Advanced Numerical Methods September 14 and 16, 2011

Lecture Notes 1: Matrix multiplication

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1 Matrix multiplication

1.1 Basic definition

- Direct multiplication

Let $A = \begin{bmatrix} a_{11} & a_{12} & \cdots & a_{1p} \\ a_{21} & a_{22} & \cdots & a_{2p} \\ \vdots & \vdots & & \vdots \\ a_{m1} & a_{m2} & \cdots & a_{mp} \end{bmatrix}, B = \begin{bmatrix} b_{11} & b_{12} & \cdots & b_{1n} \\ b_{21} & b_{22} & \cdots & b_{2n} \\ \vdots & \vdots & & \vdots \\ b_{p1} & b_{p2} & \cdots & b_{pn} \end{bmatrix}$ where $\begin{matrix} \dim(A) = (m,p) \\ \dim(B) = (p,n) \end{matrix}$

$$\text{Then } C = A \cdot B = \begin{bmatrix} c_{11} & c_{12} & \cdots & c_{1n} \\ c_{21} & c_{22} & \cdots & c_{2n} \\ \vdots & \vdots & & \vdots \\ c_{m1} & c_{m2} & \cdots & c_{mn} \end{bmatrix}$$

$$\text{where } c_{ij} = \sum_{k=1}^{p} a_{ik} b_{kj}, \forall i = 1, \cdots, m, j = 1, \cdots, n \ , \ \dim(C) = (m,n) \qquad (1)$$

$$\text{Complexity} : O(mnp) \begin{cases} \text{multiplication } \# : mnp \\ \text{addition } \# : mn(p-1) \end{cases}$$

- Inner Product form

Generally, we treat all vectors as column vectors.

Let $\vec{a}, \vec{b}$ with $\dim(\vec{a}) = \dim(\vec{b}) = n$

$\Rightarrow \vec{a} = \begin{bmatrix} a_1 \\ \vdots \\ a_n \end{bmatrix}, \vec{b} = \begin{bmatrix} b_1 \\ \vdots \\ b_n \end{bmatrix}$ and the inner product $(\vec{a} \cdot \vec{b}) = a_1 b_1 + ... + a_n b_n = \vec{a}^T \vec{b}$

Hence, if $A = \begin{bmatrix} a_{11} & \cdots & a_{1p} \\ a_{21} & \cdots & a_{2p} \\ \vdots & & \vdots \\ a_{m1} & \cdots & a_{mp} \end{bmatrix} = \begin{bmatrix} \vec{a_1}^T \\ \vec{a_2}^T \\ \vdots \\ \vec{a_m}^T \end{bmatrix}, B = \begin{bmatrix} b_{11} & b_{12} & \cdots & b_{1n} \\ \vdots & \vdots & & \vdots \\ b_{p1} & b_{p2} & \cdots & b_{pn} \end{bmatrix} = \begin{bmatrix} \vec{b_1} & \vec{b_2} & \cdots & \vec{b_n} \end{bmatrix}$

$$\text{Then } C = A \cdot B = \begin{bmatrix} \vec{a_1}^T \vec{b_1} & \vec{a_1}^T \vec{b_2} & \cdots & \vec{a_1}^T \vec{b_n} \\ \vdots & \vdots & & \vdots \\ \vec{a_m}^T \vec{b_1} & \vec{a_m}^T \vec{b_2} & \cdots & \vec{a_m}^T \vec{b_n} \end{bmatrix}$$

$$\text{where } c_{ij} = \vec{a_i}^T \vec{b_j}, i = 1, \cdots, m, j = 1, \cdots, n \qquad (2)$$

- Outer Product form

Let $A = \begin{bmatrix} a_{11} & a_{12} & \cdots & a_{1p} \\ \vdots & \vdots & & \vdots \\ a_{m1} & a_{m2} & \cdots & a_{mp} \end{bmatrix} = \begin{bmatrix} \vec{a_1} & \vec{a_2} & \cdots & \vec{a_p} \end{bmatrix}, B = \begin{bmatrix} b_{11} & \cdots & b_{1n} \\ b_{21} & \cdots & b_{2n} \\ \vdots & & \vdots \\ b_{p1} & \cdots & b_{pn} \end{bmatrix} = \begin{bmatrix} \vec{b_1}^T \\ \vec{b_2}^T \\ \vdots \\ \vec{b_p}^T \end{bmatrix}$

$$\text{Then } C = A \cdot B = \sum_{k=1}^{p} \vec{a_k} \vec{b_k}^T.$$

The elements in C are the same as (1).

Proof:

Let $C = C^{(1)} + \cdots + C^{(k)} + \cdots + C^{(p)}, C^{(k)} = \vec{a_k} \vec{b_k}^T$

$$\therefore c_{ij}^{(k)} = a_{ik} b_{kj} \Rightarrow c_{ij} = \sum_{k=1}^{p} c_{ij}^{(k)} = \sum_{k=1}^{p} a_{ik} b_{kj}$$

...the same as (1)

e.g. $A = \begin{bmatrix} 1 & 2 \\ 3 & 4 \end{bmatrix}, B = \begin{bmatrix} 1 \\ 2 \end{bmatrix} \Rightarrow C = C^{(1)} + C^{(2)} = \begin{bmatrix} 1 \\ 3 \end{bmatrix} + \begin{bmatrix} 4 \\ 8 \end{bmatrix} = \begin{bmatrix} 5 \\ 11 \end{bmatrix}$

Review Rank of a matrix.

Column(row) rank : the maximum number of linearly independent column(row) vectors.

