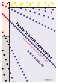
Sparse Matrices and Their Data Structures
(PSC §4.2)

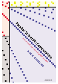


Basic sparse technique: adding two vectors

- Problem: add a sparse vector **y** of length n to a sparse vector **x** of length n, overwriting **x**, i.e.,

$$\mathbf{x} := \mathbf{x} + \mathbf{y}.$$

- **x** is a sparse vector means that $x_i = 0$ for most i.
- The number of nonzeros of **x** is c_x and that of **y** is c_y.



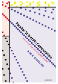
Example: storage as compressed vector

- Vectors **x**, **y** have length $n = 8$.
- Their number of nonzeros is $c_x = 3$ and $c_y = 4$.
- A compressed vector data structure for **x** and **y** is:

$x[j].a =$	2	5	1
$x[j].i =$	5	3	7

$y[j].a =$	1	4	1	4
$y[j].i =$	6	3	5	2

- Here, the jth nonzero in the array of **x** has numerical value $x_i = x[j].a$ and index $i = x[j].i$.
- How to compute $\mathbf{x} + \mathbf{y}$?



Addition is easy for dense storage

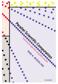
- The dense vector data structure for $\mathbf{x}$, $\mathbf{y}$, and $\mathbf{x}+\mathbf{y}$ is:

0	0	0	5	0	2	0	1
0	0	4	4	0	1	1	0
0	0	4	9	0	3	1	1

- A compressed vector data structure for $\mathbf{z} = \mathbf{x}+\mathbf{y}$ is:

$z[j].a =$	3	9	1	1	4
$z[j].i =$	5	3	7	6	2

- Conclusion: use an auxiliary dense vector!

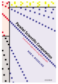


Location array

The array *loc* (initialised to -1) stores the location $j = loc[i]$ where a nonzero vector component y_i is stored in the compressed array.

$y[j].a =$	1	4	1	4
$y[j].i =$	6	3	5	2
$j =$	0	1	2	3

$y_i =$	0	0	4	4	0	1	1	0
$loc[i] =$	-1	-1	3	1	-1	2	0	-1
$i =$	0	1	2	3	4	5	6	7



Algorithm for sparse vector addition: pass 1

input:	$\mathbf{x}$: sparse vector with c_x nonzeros, $\mathbf{x} = \mathbf{x}_0$,
	$\mathbf{y}$: sparse vector with c_y nonzeros,
	loc : dense vector of length n,
	$loc[i] = -1$, for $0 \leq i < n$.
output:	$\mathbf{x} = \mathbf{x}_0 + \mathbf{y}$,
	$loc[i] = -1$, for $0 \leq i < n$.

{ Register location of nonzeros of $\mathbf{y}$}
for $j := 0$ **to** $c_y - 1$ **do**
    $loc[y[j].i] := j$;

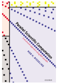
Algorithm for sparse vector addition: passes 2, 3

{ Add matching nonzeros of **x** and **y** into **x**}
for $j := 0$ **to** $c_x - 1$ **do**
    $i := x[j].i$;
    if $loc[i] \neq -1$ **then**
        $x[j].a := x[j].a + y[loc[i]].a$;
        $loc[i] := -1$;

Algorithm for sparse vector addition: passes 2, 3

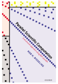
{ Add matching nonzeros of **x** and **y** into **x**}
for $j := 0$ **to** $c_x - 1$ **do**
    $i := x[j].i;$
    if $loc[i] \neq -1$ **then**
        $x[j].a := x[j].a + y[loc[i]].a;$
        $loc[i] := -1;$

{ Append remaining nonzeros of **y** to **x** }
for $j := 0$ **to** $c_y - 1$ **do**
    $i := y[j].i;$
    if $loc[i] \neq -1$ **then**
        $x[c_x].i := i;$
        $x[c_x].a := y[j].a;$
        $c_x := c_x + 1;$
        $loc[i] := -1;$

