Computational Physics 301

Exercise 1: Matrices and Linear Algebra
Submission deadline: Monday 17th Feb. 2014, 9:00am

2013-14

1 Introduction

The manipulation of matrices is a core topic in numerical analysis. Matrix methods can be used to solve many classes of physical problems, although (as with all numerical techniques) care has to be taken in the choice and implementation of appropriate algorithms.

This exercise introduces simple matrix techniques to solve mathematical problems, investigates some of the considerations of stability and efficiency in choosing appropriate algorithms.

2 Matrix Inversion for Linear Algebra

A set of simultaneous linear equations can always be written as a matrix equation. For example, two equations in two unknowns (x_1 and x_2)

$$\begin{aligned} a_{11}x_1 + a_{12}x_2 &= c_1 \\ a_{21}x_1 + a_{22}x_2 &= c_2 \end{aligned}$$

can be rewritten as

$$\begin{pmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = \begin{pmatrix} c_1 \\ c_2 \end{pmatrix}$$

An arbitrary set of equations is

$$\mathrm{A}\mathbf{x} = \mathbf{c} \tag{1}$$

where A is the matrix of coefficients, $\mathbf{x}$ is the vector of unknown variables $x_1, x_2, ...$ and $\mathbf{c}$ is the known vector of constants. The solution to Equation 1 can be obtained by pre-multiplying by the inverse of A:

$$\begin{aligned} \mathrm{A}^{-1}\mathrm{A}\mathbf{x} &= \mathrm{A}^{-1}\mathbf{c} \\ \Leftrightarrow \mathbf{x} &= \mathrm{A}^{-1}\mathbf{c} \end{aligned}$$

<u>**Task:**</u> Write **your own routine** to calculate the inverse of an arbitrary square $n \times n$ matrix with up to (at a minimum) four rows using the standard inversion formula:

$$\mathrm{A}^{-1} = \frac{1}{\det \mathrm{A}} \mathrm{C}^T$$

where C is the matrix of cofactors of A. In the process of implementing this, you may become aware of a way to perform this calculation for an arbitrary $n \times n$ matrix. Verify that your routine works by testing it against a few hand-calculated inversions, and then investigate its performance: how accurate is it, how robust is it and how does the time it takes scale with the number of rows?

3 Algorithms for Linear Algebra

A number of algorithms are used in preference to the analytical inversion method. A basic technique is "Gauss-Jordan elimination" in which a multiple of one row is subtracted from another to eliminate variables (just as you would do in solving simultaneous equations by hand). Two further common techniques are LU Decomposition and Singular Value Decomposition.

3.1 LU Decomposition

The solution to Equation 1 is straightforward if the matrix is triangular, i.e. all of the entries either above or below the diagonal are zero. For example, with a lower-diagonal matrix:

$$\begin{pmatrix} a_{11} & 0 & 0 & \dots \\ a_{21} & a_{22} & 0 & \dots \\ \vdots & & & \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ \vdots \end{pmatrix} = \begin{pmatrix} c_1 \\ c_2 \\ \vdots \end{pmatrix}$$

The first row directly gives the solution $x_1 = c_1/a_{11}$. This can then be substituted into the second row to give x_2 and so on in similar fashion.

LU decomposition works by reformulating the general matrix A as the product LU of a lower- and an upper-triangular matrix. (This is quite straightforward to do, but knowing the details is not necessary). The general solution is then reduced to the successive solution of two triangular equations:

$$\mathrm{L}\mathbf{y} = \mathbf{c}$$

and

$$\mathrm{U}\mathbf{x} = \mathbf{y}$$

3.2 Singular Value Decomposition

SVD involves writing a general matrix in the form

$$\mathrm{A} = \mathrm{UDV}$$

where U and V are orthnormal matrices, and D is a diagonal matrix containing the "singular" values.

Task: Compare the performance of LUD, SVD and the analytic formula in inverting matrices. You should use LUD and SVD routines **from GSL or another external library**. In particular, investigate the scaling with the number of rows and the behaviour when the set of equations is close to singular, e.g.

$$\begin{aligned} x + y + z &= 5 \\ x + 2y - z &= 10 \\ 2x + 3y + kz &= 15 \end{aligned}$$

for small k.

Physics Problem: A remote overhead camera at a football stadium is suspended by three cables attached to the roof. Each cable is fed from a motorised drum so the camera can be moved around by changing the lengths of the cables. The camera has a mass of 50 kg and the attachment points are all 70 m from the centre of the pitch forming an equilateral triangle in a horizontal plane. Using an appropriate matrix algorithm, calculate and plot the tension in one of the cables as a function of the camera's position as it is moved in a horizontal plane a constant depth (10 m) below the attachment points. What is the maximum tension and where does it occur? [You may ignore the mass of the cables].