in 267 of the cases the speed of Octave exceeded the speed of Matlab, with the mean speed of Octave being 12% above that of Matlab.

Finally, there are significant differences between the results for Octave and Matlab for singular matrices. The major difference is that Matlab uses Given’s rotations whereas Octave uses Householder reflections. Given’s rotations of Matlab allow row reordering to be performed to reduce the amount of work to below that of a Householder transformation. However, the underlying code used in Octave uses Householder transformation to allow the eventual use of multi-frontal techniques to the QR factorization, and so this option is not available to Octave currently.

Furthermore, Octave uses a Dulmage-Mendelsohn factorization of the matrix to allow the problems to be solved as a combination of over-determined, well-determined and under-determined parts. The advantage of this is the potential for significantly better performance and more stable results for over-determined problems. However, it is possible that the Dulmage-Mehdelsohn factorization identifies no useful structure. A case where this occurs is the GHS_indef/diag where 3 times the computation time of a straight QR solution is needed.

The Dulmage-Mendelsohn solver can be bypassed with code like

\[ [c, r] = qr(a, b); \]
\[ x = r \backslash c; \]

It should be noted that both Octave and Matlab use accelerated algorithms for the left-division operator for triangular, permuted triangular and tridiagonal matrices, as discussed in section 4 and that these cases are not treated in the matrices from the University of Florida collection used here. These are trivial cases, but important in that they should not be solved with generic code.

5. USE OF OCTAVE SPARSE MATRICES IN REAL LIFE EXAMPLE

A common application for sparse matrices is in the solution of Finite Element Models. Finite element models allow numerical solution of partial differential equations that do not have closed form solutions, typically because of the complex shape of the domain.

