### Matlab

Linear Algebra etc.

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## Please Interrupt

This course assumes a fair amount of background

- 1: that you already happy using Matlab
- E.g. basic use, syntax and error handling
- 2: that you already know some linear algebra At least up to elementary use of matrices It will refer to a bit more, but will explain
- If you don't understand, please interrupt Don't feel afraid to ask any question you want to

## Beyond the Course

```
Matlab_numerics/
```

```
http://www.mathworks.com/access/helpdesk/.../help/techdoc/
```

# Prerequisite

You need to know the basics of matrix arithmetic Including how they are used in linear algebra

No longer part of ordinary A-level mathematics
 It is only in A-level Further Pure mathematics

The following page describes places to learn it from:

matrices/

# What Is Linear Algebra?

Could call it the arithmetic of matrices It's more general than you might think

Need to explain some mathematics Don't Panic – it will be over–simplified!

You can do a great deal in Matlab

• As always, follow the motto "festina lente" "Make haste slowly" – i.e. start with simple uses

### Structure Of Course

- Overview of what analyses are possible
- Basic matrix facilities in Matlab
- Real and complex linear algebra
- Summary of more advanced matrix facilities

### What Are Matrices?

Effectively a 2-D rectangular grid of elements

```
1.2 2.3 3.4 4.5
5.6 6.7 7.8 8.9
9.0 0.1 1.2 2.3
```

1-D arrays are also called vectors

n-D arrays may be called tensors
Won't cover them, because poor in Matlab

Yes, mathematicians, I know – over-simplification!

# Terminology

Some people use matrix to mean only 2–D
Others talk about matrices of any rank
The standard term is matrix algebra not array algebra

Matlab tends to use the term array generically

- But it also uses array for other purposes
- This course often uses matrix generically But uses vector or n-D where it matters

### Elements of Matrices

- These are not limited to real numbers
   Can actually belong to any mathematical field
   Examples:
  - Real (ℝ) or complex (ℂ) numbers
  - Ratios of integers (rational numbers)
  - Ratios of polynomials/multinomials
  - And more

Course covers real but mentions complex You use them in almost exactly the same way

### Reminder

123456789 is an integer

12345.6789 is a real number

123.45+678.9i is a complex number

complex(123.45,678.9) creates the same number

### What Can We Do?

All of basic matrix arithmetic, obviously Including some quite complicated operations

Solution of simultaneous linear equations Eigenvalues and eigenvectors Matrix decompositions of quite a few types

Plus (with more hassle) their error analysis

Fourier transforms are just linear algebra, too

# Physics, Chemistry etc.

Anything expressible in normal matrix notation

That's almost everything, really!

But that isn't always practically possible Matlab is slower than NAG, but you can call NAG

 Working with expressions is not covered You need to use Mathematica for that Matlab has a few facilities, but not as much Can get more information using expressions

### Statistical Uses

- Regression and analysis of variance
- Multivariate probability functions

Calculating the errors is the tricky bit It's NOT the same as in most physics!

- Also Markov processes finite state machines
   This is where transitions are probabilistic
   Working with these is just more matrix algebra
- Standard textbooks give the matrix formulae
   You just carry on from there in theory!

### Matlab and Matrices

Will describe how Matlab provides them

And explain how to construct and display them

And perform other basic matrix operations

### Matrix Notation (1)

Conventional layout of a 4x3 matrix *A* Multiplied by a 3 vector

 $A_{3,2}$  is the value 32

530 is 
$$21 \times 7 + 22 \times 8 + 23 \times 9$$

## Matrix Notation (2)

Now we do the same thing in Matlab All of the details will be explained in due course

## Notation in Papers

There are a zillion – one for each sub-area 'Standard' tensor notation has changed, too Here is another over-simplification

 $A_i$ ,  $A^i$ ,  $\bar{A}$  or  $\tilde{A}$  is a vector  $A_i$  may also refer to element i of vector  $A_i$  or  $B_{ij}^j$  or  $B_i^j$  is a matrix

