CS601: Software Development for Scientific Computing

Autumn 2021

Week14:

Matrix Algebra

Course Progress..

- Last week: FMM, PA4, Matrix Algebra
  - FMM ideas - applying 3-step approximation (decomposition), optimizing (reuse computation), better approximation (multipole expansion), Cost.
  - PA4 discussion
  - Matrix algebra
    - Overview: matrix-matrix multiplication (motivation), program representation of a matrix, storage layout and performance implications.
- This week: Matrix algebra contd.

Matrix Multiplication

- Three fundamental ways to think of the computation
  1. Dot product

$$\begin{bmatrix}1 & 2\\3 & 4\end{bmatrix} \times \begin{bmatrix}5 & 6\\7 & 8\end{bmatrix} = \begin{bmatrix}1.5+2.7 & 1.6+2.8\\3.5+4.7 & 3.6+4.8\end{bmatrix}$$

  2. Linear combination of the columns of the left matrix

$$\begin{bmatrix}1 & 2\\3 & 4\end{bmatrix} \times \begin{bmatrix}5 & 6\\7 & 8\end{bmatrix} = \begin{bmatrix}5\begin{bmatrix}1\\3\end{bmatrix} + 7\begin{bmatrix}2\\4\end{bmatrix} & 6\begin{bmatrix}1\\3\end{bmatrix} + 8\begin{bmatrix}2\\4\end{bmatrix}\end{bmatrix}$$

  3. Sum of outer products

$$\begin{bmatrix}1 & 2\\3 & 4\end{bmatrix} \times \begin{bmatrix}5 & 6\\7 & 8\end{bmatrix} = \begin{bmatrix}\begin{bmatrix}1\\3\end{bmatrix}\begin{bmatrix}5 & 6\end{bmatrix} + \begin{bmatrix}2\\4\end{bmatrix}\begin{bmatrix}7 & 8\end{bmatrix}\end{bmatrix}$$

Dot Product

- Vector $x = \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix}$, Vector $y = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix}$ $\quad \mathrm{x_i}, \mathrm{y_i} \in \mathbb{R}$
- $x^T = [x_1 \quad x_2 \quad \cdot\cdot \quad x_n]$
- Dot Product or Inner Product: $c = x^T y$ $\mathrm{x}^\mathrm{T} \in \mathbb{R}^{1\times n}, y \in \mathbb{R}^{n\times 1}, c\ is\ scalar$

$$[x_1 \quad x_2 \quad \cdot\cdot \quad x_n] \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix} = [x_1 y_1 + x_2 y_2 + \ldots + x_n y_n]$$

- E.g. $[1 \quad 2 \quad 3] \begin{bmatrix} 4 \\ 5 \\ 6 \end{bmatrix} = [1 \times 4 + 2 \times 5 + 3 \times 6] = 32$

AXPY

- Computing the more common (a times x plus y): $y = y + ax$
- $$\begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix} = \begin{bmatrix} y \\ y_2 \\ \vdots \\ y_n \end{bmatrix} + a \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix}$$

```
..
for i=1 to n
    c[i] = c[i] +  x[i]*y[i]
..
```

- Cost? n multiplications and n additions = **`2n`** `or` **`O(n)`**

Matrix Vector Product

- Computing Matrix-Vector product: $c = c + Ax$, $A \in \mathbb{R}^{m\times r}, x \in \mathbb{R}^{r\times 1}$

$$\begin{bmatrix} c_1 \\ c_2 \\ \vdots \\ c_m \end{bmatrix} = \begin{bmatrix} c_1 \\ c_2 \\ \vdots \\ c_m \end{bmatrix} + \begin{bmatrix} a_{11} & a_{12} & .. & a_{1r} \\ a_{21} & a_{22} & .. & a_{2r} \\ & \vdots & & \\ a_{m1} & a_{m2} & .. & a_{mr} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_r \end{bmatrix} = \begin{bmatrix} c_1 \\ c_2 \\ \vdots \\ c_m \end{bmatrix} + \begin{bmatrix} a_{11}x_1 + & a_{12}x_2 + & .. & +a_{1r}x_r \\ a_{21}x_1 + & a_{22}x_2 + & .. & +a_{2r}x_r \\ & \vdots & & \\ a_{m1}x_1 + & a_{m2}x_2 + & .. & +a_{mr}x_r \end{bmatrix}$$