In order to motivate this application, we consider the boundary value Laplace equation. This system can model scalar potential fields, such as heat or electrical potential. Given a medium \( \Omega \) with boundary \( \partial \Omega \). At all points on the \( \partial \Omega \) the boundary conditions are known, and we wish to calculate the potential in \( \Omega \). Boundary conditions may specify the potential (Dirichlet boundary condition), its normal derivative across the boundary (Neumann boundary condition), or a weighted sum of the potential and its derivative (Cauchy boundary condition).
| Matrix | Order | NNZs | Execution Time for Operator (sec) | Matrix | Order | NNZs | Execution Time for Operator (sec) |
|--------|-------|------|----------------------------------|--------|-------|------|----------------------------------|
| Bai/bcsstk09 | 1813 | 8 | 0.01693 | HBB/s3 | 990 | 1814 | 8 | 0.03500 |
| Bai/bcsstk09 | 1104 | 9 | 0.01696 | HBB/s4 | 784 | 1814 | 8 | 0.03500 |
| Bai/bcsstk09 | 1105 | 1813 | 8 | 0.01693 | HBB/s5 | 990 | 1814 | 8 | 0.03500 |
| Bai/bcsstk09 | 1106 | 1300 | 8 | 0.01693 | HBB/s6 | 990 | 1814 | 8 | 0.03500 |
| Bai/bcsstk09 | 1107 | 1108 | 8 | 0.01693 | HBB/s7 | 990 | 1814 | 8 | 0.03500 |
| Bai/bcsstk09 | 1109 | 1110 | 8 | 0.01693 | HBB/s8 | 990 | 1814 | 8 | 0.03500 |
| Bai/bcsstk09 | 1111 | 1112 | 8 | 0.01693 | HBB/s9 | 990 | 1814 | 8 | 0.03500 |
| Bai/bcsstk09 | 1113 | 1114 | 8 | 0.01693 | HBB/s10 | 990 | 1814 | 8 | 0.03500 |
| Bai/bcsstk09 | 1115 | 1116 | 8 | 0.01693 | HBB/s11 | 990 | 1814 | 8 | 0.03500 |
| Bai/bcsstk09 | 1117 | 1118 | 8 | 0.01693 | HBB/s12 | 990 | 1814 | 8 | 0.03500 |
| Bai/bcsstk09 | 1119 | 1120 | 8 | 0.01693 | HBB/s13 | 990 | 1814 | 8 | 0.03500 |
| Bai/bcsstk09 | 1121 | 1122 | 8 | 0.01693 | HBB/s14 | 990 | 1814 | 8 | 0.03500 |
| Bai/bcsstk09 | 1123 | 1124 | 8 | 0.01693 | HBB/s15 | 990 | 1814 | 8 | 0.03500 |
| Bai/bcsstk09 | 1125 | 1126 | 8 | 0.01693 | HBB/s16 | 990 | 1814 | 8 | 0.03500 |
| Bai/bcsstk09 | 1127 | 1128 | 8 | 0.01693 | HBB/s17 | 990 | 1814 | 8 | 0.03500 |
| Bai/bcsstk09 | 1129 | 1130 | 8 | 0.01693 | HBB/s18 | 990 | 1814 | 8 | 0.03500 |
| Bai/bcsstk09 | 1131 | 1132 | 8 | 0.01693 | HBB/s19 | 990 | 1814 | 8 | 0.03500 |
| Bai/bcsstk09 | 1133 | 1134 | 8 | 0.01693 | HBB/s20 | 990 | 1814 | 8 | 0.03500 |
| Bai/bcsstk09 | 1135 | 1136 | 8 | 0.01693 | HBB/s21 | 990 | 1814 | 8 | 0.03500 |
| Bai/bcsstk09 | 1137 | 1138 | 8 | 0.01693 | HBB/s22 | 990 | 1814 | 8 | 0.03500 |
| Bai/bcsstk09 | 1139 | 1140 | 8 | 0.01693 | HBB/s23 | 990 | 1814 | 8 | 0.03500 |
| Bai/bcsstk09 | 1141 | 1142 | 8 | 0.01693 | HBB/s24 | 990 | 1814 | 8 | 0.03500 |
| Bai/bcsstk09 | 1143 | 1144 | 8 | 0.01693 | HBB/s25 | 990 | 1814 | 8 | 0.03500 |
| Bai/bcsstk09 | 1145 | 1146 | 8 | 0.01693 | HBB/s26 | 990 | 1814 | 8 | 0.03500 |
| Bai/bcsstk09 | 1147 | 1148 | 8 | 0.01693 | HBB/s27 | 990 | 1814 | 8 | 0.03500 |
| Bai/bcsstk09 | 1149 | 1150 | 8 | 0.01693 | HBB/s28 | 990 | 1814 | 8 | 0.03500 |
| Bai/bcsstk09 | 1151 | 1152 | 8 | 0.01693 | HBB/s29 | 990 | 1814 | 8 | 0.03500 |

Table 2. Benchmark of left-division operator on *Matlab* R14sp2 against *Octave* 2.9.5, on a Pentium 4 1.6GHz machine with 1GB of memory. † The solver used for the problem, as given in section 5.
Table 3. Benchmark of left-division operator on MatLab R14sp2 against Octave 2.9.5, on a Pentium 4 1.666GHz machine with 1GB of memory. * The solver used for the problem, as given in section 5.
Table 4. Benchmark of left-division operator on *Matlab* R14sp2 against *Octave* 2.9.5, on a Pentium 4M 1.6GHz machine with 1GB of memory. † The solver used for the problem, as given in section 5.
In a thermal model, we want to calculate the temperature in $\Omega$ and know the boundary temperature (Dirichlet condition) or heat flux (from which we can calculate the Neumann condition by dividing by the thermal conductivity at the boundary). Similarly, in an electrical model, we want to calculate the voltage in $\Omega$ and know the boundary voltage (Dirichlet) or current (Neumann condition after dividing by the electrical conductivity). In an electrical model, it is common for much of the boundary to be electrically isolated; this is a Neumann boundary condition with the current equal to zero.

