

Matrices and Eigenvalues

Many scientific problems can be represented using

3 main types of matrix problems

1)

2)

3)

Matrix types include

- Hermitian

- Real

- Positive Definite: $\operatorname{Re}\{z^t M z\} > 0$ for all complex z

For M also Hermitian: $r =$

and all eigenvalues are

- Unitary

- Diagonal

- Tridiagonal

$\left(\begin{array}{c} \\ \\ \\ \end{array} \right)$

- Upper and Lower Triangular

- Sparse Matrix

- Useful to recognize if number

Goal: manipulate matrix

Matrix Algebra

Optimal matrix manipulation depends on

in C, the matrix is stored

in Fortran, matrix is stored

C:

F:

Example: in Fortran

```
do i = 1, n
  do j = 1, n
```

```
    A(i,j)
```

```
  enddo
```

```
enddo
```

```
do j = 1, n
  do i = 1, n
    A(i,j) =
```

```
  enddo
```

```
enddo
```

F90 has built-in matrix manipulation routines

- above is just

- $A =$

is

- $A = B * C$ is

show InnerLoopROW.f90, InnerLoopCOL.f90 ...

Systems of Linear Equations

Consider solving for

$$\begin{pmatrix} \quad \\ \quad \\ \quad \end{pmatrix} \begin{pmatrix} \quad \\ \quad \\ \quad \end{pmatrix} = \begin{pmatrix} \quad \\ \quad \\ \quad \end{pmatrix}$$

- for solution to exist,

We can use Gaussian elimination

- idea: transform set of eqⁿs so that coefficient matrix is
- at each step of algorithm, eliminate

Ex 3×3 $a_{11}x_1 + a_{12}x_2 + a_{13}x_3 = b_1$ (1)

- multiply (1) by

- multiply (1) by

$$\Rightarrow a_{11}x_1 + a_{12}x_2 + a_{13}x_3 = b_1$$

where $a'_{ij} =$

$$b'_i =$$

x_1 eliminated from

Now eliminate

taking $a_{11}x_1$ and subtracting from

$$\Rightarrow a_{11}x_1 + a_{12}x_2 + a_{13}x_3 = b_1$$

where

For $n \times n$ matrix, this procedure is done
Once in n steps, we get \vec{x} through

In general

$$a_{11}x_1 + a_{12}x_2 + a_{13}x_3 + \dots + a_{1n}x_n = \tilde{b}_1$$

$$x_n =$$

$$x_i =$$

Number of operations required for a set of
is proportional to
large matrices

For matrix manipulations it is best to use efficient algorithms/routines freely available from

e.g.

- such routines, available here as reference implementations, have been incorporated in various libraries like

GSL & MKL

(But using libraries without any idea of how they work can lead to trouble sooner or later.)

Such routines are

E.g. Our simple Gaussian elimination would

These problems can be reduced by , or rearranging rows s.t.

Depending on type of matrix () different routines exist for

Manipulating matrices is often the

browse through LAPACK

Note on LAPACK routine used to solve

Employs

$$A = \begin{pmatrix} & & & \\ & & & \\ & & & \end{pmatrix}$$

$$Ax = b$$

Show use of SGESV to solve

$$\begin{pmatrix} 1 & 2 & 3 \\ 4 & 5 & 6 \\ 3 & 8 & 9 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \\ -1 \end{pmatrix}$$

$$x_1 = 0$$

$$x_2 = -2$$

$$x_3 = 5/3$$