$\downarrow$ m $\rightarrow$ r $\qquad$ $\downarrow$ m $\rightarrow$ 1

- Rewriting Matrix-Vector product using dot products:

$$\begin{bmatrix} c_1 \\ c_2 \\ \vdots \\ c_m \end{bmatrix} = \begin{bmatrix} c_1 \\ c_2 \\ \vdots \\ c_m \end{bmatrix} + \begin{bmatrix} a_{11} & a_{12} & .. & a_{1r} \\ a_{21} & a_{22} & .. & a_{2r} \\ & \vdots & & \\ a_{m1} & a_{m2} & .. & a_{mr} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_r \end{bmatrix} = \begin{bmatrix} c_1 \\ c_2 \\ \vdots \\ c_m \end{bmatrix} + \begin{bmatrix} a_1^T x \\ a_2^T x \\ \vdots \\ a_m^T x \end{bmatrix}$$

- Cost? m rows involving dot products and having the form $c_i = c_i + x^T y$ (Per row cost = 2r (because $a_i, x \in \mathbb{R}^r$), Total cost = **2mr** or **O(mr)**)

Matrix-Matrix Product

- Computing Matrix-Matrix product $C = C + AB, A \in \mathbb{R}^{m\times r}, B \in \mathbb{R}^{r\times n}$, $C \in \mathbb{R}^{m\times n}$

$$\begin{bmatrix} c_{11} & c_{12} & .. & c_{1n} \\ c_{21} & c_{22} & .. & c_{2n} \\ & & \vdots & \\ c_{m1} & c_{m2} & .. & c_{mn} \end{bmatrix} = \begin{bmatrix} c_{11} & c_{12} & .. & c_{1n} \\ c_{21} & c_{22} & .. & c_{2n} \\ & & \vdots & \\ c_{m1} & c_{m2} & .. & c_{mn} \end{bmatrix} + \begin{bmatrix} a_{11} & a_{12} & .. & a_{1r} \\ a_{21} & a_{22} & .. & a_{2r} \\ & & \vdots & \\ a_{m1} & a_{m2} & .. & a_{mr} \end{bmatrix} \begin{bmatrix} b_{11} & b_{12} & .. & b_{1n} \\ b_{21} & b_{22} & .. & b_{2n} \\ & & \vdots & \\ b_{r1} & b_{r2} & .. & b_{rn} \end{bmatrix}$$

$\downarrow m \; \rightarrow n \qquad \downarrow m \; \rightarrow r \qquad \downarrow r \; \rightarrow n$

- Consider the AB part first.

$$\begin{bmatrix} a_{11} & a_{12} & .. & a_{1r} \\ a_{21} & a_{22} & .. & a_{2r} \\ & & \vdots & \\ a_{m1} & a_{m2} & .. & a_{mr} \end{bmatrix} \begin{bmatrix} b_{11} & b_{12} & .. & b_{1n} \\ b_{21} & b_{22} & .. & b_{2n} \\ & & \vdots & \\ b_{r1} & b_{r2} & .. & b_{rn} \end{bmatrix}$$

Matrix-Matrix Product

$$\begin{array}{cc} A & B \\ \begin{bmatrix} a_{11} & a_{12} & .. & a_{1r} \\ a_{21} & a_{22} & .. & a_{2r} \\ & : & & \\ a_{m1} & a_{m2} & .. & a_{mr} \end{bmatrix} & \begin{bmatrix} b_{11} & b_{12} & .. & b_{1n} \\ b_{21} & b_{22} & .. & b_{2n} \\ & : & & \\ b_{r1} & b_{r2} & .. & b_{rn} \end{bmatrix} \end{array}$$

$$= \begin{bmatrix} a_{11}b_{11} + a_{12}b_{21} + .. + a_{1r}x_{r1} & . & . & a_{11}b_{1n} + a_{12}b_{2n} + .. + a_{1r}x_{rn} \\ . & & . & \\ a_{m1}b_{11} + a_{m2}b_{21} + .. + a_{mr}x_{r1} & . & . & a_{m1}b_{1n} + a_{m2}b_{2n} + .. + a_{mr}x_{rn} \end{bmatrix}$$

$$= \begin{bmatrix} a_1^T b_1 & . & . & a_1^T b_n \\ . & . & & \\ a_m^T b_1 & . & . & a_m^T b_n \end{bmatrix}$$