 $A_i B_{ij}$  often means  $\sum_i A_i imes B_{ij}$ 

Algorithms may use A(i) or A[i] and B(i,j) or B[i,j]

### Matrices as Lists (1)

We can input a list of values

You use commas (,) between numbers in rows And semicolons (;) between successive columns

## Matrices as Lists (2)

Values need not be simple numbers

Expressions using defined variables are allowed

```
x = 1.23

y = 4.56

c = [1 + x^2, x * y; -x * y, 1 + y^2]

2.5129 5.6088

-5.6088 21.7936
```

# Row Major or Column Major?

I find those terms seriously confusing We want to know which subscript varies fastest

Matlab like Mathematica and C, NOT Fortran
 First subscript (rows) varies slowest
 Last subscript (columns) varies fastest

```
a = [11, 12, 13; 21, 22, 23; 31, 32, 33; 41, 42, 43]

a(3,2) \rightarrow 32
```

11, 12, 13 is the first of 4 rows 11, 21, 31, 41 is the first of 3 columns

### **Vectors**

A vector can be either a row or column

And you need to use the right one

# Index Ranges (1)

a: b means all values from a to b

$$a = [1, 2, 3, 4, 5, 6, 7, 8, 9, 10]$$
 $a(5:7) \rightarrow [5, 6, 7]$ 
 $a = [1, 2, 3; 4, 5, 6; 7, 8, 9]$ 
 $a(1:2, 2:3) \rightarrow [2, 3; 5, 6]$ 

# Index Ranges (2)

Just a: means all values in a row or column
Can be combined with indices and index ranges

## Matrix Constructors (1)

```
zeros (2) -> [0,0;0,0]

zeros (1,2) -> [0,0]

zeros (2,1) -> [0;0]

1.23 * ones (2) -> [1.23,1.23;1.23,1.23]

rand (2) -> [0.9649,0.9706;0.1576,0.9572]

eye (3) -> [1,0,0;0,1,0;0,0,1]
```

Most have several options and extra features

## Matrix Constructors (2)

There are also many specialised standard matrices
These are Hilbert and inverse Hilbert ones

```
hilb (3)
1.0000 0.5000 0.3333
0.5000 0.3333 0.2500
0.3333 0.2500 0.2000
invhilb (3)
9 -36 30
-36 192 -180
30 -180 180
```

Also companion, Hankel, Toeplitz matrices, etc.

Look them up when and if you need them!

## Matrix Constructors (3)

You can construct linear sequence vectors

```
linspace (-2.3, 8.9, 7)
-2.3000 -0.4333 1.4333 3.3000 5.1667
7.0333 8.9000
```

And then assign them to rows or columns Try this and see what it does:

```
a = zeros(7,3);

a(:,1) = linspace(1,7,7);

a(:,2) = linspace(-2.3,8.9,7);

a(:,3) = linspace(5.6,7.8,7);
```

### **Advanced Construction**

Matlab has lots of more advanced features
If you can't do what you want, look for something

```
a = [11,12,13; 21,22,23; 31,32,33]
[a,a,a]
[a;a;a]
repmat(a,5,7)
```

Look in Elementary Matrices and Arrays And in Array Manipulation

## Importing Data

Unfortunately, Matlab isn't brilliant at this This course won't go into how to do it General advice:

- Use load and save for storage
   Uses Matlab's own format version dependent
- Use importdata for numbers in text form Input them in the format that Matlab expects
- Use Python (or Perl) for other formats
   Write the data out in importdata format

### Basic Functions (1)

disp(A) displays A – compare that with A

$$a = [11, 12, 13]$$

a

disp(a)

11 12 13

### Basic Functions (2)

ndims is the rank (number of dimensions) size gives the actual dimensions

```
a = [11,12,13; 21,22,23]

ndims(a)
2

size(a)
2 3
```

### A Vector 'Gotcha'

The rank of a vector is one (1), right?