The simplest finite element models will divide $\Omega$ into simplexes (triangles in 2D, pyramids in 3D). A 3D example is shown in Figure 1G and represents a cylindrical liquid filled tank with a small non-conductive ball [9, 10]. This model is designed to reflect an application of electrical impedance tomography, where current patterns are applied to such a tank in order to image the internal conductivity distribution. In order to describe the FEM geometry, we first calculate the voltage in $\Omega$ and know the boundary temperature (Dirichlet condition) or heat flux (from which we can calculate the thermal conductivity at the boundary). Similarly, in an electrical model, we want to calculate the voltage in $\Omega$ and know the boundary voltage (Dirichlet) or current (Neumann condition by dividing by the electrical conductivity). In an electrical model, it is common for much of the boundary to be electrically isolated; this is a Neumann boundary condition with the current equal to zero.

The following example creates a simple rectangular 2D electrically conductive medium with 10 V and 20 V imposed on opposite sides (Dirichlet boundary conditions). All other edges are electrically isolated.

```matlab
node_x = [1:1:2,1:5,1:8,2] * ones(1,11);
node_y = ones (5,1)+[1,1.05,1,1,1.2,. . ., 1.3,1.5,1.7,1.8,1.9,1.95,2];
nodes = [node_x(:,), node_y (:)];

[h,w]= size (node_x);
elems = [ ];
for idx= 1:w-1
    widx = (idx-1)+h;
elems = [elems; . . .
          widx+[((1:h-1):(2:h);h+(1:h-1))'; . . .
          widx+[(2:h);h+(2:h);h+(1:h-1)]'
    ];
endfor

E= size(elems,1); # No. of simplices
N= size(nodes,1); # No. of vertices
D= size(elems,2); # dimensions+1

This creates a $N \times 2$ matrix nodes and a $E \times 3$ matrix elems with values, which define finite element triangles:

```matlab
nodes(1:7,:)'
  1.00 1.00 1.00 1.00 1.05 1.05 . . .
  1.00 1.20 1.50 1.80 2.00 1.00 1.20

elems(1:7,:)'
  1 2 3 4 2 3 4 . . .
  2 3 4 5 7 8 9 . . .
  6 7 8 9 6 7 8

Using a first order FEM, we approximate the electrical conductivity distribution in $\Omega$ as constant on each simplex (represented by the vector conductivity). Based on the finite element geometry, we first calculate a system (or stiffness) matrix for each simplex (represented as $3 \times 3$ elements on the diagonal of the element-wise system matrix SE). Based on SE and a $N \times DE$ connectivity matrix C, representing the connections between simplexes and vertices, the global connectivity matrix $S$ is calculated.

```matlab
# Element conductivity
conductivity = [1*ones (1,16), . . .
              2*ones (1,48), 1*ones (1,16)];

# Connectivity matrix
C = sparse ((1:D+E), reshaped (elems', . . .
            D+E, 1), 1, D+E, N);

# Calculate system matrix
Siidx = floor ([0:D+E-1]' / D) * D + . . .
       ones (1,D) + ones (D+E,1)*(1:D);
Sjidx = [1:D+E]' *ones (1,D);
Sdata = zeros (D+E,D);
dfact = factor (D-1);
for j=1:E
    a = inv ([ones (D,1), . . .
             nodes (elems (j,:), :) ]);
    const = conductivity (j) * 2 /
            dfact / abs (det (a));
    Sdata (D*(j-1)+(1:D),:) = const * . . .
                          a (2:D,:)' * a (2:D,:);
endfor

# Element-wise system matrix
SE= sparse (Siidx, Sjidx, Sdata);

# Global system matrix
S= C' * SE * C;

The system matrix acts like the conductivity $S$ in Ohm's law $SV = I$. Based on the Dirichlet and Neumann boundary conditions, we are able to solve for the voltages at each vertex $V$.

