CS601: Software Development for Scientific Computing

Autumn 2022

Week6: Motifs – Matrix Computations with Dense and Sparse Matrices

Last week..

- Three fundamental ways to multiply two matrices
  - Comprising of dot products, linear combination of the left matrix columns, outer product updates
    - Commonly occurring algorithmic patterns / kernels :

      Dot product, AXPY and GAXPY, outer product, matrix-vector product, matrix-matrix product
- Linear algebra software (BLAS, LAPACK)
  - BLAS routines and categorization
- Algorithmic costs
  - Arithmetic cost
  - Data movement cost
- Computational intensity (examples: `axpy, matvec, matmul`)

Last week - Communication Cost

```
//Assume A, B, C are all nxn
for i=1 to n
  for j=1 to n
    for k=1 to n
      C(i,j)=C(i,j) + A(i,k)*B(k,j)
```

- n^2 words read: each row of A read once for each i.
- Assume that row i of A stays in fast memory during j=2, .. J=n
- Reading a row i of A

- loop k=1 to n: read C(i,j) into fast memory and update in fast memory
- End of loop k=1 to n: write C(i,j) back to slow memory

n^2 words read and n^2 words written (each entry of C read/written to memory once). = 2 n^2 words read/written

total cost = 3 n^2 + n^3 (if the cache size is n+n+1)

- Reading column j of B
- Suppose there is space in fast memory to hold only one column of B (in addition to one row of A and 1 element of C), then every column of B is read from slow memory to fast memory once in **inner two loops.**
- Each column of B read n times including **outer i loop =** n^3 words read

Last week – Computational Intensity of Matmul (ijk)

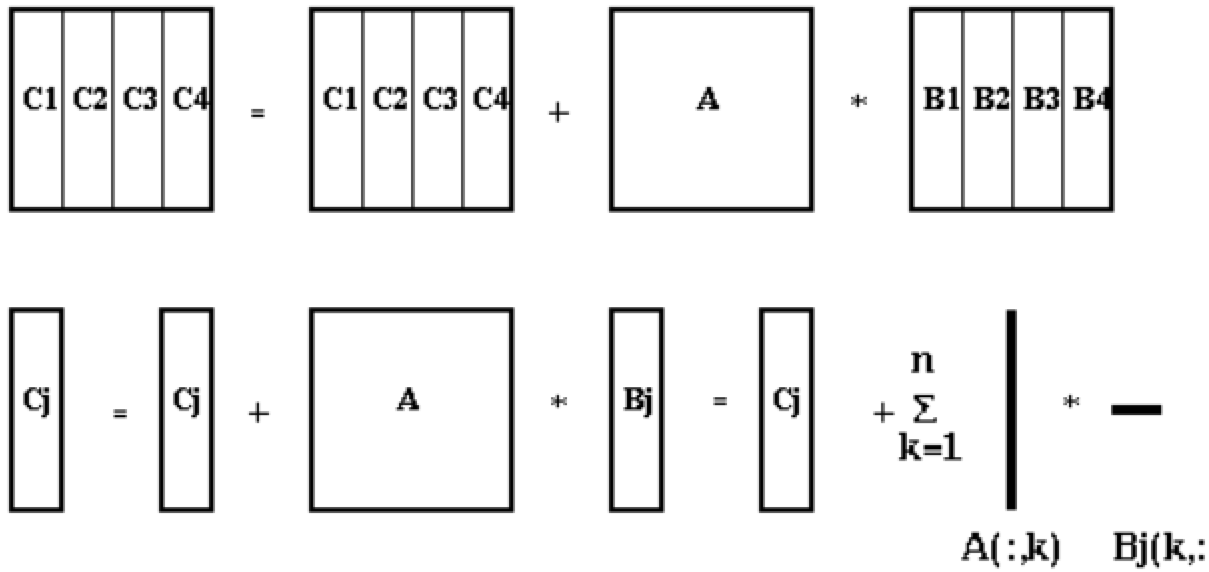
- Words moved = $n^3+3n^2 = n^3+O(n^2)$
- Number of arithmetic operations = $2n^3$ (from slide 35)
- computational intensity $q \approx 2n^3/n^3 = 2$. (computation to communication ratio)

  Same as q for matrix-vector?
  What if the fast memory has more space ? more than just two columns + one element space?

- Can we do better?