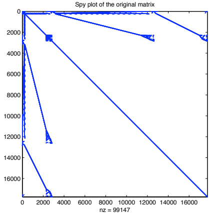


Analysis of sparse vector addition

- The total number of operations is $\mathcal{O}(c_x + c_y)$, since there are $c_x + 2c_y$ loop iterations, each with a small constant number of operations.
- The number of flops equals the number of nonzeros in the intersection of the sparsity patterns of $\mathbf{x}$ and $\mathbf{y}$. 0 flops can happen!
- Initialisation of array *loc* costs n operations, which will dominate the total cost if only one vector addition has to be performed.
- *loc* can be reused in subsequent vector additions, because each modified element $loc[i]$ is reset to -1.
- If we add two $n \times n$ matrices row by row, we can amortise the $\mathcal{O}(n)$ initialisation cost over n vector additions.

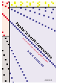


Accidental zero



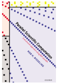
$17,758 \times 17,758$ matrix `memplus` with $126,150$ entries, including 27,003 accidental zeros.

- An accidental zero is a matrix element that is numerically zero but still occurs as a nonzero pair $(i, 0)$ in the data structure.
- Accidental zeros are created when a nonzero $y_i = -x_i$ is added to a nonzero x_i and the resulting zero is retained.
- Testing all operations in a sparse matrix algorithm for zero results is more expensive than computing with a few additional nonzeros.
- Therefore, accidental zeros are usually kept.



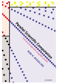
No abuse of numerics for symbolic purposes!

- Instead of using the symbolic location array, initialised at -1, we could have used an auxiliary array storing numerical values, initialised at 0.0.
- We could then add $\mathbf{y}$ into the numerical array, update $\mathbf{x}$ accordingly, and reset the array.
- Unfortunately, this would make the resulting sparsity pattern of $\mathbf{x}+\mathbf{y}$ dependent on the numerical values of $\mathbf{x}$ and $\mathbf{y}$: an accidental zero in $\mathbf{y}$ would never lead to a new entry in the data structure of $\mathbf{x}+\mathbf{y}$.
- This dependence may prevent reuse of the sparsity pattern in case the same program is executed repeatedly for a matrix with different numerical values but the same sparsity pattern.
- Reuse often speeds up subsequent program runs.



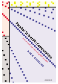
Sparse matrix data structure: coordinate scheme

- In the coordinate scheme or triple scheme, every nonzero element a_{ij} is represented by a triple (i, j, a_{ij}), where i is the row index, j the column index, and a_{ij} the numerical value.
- The triples are stored in arbitrary order in an array.
- This data structure is easiest to understand and is often used for input/output.
- It is suitable for input to a parallel computer, since all information about a nonzero is contained in its triple. The triples can be sent directly and independently to the responsible processors.
- Row-wise or column-wise operations on this data structure require a lot of searching.



Compressed Row Storage

- In the Compressed Row Storage (CRS) data structure, each matrix row i is stored as a compressed sparse vector consisting of pairs (j, a_{ij}) representing nonzeros.
- In the data structure, $a[k]$ denotes the numerical value of the kth nonzero, and $j[k]$ its column index.
- Rows are stored consecutively, in order of increasing i.
- $start[i]$ is the address of the first nonzero of row i.
- The number of nonzeros of row i is $start[i+1] - start[i]$, where by convention $start[n] = nz(A)$.



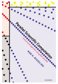
Example of CRS

$$A = \begin{bmatrix} 0 & 3 & 0 & 0 & 1 \\ 4 & 1 & 0 & 0 & 0 \\ 0 & 5 & 9 & 2 & 0 \\ 6 & 0 & 0 & 5 & 3 \\ 0 & 0 & 5 & 8 & 9 \end{bmatrix}, \; n = 5, \; nz(A) = 13.$$

The CRS data structure for A is:

$a[k] =$	3	1	4	1	5	9	2	6	5	3	5	8	9
$j[k] =$	1	4	0	1	1	2	3	0	3	4	2	3	4
$k =$	0	1	2	3	4	5	6	7	8	9	10	11	12