```matlab
# Dirichlet boundary conditions
D_nodes=[1:5, 51:55];
D_value=[10+ones (1,5), 20+ones (1,5)];
V= zeros (N,1);
V(D_nodes) = D_value;
idx = 1:N; # vertices without Dirichlet
# boundary condns
idx (D_nodes) = [ ];

# Neumann boundary conditions. Note that
# N_value must be normalized by the
# boundary length and element conductivity
N_nodes=[];
N_value=[];
Q = zeros (N,1);
Q(N_nodes) = N_value;
V(idx) = S (idx, idx) \ ( Q (idx) - ...
Fig. 7. Example finite element model the showing triangular elements. The height of each vertex corresponds to the solution value $S(\text{idx},\text{D}\_\text{nodes}) = V(\text{D}\_\text{nodes})$;

Finally, in order to display the solution, we show each solved voltage value in the z-axis for each simplex vertex in Figure 7:

\[
\text{elemx} = \text{elems}(:,[1,2,3,1])';
\text{xelems} = \text{reshape} (\text{nodes} (\text{elemx}, 1), 4, \text{E});
\text{yelems} = \text{reshape} (\text{nodes} (\text{elemx}, 2), 4, \text{E});
\text{velems} = \text{reshape} (\text{V} (\text{elemx}), 4, \text{E});
\text{plot3} (\text{xelems}, \text{yelems}, \text{velems}, 'k');
\text{print} ('\text{grid}\_\text{eps}');
\]

6. USING SPARSE MATRICES IN OCT-FILES

An oct-file is a means of writing an Octave function in a compilable language like C++, rather than as a script file. This can result in a significant acceleration in the code. It is not the purpose of this section to discuss how to write an oct-file, or discuss what they are. Users wishing to find out more about oct-files themselves are referred to the articles by Cristophe Spiel [17] and Paul Thomas [18]. Users who are not familiar with oct-files are urged to read these references to fully understand this section. The examples discussed here assume that the oct-file is written entirely in C++.

There are three classes of sparse objects that are of interest to the user.

- SparseMatrix - double precision sparse matrix class
- SparseComplexMatrix - Complex sparse matrix class
- SparseBoolMatrix - boolean sparse matrix class

All of these classes inherit from the Sparse$<T>$ template class, and so all have similar capabilities and usage. The Sparse$<T>$ class was based on Array$<T>$ class, and so users familiar with Octave’s array classes will be comfortable with the use of the sparse classes.

The sparse classes will not be entirely described in this section, due to their similar with the existing array classes. However, there are a few differences due the different nature of sparse objects, and these will be described. Firstly, although it is fundamentally possible to have N-dimensional sparse objects, the Octave sparse classes do not allow them at this time. So all operations of the sparse classes must be 2-dimensional. This means that in fact SparseMatrix is similar to Octave’s Matrix class rather than its NDArray class.

6.1. Differences between the Array and Sparse Classes

The number of elements in a sparse matrix is considered to be the number of non-zero elements rather than the product of the dimensions. Therefore

```
\text{SparseMatrix sm;}
\ldots
\text{int nel = sm.nelem();}
```

returns the number of non-zero elements. If the user really requires the number of elements in the matrix, including the non-zero elements, they should use numel rather than nelem. Note that for very large matrices, where the product of the two dimensions is larger than the representation of the an octave currents type, then numel can overflow. An example is `speye(1e6)` which will create a matrix with a million rows and columns, but only a million non-zero elements. Therefore the number of rows by the number of columns in this case is more than two hundred times the maximum value that can be represented by an unsigned int on a 32-bit platform. The use of numel should therefore be avoided useless it is known it won’t overflow.

Extreme care must be taken with the elem method and the () operator, which perform basically the same function. The reason is that if a sparse object is non-const, then Octave will assume that a request for a zero element in a sparse matrix is in fact a request to create this element so it can be filled. Therefore a piece of code like

```
\text{SparseMatrix sm;}
\ldots
\text{for} (\text{int j = 0; j < nc; j++})
\text{for} (\text{int i = 0; i < nr; i++})
\text{std::cerr} \ll " (" \ll i \ll ","
\ll j \ll ": " \ll \text{sm}(i,j)
\ll \text{std::endl};
```

is a great way of turning the sparse matrix into a dense one, and a very slow way at that since it reallocates the sparse object at each zero element in the matrix.
An easy way of preventing the above from happening is to create a temporary constant version of the sparse matrix. Note that only the container for the sparse matrix will be copied, while the actual representation of the data will be shared between the two versions of the sparse matrix. So this is not a costly operation. For example, the above would become

```cpp
SparseMatrix sm;
...
const SparseMatrix tmp (sm);
for (int j = 0; j < nc; j++)
    for (int i = 0; i < nr; i++)
        std::cerr << "( " << i << ", ",
                 << j << ") : " << tmp(i, j)
                 << std::endl;
```