Not usually in Matlab, it isn't
 Most 'vectors' are actually degenerate matrices

#### IEEE 754 Features

Matlab has a large collection of IEEE 754 functions Matlab's support is not IEEE 754-compliant Nor is Java's, or most other languages'

I strongly recommend NOT using them
 See the course How Computers Handle Numbers

The reasons are far to complicated to go into here But not even experts can use them reliably Please ask if you want to know more details

# **Basic Operations**

```
    A + B addition
    A - B subtraction
    A * B matrix multiplication
    A ^ K Kth power of matrix
    A ' normal transpose (conjugated)
```

A .'

All of those work as in normal mathematics Generally, use only positive integer power K

transpose (non-conjugated)

# Matrix Multiplication

Remember that this is NOT commutative A\*B is generally not equal to B\*A

Try the following if you need to convince yourself

```
A = rand(5)

B = rand(5)

A*B

B*A
```

And the product of two symmetric matrices will usually be unsymmetric

### **Matrix Division**

- A / B matrix (right) division
- A.\B matrix left division
- Take care about numerical problems with these
   Serious ones with both accuracy and range
- They are effectively linear equation solvers
   We will discuss that in more detail later

It is easy to get confused when using these

# Elementwise Operations

You can also do elementwise operations

```
A .* B elementwise multiplication
```

A . ^ K elementwise Kth power

A ./ B elementwise (right) division

A.\ B elementwise left division

You can use any power that makes sense

## Diagonalisation (1)

Can construct a diagonal matrix from a vector Or convert a matrix into its diagonal vector

```
diag ([1.23, 4.56]) \rightarrow [1.23, 0; 0, 4.56]
diag ([1.23; 4.56]) \rightarrow [1.23, 0; 0, 4.56]
b = [1.2, 2.3, 3.4; 4.5, 5.6, 6.7; 7.8, 8.9, 9.0]
diag (b) \rightarrow [1.2; 5.6; 9.0]
```

That dual use is counter-intuitive, but this is useful:

```
diag (diag (b))
```

# Diagonalisation (2)

You can also construct block diagonal matrices The block matrices can be of any shape

```
a = [11,12,13; 21,22,23; 31,32,33]
b = [100,200; 300,400]
c = 5
blkdiag(a,b,c,c,c,b,a)
```

I strongly recommend experimenting before use Especially if any of your blocks aren't square

#### More Functions (1)

max and min collapse along one dimension

```
a = [11, 12, 13; 21, 22, 23; 31, 32, 33]
max (a)
   31 32 33
min(a)
   11 12 13
max (a,[],2)
    13
    23
    33
```

#### More Functions (2)

prod and sum use a different syntax

```
a = [11, 12, 13; 21, 22, 23; 31, 32, 33]
sum (a)
    63 66 69
prod (a)
    7161 8448 9867
sum (a, 2)
    36
    66
    96
```

#### More Functions (3)

Most basic mathematical functions work elementwise

$$a = [1, 2, 3]$$
 $b = [-2, 0, 1]$ 

sqrt(a)

1.0000 1.4142 1.7321
exp(a)

2.7183 7.3891 20.0855
atan2(a,b)

2.6779 1.5708 1.2490

arrayfun can be used for your functions

#### More Functions (4)

The usual inner and cross products of vectors dot(V1,V2) and cross(V1,V2)

But no outer product nor normalisation You have to program those yourself, by hand; e.g.

$$a = [1, 2, 3]$$
  
 $b = a / sqrt (dot (a, a))$   
 $0.2673 \quad 0.5345 \quad 0.8018$ 

Other absences for multi-dimensional matrices

#### Practical Break

We shall now stop for some practical exercises
These are mainly for inexperienced Matlab users

• I don't care which system you use Just don't expect any help with Microsoft!