The column rank and the row rank are always equal and hence it is simply called the rank of a matrix.

- Block form

$A = \begin{bmatrix} A_{11} & A_{12} & \cdots & A_{1P} \\ \vdots & \vdots & & \vdots \\ A_{M1} & A_{M2} & \cdots & A_{MP} \end{bmatrix}$ which contains P (M) blocks per row (column).

e.g. If $\dim(A)$=(1024, 1024), $\dim(A_{ij})$ could be (64,64)$\cdots$ all the same

e.g. $\begin{bmatrix} \dim(5,6) & \dim(5,8) & \dim(5,7) \\ \dim(3,6) & \dim(3,8) & \dim(3,7) \\ \dim(2,6) & \dim(2,8) & \dim(2,7) \end{bmatrix}$ whose all boxes in the same row(column) have the same height(width).

Let B= $\begin{bmatrix} B_{11} & \cdots & B_{1N} \\ \vdots & & \vdots \\ B_{P1} & \cdots & B_{PN} \end{bmatrix}$, if we want to do block form multiplication, $\dim(A_{IK})_2 = \dim(B_{KJ})_1$ should be true $\forall 1 \le I \le M, 1 \le J \le N, 1 \le K \le P$.

That is, $C = A \cdot B = \begin{bmatrix} C_{11} & C_{12} & \cdots & C_{1N} \\ \vdots & \vdots & & \vdots \\ C_{M1} & C_{M2} & \cdots & C_{MN} \end{bmatrix}, C_{IJ} = \sum_{k=1}^{P} A_{IK} B_{KJ}$

Question How to prove it the same as (2)? (Homework problem)

1.2 Performance Consideration

- Performance
  (1)computation
  (2)bandwidth
  (3)memory latency

  Computation $\rightarrow T_c$, bandwidth, memory latency $\rightarrow T_d$.
  Assume two $n \times n$ matrices A and B, then $C = A \cdot B$ is also $n \times n$. $\Rightarrow$ Totally $3n^2$ data to be stored.

  $\therefore T_d$ is related to $3n^2$, T_c is related to $2n^3$.

  What if the storing spaces are much less?

  If we only have $3b^2$ spaces, $b \ll n$, in our "fast"memory and assume $b^2 \approx n$. In order to compute C, A will be loaded n times, each of them is a complete A (i.e. n^2 elements), as shown in Fig. 1. So the total data movement is $O(n^3)$.

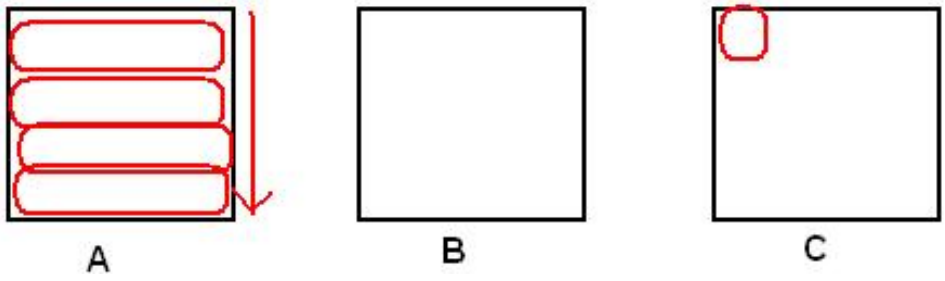

Figure 1: If the spaces are much less.

How about using block form?

Computing a block C_{ij} needs $2b^2 \times \frac{n}{b} = 2bn$ data movement and $2b^3 \times \frac{n}{b} = 2b^2 n$ computations, as shown in Fig. 2.

$\therefore$ We have $(\frac{n}{b})^2$ C_{ij} blocks and hence require $2bn \times \frac{n^2}{b^2} = \frac{2n^3}{b}$ loadings, $2b^2 n \times \frac{n^2}{b^2} = 2n^3$ computations.$\Rightarrow T_c = 2n^3, T_d = \frac{2n^3}{b} \cdots$ b times less data movement.

- A brief history of (Dense) Linear Algebra software

  – BLAS (1973-1977)
  Also called BLAS 1, do $O(n^1)$ ops on $O(n^1)$ data. Standard library of 15 operations (mostly) on vectors.

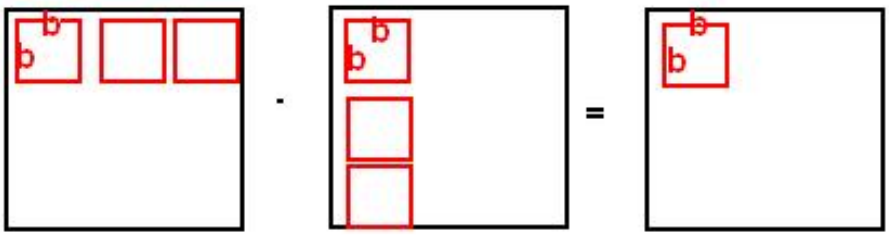

Figure 2: Using block form.

– BLAS 2 (1984-1986)
Standard library of 25 operations (mostly) on matrix/vector pairs. Do $O(n^2)$ ops on $O(n^2)$ data.

– BLAS 3 (1987-1988)
Standard library of 9 operations (mostly) on matrix/matrix pairs, functions are integrated. Do $O(n^3)$ ops on $O(n^2)$ data...much higher computational intensity.

– LAPACK (1989-now)
"Linear Algebra PACKage"-uses BLAS-3. Much more generalized.

– ScaLAPACK (1995-now)
"Scalable LAPACK", uses MPI to parallelize. More complex data structures, algorithms than LAPACK.