Finally, as the sparse types aren’t just represented as a contiguous block of memory, the fortran_vec method of the Array<T> class is not available. It is however replaced by three separate methods ridx, cidx and data, that access the raw compressed column format that the Octave sparse matrices are stored in. Additionally, these methods can be used in a manner similar to elem, to allow the matrix to be accessed or filled. However, in that case it is up to the user to respect the sparse matrix compressed column format discussed previous.

### 6.2. Creating Spare Matrices in Oct-Files

The user has several alternatives in how to create a sparse matrix. They can first create the data as three vectors representing the row and column indexes and the data, and from those create the matrix. Or alternatively, they can create a sparse matrix with the appropriate amount of space and then fill in the values. Both techniques have their advantages and disadvantages.

An example of how to create a small sparse matrix with the first technique might be seen the example

```cpp
int nz = 4, nr = 3, nc = 4;
ColumnVector ridx (nz);
ColumnVector cidx (nz);
ColumnVector data (nz);

ridx(0) = 0; ridx(1) = 0;
ridx(2) = 1; ridx(3) = 2;
cidx(0) = 0; cidx(1) = 1;
cidx(2) = 3; cidx(3) = 3;
data(0) = 1; data(1) = 2;
data(2) = 3; data(3) = 4;

SparseMatrix sm(data, ridx, cidx, nr, nc);
```

As previously mentioned, the values of the sparse matrix are stored in increasing column-major ordering. Although the data passed by the user does not need to respect this requirement, the pre-sorting the data significantly speeds up the creation of the sparse matrix.

The disadvantage of this technique of creating a sparse matrix is that there is a brief time where two copies of the data exists. Therefore for extremely memory constrained problems this might not be the right technique to create the sparse matrix.

The alternative is to first create the sparse matrix with the desired number of non-zero elements and then later fill those elements in. The easiest way to do this is

```cpp
int nz = 4, nr = 3, nc = 4;
SparseMatrix sm(nz, nc, nz);
sm(0, 0) = 1; sm(0, 1) = 2;
sm(1, 3) = 3; sm(2, 3) = 4;
```

That creates the same matrix as previously. Again, although it is not strictly necessary, it is significantly faster if the sparse matrix is created in this manner that the elements are added in column-major ordering. The reason for this is that if the elements are inserted at the end of the current list of known elements then no element in the matrix needs to be moved to allow the new element to be inserted. Only the column indexes need to be updated.

There are a few further points to note about this technique of creating a sparse matrix. Firstly, it is not illegal to create a sparse matrix with fewer elements than are actually inserted in the matrix. Therefore

```cpp
int nz = 4, nr = 3, nc = 4;
SparseMatrix sm(nz, nc, nz);
sm(0, 0) = 1; sm(0, 1) = 2;
sm(1, 3) = 3; sm(2, 3) = 4;
```

is perfectly legal, but will be very slow. The reason is that as each new element is added to the sparse matrix the space allocated to it is increased by reallocating the memory. This is an expensive operation, that will significantly slow this means of creating a sparse matrix. Furthermore, it is not illegal to create a sparse matrix with too much storage, so having nz above equaling 6 is also legal. The disadvantage is that the matrix occupies more memory than strictly needed.

It is not always easy to know the number of non-zero elements prior to filling a matrix. For this reason the additional storage for the sparse matrix can be removed after its creation with the maybe_compress function. Furthermore, maybe_compress can deallocate the unused storage, but it can equally remove zero elements from the matrix.