I use matlab -nodisplay under Linux

## Numeric Linear Algebra

This is defined only for real and complex Matlab uses IEEE 754 64-bit – c.15 sig. figs

- This has some special mathematics to itself
   Can do a lot more than for general matrices
- Are going to cover only the simplest analyses
   There's a huge amount more in Matlab
   And even more in books and papers

#### Determinant

det gives the determinant As usual, watch out for numerical problems

So far, so good. Now let's try a harder problem

#### Norms

norm gives a choice of induced norms Calculate other norms using the usual formulae

norm(A) is the 2-norm of A

I.e. the largest singular value of A norm(A,1) is the 1-norm or largest column sum norm(A,inf) is the  $\infty$ -norm or largest row sum norm(A,inf) is the Frobenius norm norm(A,inf) is an approximation to norm

norm(V,p) is the p-norm for vector V and integer p

#### **Condition Numbers**

cond(A) is the 2-norm condition number
cond(A,opt) is the opt-norm condition number
 opt can be anything allowed in norm

rcond(A) is LAPACK approx. reciprocal cond. no

condeig(A) is the vector of eigenvalue cond. nos Relevant only for unsymmetric matrices

#### Other Functions

trace(A) is the sum of diagonal elements

expm(A) is the matrix exponential

inv(A) is the matrix inverseYou very rarely should be using this

rank, null, orth etc. for subspaces Most of these are for relatively advanced use

Watch out for serious numerical 'gotchas'

### Linear Equations (1)

In the common, simple cases, Just Do It

$$a = [4.2, 2.2, -3.9, 9.3, 0.1; 8.6, 0.0, 0.7, -2.3, -0.3; 8.4, -5.9, -8.1, 9.6, 3.8 -0.8, -9.4, -9.9, 9.9, 5.0; -1.3, -8.1, 0.6, -9.2, -7.3]$$

$$b = [-6.8, 2.3, 2.7, -7.0, 2.0]$$

$$linsolve(a, b')$$

$$[1.45411, -12.4949, 24.5078, 11.8408, 0.422917]$$

# Linear Equations (2)

How do these relate to matrix division? Yes, I find this very confusing, too!

```
a = rand (5)
b = rand (5)
linsolve (a,b)
a \ b
(b' / a')'
```

All of the above are more-or-less equivalent

# Linear Equations (3)

How did I work that out? Trying every combination ... I then worked out what Matlab's authors were thinking

• Always run a cross-check when doing that I.e. check you have done the right calculation

```
a * linsolve(a,b) \rightarrow b
(b/a) * a -> b
```

# Linear Equations (4)

It's critical to look for its warnings

```
linsolve ([1.2, 3.4; 2.4, 6.8], [1.0; 1.0])
Warning: Matrix is singular to working precision.
-Inf
Inf
linsolve (hilb (20), rand(20, 1))
```

Warning: Matrix is close to singular or badly scaled. Results may be inaccurate. RCOND = 1.995254e-19.

# Linear Equations (5)

- If any, the results are often complete nonsense They may be NaNs, infinities, zeroes
- → Or plausible values that are just plain wrong
- Matlab won't stop by itself on a warning You have to do the checking, by hand

The command dbstop if warning looks useful here But works only if you are running the debugger!

Naturally, this applies to all warnings
 Not just ones that occur in linear equations

### Decompositions

You can get just the decompositions

The main ones are chol(A) and lu(A)
Cholesky for real positive definite symmetric only
LU for pretty well any square matrix

qr(A) is also used for eigenvalues

pinv(A) is the Moore–Penrose pseudo–inverse

## Least Squares Solutions (1)

Matlab uses these for over-determined problems Generally, everything does what you expect

```
a = rand (10,3)
b = rand (10,1)
linsolve (a,b)

0.5731
0.1851
0.2837
```

You will get different random results, of course

## Least Squares Solutions (2)

Iscov can handle known covariances
Look it up if you need to do that

But what if you need to do more advanced work? Including any serious statistics or regression

