HPC Doctoral Taught Centre: Autumn Academy

Preliminary Exercises by J.H. Davenport — J.H.Davenport@bath.ac.uk

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1 Matrices

Much of High-Performance Computing deals with *regular* mathematical structures, of which the most obvious kinds are vectors and matrices. Unfortunately there are not in everyone's mathematical background:

- the simplest (and cheapest) reference text that we have found that covers this seems to be: A Level Mathematics for Edexcel: Further Pure FP1 (ISBN 9780435519230);
- the Wikipedia page on Matrix (mathematics) and its linked pages are not bad (except that it uses [...] where I am using (...): I hope this doesn't confuse, but both notations are in use).

2 Exercises

All of you should be familiar with programming in *some* language. These exercises are to be carried out in whatever language you feel most comfortable with: we will show C/Fortran equivalents at the Academy itself. For those of you whose programming language of choice is MatLab, please use MatLab for or while statements, rather than the built-in MatLab features, and the same applies to other languages with built-in matrix manipulation.

I say "Write a function to" — the precise method will depend on your langauge: it might be a method, function, procedure or subroutine.

1. Write a function to add two $m \times n$ matrices together, i.e. input the matrices of $a_{i,j}$ and $b_{i,j}$, and output the matrix of $c_{i,j}$:

$$\left(\begin{array}{ccc}a_{1,1}&\ldots&a_{1,n}\\\vdots&\ddots&\vdots\\a_{m,1}&\ldots&a_{m,n}\end{array}\right)+\left(\begin{array}{ccc}b_{1,1}&\ldots&b_{1,n}\\\vdots&\ddots&\vdots\\b_{m,1}&\ldots&b_{m,n}\end{array}\right)=\left(\begin{array}{ccc}c_{1,1}&\ldots&c_{1,n}\\\vdots&\ddots&\vdots\\c_{m,1}&\ldots&c_{m,n}\end{array}\right),$$

where $c_{i,j} = a_{i,j} + b_{i,j}$.

2. Write a function to multiply an $m \times n$ matrix by an *n*-vector, i.e. input the matrix of $a_{i,j}$ and the vector of c_j and output the vector of v_j :

$$\left(\begin{array}{ccc}a_{1,1}&\ldots&a_{1,n}\\\vdots&\ddots&\vdots\\a_{m,1}&\ldots&a_{m,n}\end{array}\right)\times\left(\begin{array}{c}c_{1}\\\vdots\\c_{n}\end{array}\right)=\left(\begin{array}{c}d_{1}\\\vdots\\d_{m}\end{array}\right),$$

where $d_i = \sum_{j=1}^n a_{i,j} c_j$.

3. Write a function to multiply an $m \times n$ matrix by an $n \times p$ matrix, i.e. input the matrices of $a_{i,j}$ and $b_{i,j}$, and output the matrix of $c_{i,j}$:

$$\left(\begin{array}{ccc}a_{1,1}&\ldots&a_{1,n}\\\vdots&\ddots&\vdots\\a_{m,1}&\ldots&a_{m,n}\end{array}\right)\times\left(\begin{array}{ccc}b_{1,1}&\ldots&b_{1,p}\\\vdots&\ddots&\vdots\\b_{n,1}&\ldots&b_{n,p}\end{array}\right)=\left(\begin{array}{ccc}c_{1,1}&\ldots&c_{1,p}\\\vdots&\ddots&\vdots\\c_{m,1}&\ldots&c_{m,p}\end{array}\right),$$

where $c_{i,k} = \sum_{j=1}^{n} a_{i,j} b_{j,k}$.

Note that, depending on the system you are using, you may or may not find it easier to re-use exercise 2 here.

4, harder Write a function to solve a set of linear equations, i.e. input the matrix of $a_{i,j}$ and the vector of c_j and output the vector of x_j :

$$\left(\begin{array}{ccc}a_{1,1}&\ldots&a_{1,n}\\\vdots&\ddots&\vdots\\a_{n,1}&\ldots&a_{n,n}\end{array}\right)\times\left(\begin{array}{c}x_1\\\vdots\\x_n\end{array}\right)=\left(\begin{array}{c}c_1\\\vdots\\c_n\end{array}\right),$$

where $d_i = \sum_{j=1}^n a_{i,j}c_j$. This is a process known as *Gaussian elimination*, and actually has many subtleties when translated into a numerical process, some of which will be discussed during the Academy.