The removal of zero elements from the matrix is controlled by setting the argument of the maybe_compress function to be ‘true’. However, the cost of removing the zeros is high because it implies resorting the elements. Therefore, if pos-
sible it is better is the user doesn’t add the zeros in the first place. An example of the use of \texttt{maybe	extunderscore compress} is
\begin{verbatim}
int nz = 6, nr = 3, nc = 4;
SparseMatrix sml (nr, nc, nz);
sml(0,0) = 1; sml(0,1) = 2;
sml(1,3) = 3; sml(2,3) = 4;
// No zero elements were added
sml.maybe	extunderscore compress ( );
\end{verbatim}

\begin{verbatim}
SparseMatrix sm2 (nr, nc, nz);
sm2(0,0) = 1; sm2(0,1) = 2; sm2(0,2) = 0; sm2(1,2) = 0;
sm2(1,3) = 3; sm2(2,3) = 4;
// Zero elements were added
sm2.maybe	extunderscore compress (true);
\end{verbatim}

The \texttt{maybe	extunderscore compress} function should be avoided if possible, as it will slow the creation of the matrices.

A third means of creating a sparse matrix is to work directly with the data in compressed row format. An example of this technique might be
\begin{verbatim}
octave	extunderscore value arg;
...
// Assume we know the max no nz
int nz = 6, nr = 3, nc = 4;
SparseMatrix sm (nr, nc, nz);
Matrix m = arg.matrix	extunderscore value ( );
int ii = 0;
sm.cidx (0) = 0;
for (int j = 1; j < nc; j++)
{
    for (int i = 0; i < nr; i++)
    {
        double tmp = foo (m(i,j));
        if (tmp != 0.)
        {
            sm.data(ii) = tmp;
            sm.ridx(ii) = i;
            ii++;
        }
    }
    sm.cidx(j+1) = ii;
}
// Don’t know a	extunderscore priori the final no of nz.
sm.maybe	extunderscore compress ( );
\end{verbatim}

Note that both increasing and decreasing the number of non-zero elements in a sparse matrix is expensive, as it involves memory reallocation. Also as parts of the matrix, though not its entirety, exist as the old and new copy at the same time, additional memory is needed. Therefore, if possible this should be avoided.

6.3. Using Sparse Matrices in Oct-Files

Most of the same operators and functions on sparse matrices that are available from the \texttt{Octave} are equally available with \texttt{oct	extunderscore files}. The basic means of extracting a sparse matrix from an \texttt{octave	extunderscore value} and returning them as an \texttt{octave	extunderscore value}, can be seen in the following example
\begin{verbatim}
octave	extunderscore value list retval;

SparseMatrix sm =
    args(0).sparse	extunderscore matrix	extunderscore value ( );
SparseComplexMatrix scm =
    args(1).sparse	extunderscore complex	extunderscore matrix	extunderscore value ( );
SparseBoolMatrix sbm =
    args(2).sparse	extunderscore bool	extunderscore matrix	extunderscore value ( );
...
retval(2) = sbm;
retval(1) = scm;
\end{verbatim}
The conversion to an octave-value is automatically handled by the sparse `octave_value` constructors, and so no special care is needed.

7. CONCLUSION

This paper has presented the implementation of sparse matrices with recent versions of Octave. Their storage, creation, fundamental algorithms used, their implementations and basic operations were also discussed. Important considerations for the use of sparse matrices were discussed include efficient manners to create and use them as well as the return types of several operations.

Furthermore, the Octave sparse matrix implementation in Octave version 2.9.5 was compared against Matlab version R14sp2 for the fundamental addition, multiplication and left-division operators. It was found that Octave outperformed Matlab in most cases, with the exceptions often being for smaller, lower density problems. The efficiency of the basic Octave sparse matrix implementation has therefore been demonstrated.

Furthermore, we discussed the use of the Octave sparse matrix type in the context of a real finite element model. The case of a boundary value Laplace equation, treating the case of a 2D electrically conductive strip.

Finally, we discussed the use of Octave’s sparse matrices from within Octave’s dynamically loadable `oct-files`. The passing, means of creating, manipulating and returning sparse matrices within Octave were discussed. The differences with the Octave’s `Array<T>` were discussed.

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