Last week - Blocked Matrix Multiply

- For N=4:




```
for j=1 to N
//Read entire Bj into fast memory
//Read entire Cj into fast memory
  for k=1 to n
   //Read column k of A into fast memory
   Cj=Cj + A(*,k) * Bj(k,*)
   //Write Cj back to slow memory
```


source: http://people.eecs.berkeley.edu/~demmel/cs267/lecture02.html

Last week – Computational Intensity

```
for j=1 to N
//Read entire Bj into fast memory
//Read entire Cj into fast memory
  for k=1 to n
   //Read column k of A into fast memory
   C(*,j)=C(*,j) + A(*,k)*Bj(k,*) //outer-product
        //Write Cj back to slow memory
```

n^2 words read: each column of B read once.

Nn^2 words read: each column of A read N times

$2n^2$ words read: read/write each entry of C to memory once.

- Number of arithmetic operations = $2n^3$
- $\boldsymbol{q = 2n^3/(N+3)n^2 = 2n/N}$**. Good!**

Blocked Matrix Multiply - General

$$C = \begin{bmatrix} C_{11} & C_{12} & .. & C_{1r} \\ C_{21} & C_{22} & .. & C_{2r} \\ & \vdots & & \\ C_{q1} & C_{q2} & .. & C_{qr} \end{bmatrix} \quad A = \begin{bmatrix} A_{11} & A_{12} & .. & A_{1p} \\ A_{21} & A_{22} & .. & A_{2p} \\ & \vdots & & \\ A_{q1} & A_{q2} & .. & A_{qp} \end{bmatrix} \quad B = \begin{bmatrix} B_{11} & B_{12} & .. & B_{1r} \\ B_{21} & B_{22} & .. & B_{2r} \\ & \vdots & & \\ B_{p1} & B_{p2} & .. & B_{pr} \end{bmatrix}$$

q r   q p   p r

- $A, B, C \in \mathbb{R}^{n \times n}$
- We wish to update C block-by-block: $C_{ij} = C_{ij} + \Sigma_{k=1}^{p} A_{ik}B_{kj}$
  - Assume that blocks of A, B, and C fit in cache. C_{ij} is roughly n/q by n/r, A_{ij} is roughly n/q by n/p, B_{ij} is roughly n/p by n/r.
  - But how to choose block parameters p, q, r such that assumption holds for a cache of size M?
    - i.e. given the constraint that $\frac{n}{q} \times \frac{n}{r} + \frac{n}{q} \times \frac{n}{p} + \frac{n}{p} \times \frac{n}{r} \leq M$

Blocked Matrix Multiply - General

- Maximize $\frac{2n^3}{qrp}$ subject to $\frac{n}{q} \times \frac{n}{r} + \frac{n}{q} \times \frac{n}{p} + \frac{n}{p} \times \frac{n}{r} \leq M$
  - $q_{opt} = p_{opt} = r_{opt} \approx \sqrt{\frac{3n^2}{M}}$
- Each block should roughly be a square matrix and occupy one third of the cache size
- Can we design algorithms that are independent of cache size?

Recursive Matrix Multiply

- Cache-oblivious algorithm
  - No matter what the size of the cache is, the algorithm performs at a near-optimal level
- Divide-conquer approach

$$\begin{bmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{bmatrix} \times \begin{bmatrix} B_{11} & B_{12} \\ B_{21} & B_{22} \end{bmatrix} = \begin{bmatrix} A_{11}B_{11} + A_{12}B_{21} & A_{11}B_{12} + A_{12}B_{22} \\ A_{21}B_{11} + A_{22}B_{21} & A_{21}B_{12} + A_{22}B_{22} \end{bmatrix}$$

- Apply the formula recursively to $A_{11}B_{11}$ etc.
  - Works neat when n is a power of 2.
- What layout format is preferred for this algorithm?
  - Row-major or Col-major? Neither.

Recursive Matrix Multiply

- Cache-oblivious Data structure

$$
\begin{bmatrix}
1 & 2 & 5 & 6 & 17 & 18 & 21 & 22 \\
3 & 4 & 7 & 8 & 19 & 20 & 23 & 24 \\
9 & 10 & 13 & 14 & 25 & 26 & 29 & 30 \\
11 & 12 & 15 & 16 & 27 & 28 & 31 & 32 \\
33 & 34 & 37 & 38 & 49 & 50 & 53 & 54 \\
35 & 36 & 39 & 40 & 51 & 52 & 55 & 56 \\
41 & 42 & 45 & 46 & 57 & 58 & 61 & 62 \\
43 & 44 & 47 & 48 & 59 & 60 & 63 & 64
\end{bmatrix} .
$$

- Matrix entries are stored in the order shown
  - E.g. row-major would have 1-8 in the first row, followed by 9-16 in the second and so on.