$a_i^T \in \mathbb{R}^{1\times r}, b_j \in \mathbb{R}^{r\times 1}$

i ranges from 1 to m

j ranges from 1 to n

Matrix-Matrix Product using Dot Product Formulation

- Pseudocode - Matrix-Matrix product: $C = C + AB,\ A \in \mathbb{R}^{m \times r}, B \in \mathbb{R}^{r \times n}, C \in \mathbb{R}^{m \times n}$

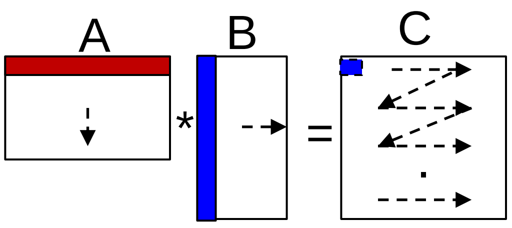
```
..
for i=1 to m
    for j=1 to n
        //compute updates involving dot products
```

$$c_{ij} = c_{ij} + a_i^T b_j$$

- Expanded:

```
..
for i=1 to m
    for j=1 to n
        for k=1 to r
```

$$c_{ij} = c_{ij} + a_{ik} b_{kj}$$



Elements of C matrix are computed from top to bottom, left to right. Per element computation, you need a row of A and a column of B.

Matrix-Matrix Product using Dot Product Formulation

- Pseudocode - Matrix-Matrix product: $C = C + AB,\ A \in \mathbb{R}^{m \times r}, B \in \mathbb{R}^{r \times n}, C \in \mathbb{R}^{m \times n}$

```
..
for i=1 to m
    for j=1 to n
        //compute updates involving dot products
```

$$c_{ij} = c_{ij} + a_i^T b_j$$

- Cost?
  - Per dot-product cost = `2r` $(a_i, b_j \in \mathbb{R}^r)$ Total cost = **`2mnr`** `or` **`O(mnr)`**

Common Computational Patterns

Some patterns that we see while doing Matrix-Matrix product:

- Dot Product or Inner Product: $x^T y$ ← Slide 4, Method 1
- Scalar **a** times **x** **p**lus **y**: y=y+ax OR `axpy` ← Slide 4, Method 2
- Scalar times **x**: αx
- **M**atrix times **x** **p**lus **y**: y=y+Ax ← Slide 4, Method 1
  - generalized `axpy` OR `gaxpy`
- Outer product: C=C+xy^T ← Slide 4, Method 3
- **M**atrix times **M**atrix plus Matrix
  - `GEMM` or generalized matrix multiplication