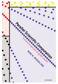
$start[i] =$	0	2	4	7	10	13
$i =$	0	1	2	3	4	5



Sparse matrix–vector multiplication using CRS

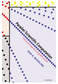
input:	A: sparse $n \times n$ matrix,
	$\mathbf{v}$: dense vector of length n.
output:	$\mathbf{u}$: dense vector of length n, $\mathbf{u} = A\mathbf{v}$.

for $i := 0$ **to** $n - 1$ **do**
    $u[i] := 0;$
    for $k := start[i]$ **to** $start[i+1] - 1$ **do**
        $u[i] := u[i] + a[k] \cdot v[j[k]];$



Incremental Compressed Row Storage

- Incremental Compressed Row Storage (ICRS) is a variant of CRS proposed by Joris Koster in 2002.
- In ICRS, the location (i, j) of a nonzero a_{ij} is encoded as a 1D index $i \cdot n + j$.
- Instead of the 1D index itself, the difference with the 1D index of the previous nonzero is stored, as an increment in the array *inc*.
- The nonzeros within a row are ordered by increasing j, so that the 1D indices form a monotonically increasing sequence and the increments are positive.
- An extra dummy element $(n, 0)$ is added at the end.



Example of ICRS

$$A = \begin{bmatrix} 0 & 3 & 0 & 0 & 1 \\ 4 & 1 & 0 & 0 & 0 \\ 0 & 5 & 9 & 2 & 0 \\ 6 & 0 & 0 & 5 & 3 \\ 0 & 0 & 5 & 8 & 9 \end{bmatrix}, \quad n = 5, \quad nz(A) = 13.$$

The ICRS data structure for A is:

$a[k] =$	3	1	4	1	5	9	2	$\ldots$	0
$j[k] =$	1	4	0	1	1	2	3	$\ldots$	0
$i[k] \cdot n + j[k] =$	1	4	5	6	11	12	13	$\ldots$	25
$inc[k] =$	1	3	1	1	5	1	1	$\ldots$	1
$k =$	0	1	2	3	4	5	6	$\ldots$	13

Sparse matrix–vector multiplication using ICRS

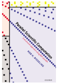
input: A: sparse $n \times n$ matrix,
$\mathbf{v}$: dense vector of length n.
output: $\mathbf{u}$: dense vector of length n, $\mathbf{u} = A\mathbf{v}$.

$k := 0$; $j := inc[0]$;
for $i := 0$ **to** $n-1$ **do**
  $u[i] := 0$;
  while $j < n$ **do**
    $u[i] := u[i] + a[k] \cdot v[j]$;
    $k := k + 1$;
    $j := j + inc[k]$;
  $j := j - n$;

Slightly faster: increments translate well into pointer arithmetic of programming language C; no indirect addressing $v[j[k]]$.

A few other data structures

- Compressed column storage (CCS), similar to CRS.
- Gustavson's data structure: both CRS and CCS, but storing numerical values only once. Offers row-wise and column-wise access to the sparse matrix.
- The two-dimensional doubly linked list: each nonzero is represented by i, j, a_{ij}, and links to a next and a previous nonzero in the same row and column. Offers maximum flexibility: row-wise and column-wise access are easy and elements can be inserted and deleted in $\mathcal{O}(1)$ operations.
- Matrix-free storage: sometimes it may be too costly to store the matrix explicitly. Instead, each matrix element is recomputed when needed. Enables solution of huge problems.



Summary

- Sparse matrix algorithms are more complicated than their dense equivalents, as we saw for sparse vector addition.
- Sparse matrix computations have a larger integer overhead associated with each floating-point operation.
- Still, using sparsity can save large amounts of CPU time and also memory space.
- We learned an efficient way of adding two sparse vectors using a dense initialised auxiliary array. You will be surprised to see how often you can use this trick.
- Compressed row storage (CRS) and its variants are useful data structures for sparse matrices.
- CRS stores the nonzeros of each row together, but does not sort the nonzeros within a row. Sorting is a mixed blessing: it may help, but it also takes time.