Summary- matmul

- Unblocked Matrix Multiplication - Loop Orderings and Properties

Loop Order	Inner Loop	Inner Two Loops	Inner Loop Data Access
i j k	dot	Vector x Matrix	A by row, B by column
j k i	saxpy	gaxpy	A by column, C by column
k j i	saxpy	Outer product	A by column, C by column
.. (3 more rows here..)			

Ref: Matrix Computations, 4th Ed., Golub and Van Loan

- Blocked matrix multiplication
  - Column blocking, row blocking, tiling
- Recursive matrix multiplication
  - Divide-conquer, Strassen's
- Many more?

Efficiency Considerations for a High-Performing Implementation

- Cache details (size)
- Data movement overhead
- Storage layout
- Parallel and ‘special’ functional Units (e.g. Vector units and fused multiply-add)

Parallel Functional Units

- IBM's RS/6000 and Fused Multiply Add (FMA)
  - Fuses multiply and an add into one functional unit (c=c+a*b)
  - The functional unit consists of 3 independent subunits : *Pipelining*
  - Example: Suppose the FMA unit takes 3 cycles to complete,

```
sum=0.0
for (i=0;i<n;i++)
  sum=sum+a[i]*b[i]
```

how many cycles do you need to execute this code snippet?

```
sum=0.0
for (i=0;i<n;i+=4)
  sum1=sum1+a[i]*b[i]
  sum2=sum2+a[i+1]*b[i+1]
  sum3=sum3+a[i+2]*b[i+2]
  sum4=sum4+a[i+3]*b[i+3]
```

how many cycles do you need to execute this code snippet?

Matrix Structure and Efficiency

- Sparse Matrices
  - E.g. banded matrices
  - Diagonal
  - Tridiagonal etc.
- Symmetric Matrices

Admit optimizations w.r.t.

- Storage
- Computation

Sparse Matrices - Motivation

- Matrix Multiplication with Upper Triangular Matrices (C=C+AB)

$$\underbrace{\begin{bmatrix} a_{11} & a_{12} & a_{13} \\ 0 & a_{22} & a_{23} \\ 0 & 0 & a_{33} \end{bmatrix}}_{A} \underbrace{\begin{bmatrix} b_{11} & b_{12} & b_{13} \\ 0 & b_{22} & b_{23} \\ 0 & 0 & b_{33} \end{bmatrix}}_{B} =$$

$$\underbrace{\begin{bmatrix} a_{11}b_{11} & a_{11}b_{12}+a_{12}\, b_{22} & a_{11}b_{13}+a_{12}\, b_{23} + a_{13}\, b_{13} \\ 0 & a_{22}b_{22} & a_{22}b_{23}+a_{23}\, b_{33} \\ 0 & 0 & a_{33}b_{33} \end{bmatrix}}_{AB}$$

The result, A*B, is also upper triangular.

The non-zero elements appear to be like the result of *inner-product*

Sparse Matrices - Motivation

- C=C+AB when A, B, C are upper triangular

```
for i=1 to N
   for j=i to N
       for k=i to j
           C[i][j] = C[i][j] + A[i][k]*B[k][j]
```

- Cost = $\Sigma_{i=1}^{N}\Sigma_{j=i}^{N}2(j-i+1)$ flops (why 2?)
- Using $\Sigma_{i=1}^{N}i \approx \frac{n^2}{2}$ and $\Sigma_{i=1}^{N}i^2 \approx \frac{n^3}{3}$
- $\Sigma_{i=1}^{N}\Sigma_{j=i}^{N}2(j-i+1) \approx \frac{n^3}{3}$, 1/3rd the number of flops required for dense matrix-matrix multiplication

Sparse Matrices

- Have lots of zeros (a *large* fraction)

x	x	o	o	x	o	o	o	x
o	x	o	o	x	o	x	o	o
o	x	x	x	o	x	o	o	x
x	o	o	x	o	o	x	o	o
o	x	o	x	x	o	o	o	x
o	x	x	o	o	o	x	x	x

- Representation
  – Many formats available
  – Compressed Sparse Row (CSR)

Implementation:Three arrays:

```
double *val;
int *ind;
int *rowstart;
```

Sparse Matrices - Example

- Using Arrays

```
double *val; //size= NNZ
int *ind; //size=NNZ
int *rowstart; //size=M=Number of rows
```