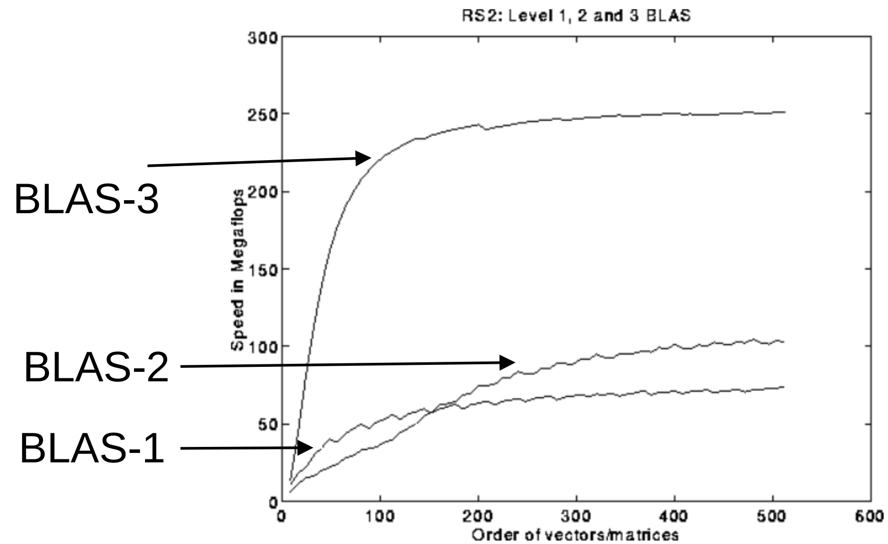
BLAS – Basic Linear Algebra Subroutines

- Level-1 or BLAS-1 (46 operations, routines operating on vectors mostly)
  - axpy, dot product, rotation, scale, etc.
  - 4 versions each: **S**ingle-precision, **d**ouble-precision, **c**omplex, complex-double (**z**)
  - E.g. saxpy, daxpy, caxpy etc.
  - **Do O(n) operations on O(n) data.**
- Level-2 or BLAS-2 (25 operations, routines operating on matrix-vectors mostly)
  - E.g. GEMV ($\alpha A.x + \beta y$), GER (Rank-1 update $A = A + y.x^T$), Triangular solve ($y = T.x, T\ is\ a\ triangular\ matrix$) etc.
  - 4 versions each, **do $O(n^2)$ operations on $O(n^2)$ data.**

BLAS – Basic Linear Algebra Subroutines

- Level-3 or BLAS-3 (9 basic operations, routines operating on matrix-matrix mostly)
  - GEMM ($C = \alpha A.B + \beta C$),
  - Multiple triangular solve ($Y = TX$, T is triangular, X is rectangular)
  - **Do O(n^3) operations on O(n^2) data.**

- *Why categorize as BLAS-1, BLAS-2, BLAS-3?*
  - *Performance*



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

Computational Intensity

- Average number of operations performed per data element (word) read/written from slow memory
  - E.g. Read/written m words from memory. Perform f operations on m words.
  - Computational Intensity $q = f/m$ (*flops per word*).
- We want to *maximize* the computational intensity
- What is q for axpy? Matrix-vector product? Matrix-Matrix product?

Computational Intensity - axpy

$$\begin{bmatrix} c_1 \\ c_2 \\ \vdots \\ c_n \end{bmatrix} = \begin{bmatrix} c_1 \\ c_2 \\ \vdots \\ c_n \end{bmatrix} + \begin{bmatrix} x_1 & x_2 & \cdots & x_n \end{bmatrix} \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix} = \begin{bmatrix} c_1 \\ c_2 \\ \vdots \\ c_n \end{bmatrix} + \begin{bmatrix} x_1 \times y_1 \\ x_2 \times y_2 \\ \vdots \\ x_n \times y_n \end{bmatrix}$$

```
Read(x) //read x from slow memory
Read(y) //read y from slow memory
Read(c) //read c from slow memory
for i=1 to n
   c[i] = c[i] +  x[i]*y[i]  //do arithmetic on data read
Write(c) //write c back to slow memory
```

- Number of memory operations = 4n (assuming one word of storage for each component (x_i, y_i, c_i) of vectors x, y, c resp.)
- Number of arithmetic operations = 2n (one addition and one multiplication per row.)
- **q=2n/4n = 1/2**

Computational Intensity – matrix-vector

- Assume m=r=n =n

$$\begin{bmatrix} c_1 \\ c_2 \\ \vdots \\ c_m \end{bmatrix} = \begin{bmatrix} c_1 \\ c_2 \\ \vdots \\ c_m \end{bmatrix} + \begin{bmatrix} a_{11} & a_{12} & .. & a_{1r} \\ a_{21} & a_{22} & .. & a_{2r} \\ & & \vdots & \\ a_{m1} & a_{m2} & .. & a_{mr} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_r \end{bmatrix} = \begin{bmatrix} c_1 \\ c_2 \\ \vdots \\ c_m \end{bmatrix} + \begin{bmatrix} a_{11}x_1 + & a_{12}x_2 + & .. & +a_{1r}x_r \\ a_{21}x_1 + & a_{22}x_2 + & .. & +a_{2r}x_r \\ & & \vdots & \\ a_{m1}x_1 + & a_{m2}x_2 + & .. & +a_{mr}x_r \end{bmatrix}$$