A

$$A = \begin{bmatrix} a_{11} & a_{12} & 0 & 0 & a_{15} & 0 & 0 & 0 & a_{19} \\ 0 & a_{22} & 0 & 0 & a_{25} & 0 & a_{27} & 0 & 0 \\ 0 & a_{32} & a_{33} & a_{34} & 0 & a_{36} & 0 & 0 & a_{39} \\ a_{41} & 0 & 0 & a_{44} & 0 & 0 & a_{47} & 0 & 0 \\ 0 & a_{52} & 0 & a_{54} & a_{55} & 0 & 0 & 0 & a_{59} \\ 0 & a_{62} & a_{63} & 0 & 0 & 0 & a_{67} & a_{68} & a_{69} \end{bmatrix}$$

val:

a_{11}	a_{12}	a_{15}	a_{19}	a_{22}	a_{25}	a_{27}	a_{32}	a_{33}	a_{34}	a_{36}	a_{39}	a_{41}	a_{44}	a_{47}	a_{52}	a_{54}	a_{55}	a_{59}	a_{62}	a_{63}	a_{67}	a_{68}	a_{69}

ind:

1	2	5	9	2	5	7	2	3	4	6	9	1	4	7	2	4	5	9	2	3	7	8	9

rowstart:

0	4	7	12	15	19	

Sparse Matrices: y=y+Ax

- Using arrays

```
for i=0 to numRows
  for j=rowstart[i] to rowstart[i+1]-1
     y[i] = y[i] + val[j]*x[ind[j]]
```

- Does the above code reuse y, x, and val ? (we want our code to reuse as much data elements as possible while they are in fast memory):
  - y? Yes. Read and written in close succession.
  - x? Possible. Depends on how data is scattered in val.
  - val? Less likely for a sparse matrix.

Sparse Matrices: y=y+Ax

- Optimization strategies:

```
for i=0 to numRows
  for j=rowstart[i] to rowstart[i+1]-1
     y[i] = y[i] + val[j]*x[ind[j]]
```

  - Unroll the j loop // we need to know the number of non-zeros per row
  - Move y[i] outside the loop //Possible only if y is not aliased.
  - Eliminate ind[i] and thereby the indirect access to elements of x. Indirect access is not good because we cannot predict the pattern of data access in x. //We need to know the column numbers
  - Reuse elements of x //The elements of a should be e.g. located closely

Sparse Matrices

- Further reading:

Refer to Lecture 15 (Spring 2018) at
https://inst.eecs.berkeley.edu/~cs267/archives.html

Banded Matrices

- Special case of sparse matrices, characterized by two numbers:
  - Lower bandwidth p, and upper bandwidth q
  - $a_{ij} = 0$ if $i > j+p$
  - $a_{ij} = 0$ if $j > i+q$
  - E.g. p=1, q=2
    for a 8x5 matrix

  (x represents non-zero element)

$$\begin{bmatrix} x & x & x & 0 & 0 \\ x & x & x & x & 0 \\ 0 & x & x & x & x \\ 0 & 0 & x & x & x \\ 0 & 0 & 0 & x & x \\ 0 & 0 & 0 & 0 & x \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{bmatrix}$$

Banded Matrices - Representation

- Optimizing storage (specific to banded matrices)

$$A = \begin{bmatrix} a_{11} & a_{12} & a_{13} & 0 & 0 \\ a_{21} & a_{22} & a_{23} & a_{24} & 0 \\ 0 & a_{32} & a_{33} & a_{34} & a_{35} \\ 0 & 0 & a_{43} & a_{44} & a_{45} \\ 0 & 0 & 0 & a_{54} & a_{55} \\ 0 & 0 & 0 & 0 & a_{65} \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{bmatrix} \Rightarrow \begin{array}{|ccccc|} \hline * & * & a_{13} & a_{24} & a_{35} \\ * & a_{12} & a_{23} & a_{34} & a_{45} \\ a_{11} & a_{22} & a_{33} & a_{44} & a_{55} \\ a_{21} & a_{32} & a_{43} & a_{54} & a_{65} \\ \hline \end{array}$$

A

A*band*

$A_{ij}=Aband(i-j+q+1, j)$

E.g. $A_{44} = Aband_{34}$

Banded Matrices: y= y + Aband x

- A=Aband: optimizing computation and storage

```
for j=1 to n
  alpha1=max(1, j-q)
  alpha2=min(n, j+p)
  beta1=max(1, q+2-j)
  for i=alpha1 to alpha2
     y[i]=y[i] + Aband(beta1+i-alpha1,j)*x[j]
```

- Cost? 2n(p+q+1) time! Much lesser than $2N^2$ time required for regular y=y+Ax (assuming p and q are much smaller than n)