- Number of memory operations = $n^2 + 3n$ = $n^2 + O(n)$
- Number of arithmetic operations = $2n^2$
- $\boldsymbol{q \approx 2n^2/n^2 \ = \ 2}$

Computational Intensity – matrix-matrix

```
for i=1 to n
//Read row i of A into fast memory
        for j=1 to n
        //Read C(i,j) into fast memory
        //Read column j of B into fast memory
        for k=1 to n
               C(i,j)=C(i,j) + A(i,k)*B(k,j)
        //Write C(i,j) back to slow memory
```

n^2 words read: each row of A read once for each i. Assume that the row read stays in fast memory during the execution of inner two loops.

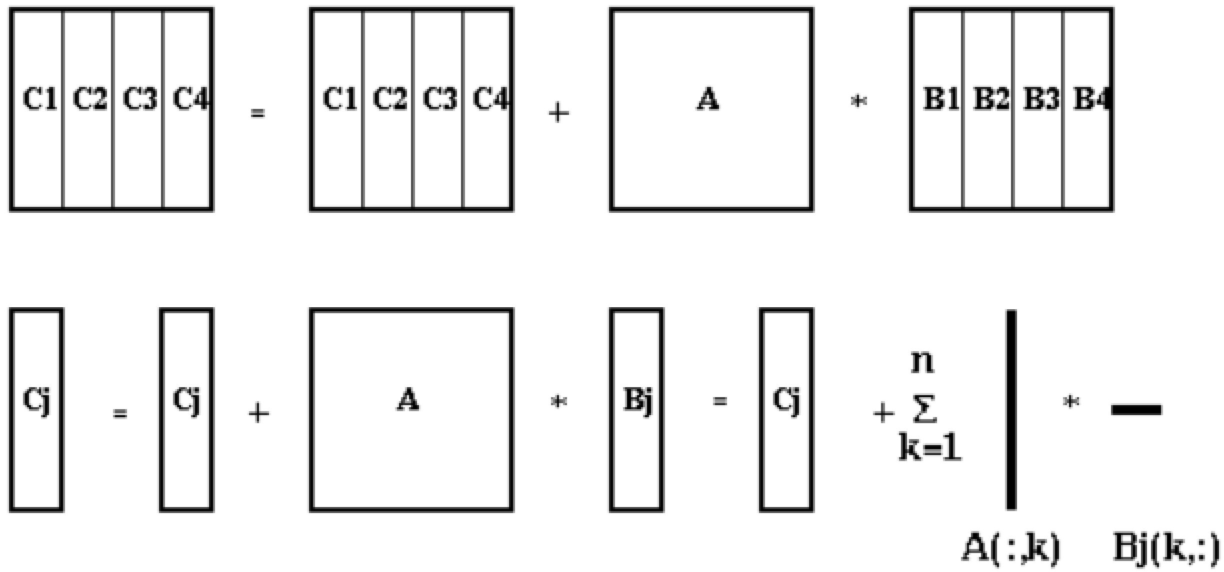
n^3 words read: each column of B read n^2 times

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

- Number of memory operations = $n^3 + 3n^2 = n^3 + O(n^2)$
- Number of arithmetic operations = $2n^3$
- $\boldsymbol{q \approx 2n^3/n^3 \ = \ 2.}$ *Same as matrix-vector?*
- What if the fast memory has space to hold entire B matrix, a row of A matrix, and one element of C matrix?

Blocked Matrix Multiply

- For N=4:




```
for j=1 to N
//Read column j of B into fast memory
//Read column j of C 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 C(i,j) back to slow memory
```


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

Computational Intensity - Blocked Matrix Multiply

```
for j=1 to N
//Read column j of B into fast memory
//Read column j of C 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 C(i,j) 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!**