- Use the Matlab statistics toolbox (extra cash)
- Statistical package, like Genstat or SPSS
- Program the formulae yourself, if you can

#### Fourier Transforms (1)

Matlab doesn't call them linear algebra Look under Data Analysis for fft\*

```
a = [-0.92, 9.1, 2.3, 5.7, 4.9, -2.8, -5.6, 6.7, -7.0, 9.0]
b = fftn (a)
21.4, 11.8 - 14.1i, -4.6 + 3.8i, 9.9 - 5.2i, -15.4 + 15.9i, -34.0, -15.4 - 15.9i, 9.9 + 5.2i, -4.6 - 3.8i, 11.8 + 14.1i
ifftn (b)
-0.92, 9.1, 2.3, 5.7, 4.9, -2.8, -5.6, 6.7, -7.0, 9.0
```

#### Fourier Transforms (2)

• fftn and fftn work on matrices, too
They are the multi-dimensional array forms

fft/ifft and fft2/ifft2 look more obvious

But they have a very serious 'gotcha'
 Unexpected behaviour on too many dimensions

fft/ifft work on the first dimension only I.e. they apply multiple 1-dimensional FFTs

I haven't experimented with what fft2/ifft2 do

#### Fourier Transforms (3)

You can make fft/ifft work on another dimension Using the same nasty syntax as for max/min The following two operations are equivalent – try them

```
a = rand(5)

fft2(a)

fft(fft(a,[],2))
```

# Eigenanalysis (1)

- Things start to get a bit hairier, here That is because the mathematics does
- All square matrices have all eigenvalues
   But real matrices may have complex eigenvalues
- All real symmetric matrices have all eigenvectors
   And those are always orthogonal
   The same applies to all complex Hermitian ones
- But unsymmetric matrices may be nasty

# Eigenanalysis (2)

Simple use is, er, simple

```
a = [4.2, 2.2, -3.9, 9.3, 0.1;
       8.6, 0.0, 0.7, -2.3, -0.3;
       8.4, -5.9, -8.1, 9.6, 3.8;
       -0.8, -9.4, -9.9, 9.9, 5.0;
       -1.3, -8.1, 0.6, -9.2, -7.3
eig (a)
       6.4585 + 9.8975i
       6.4585 - 9.8975i
      -7.2840 + 4.4546i
      -7.2840 - 4.4546i
       0.3510
```

## Characteristic Polynomial

Eigenvalues are the roots of that You can calculate it directly, if you want

```
a = [4.2, 2.2, -3.9, 9.3, 0.1;
      8.6, 0.0, 0.7, -2.3, -0.3;
      8.4, -5.9, -8.1, 9.6, 3.8;
      -0.8, -9.4, -9.9, 9.9, 5.0;
      -1.3, -8.1, 0.6, -9.2, -7.3
poly (a)
 1.0e+03 *
    0.0010 0.0013 0.0238 1.0845 9.7983 -3.5741
```

# Eigenvectors (1)

You can get the eigenvectors almost as easily

If you don't know the following syntax, just use it It just assigns two results, rather than one

$$a = [4.2, 2.2, -3.9; 8.6, 0.3, 0.7; 8.4, -5.9, -8.1]$$

$$[p,q] = eig(a)$$

Returns the eigenvectors in the columns of p And the eigenvalues as a diagonal matrix in q

# Eigenvectors (2)

The output is omitted because of verbosity – try it Let's check that we have got the right answer p \* q / p should be the matrix a

# Eigenvectors (3)

Here, really don't rely on the diagnostics

Oops! Not even a warning

# Eigenvectors (4)

Let's try another of the same level of nastiness

$$a = [0.0, 1.0; 0.0, 0.0]$$
 
$$[p,q] = eig(a)$$
 
$$p*q/p$$
 Warning: Matrix is close to singular or badly scaled. Results may be inaccurate. RCOND = 2.004168e-292. 0 0

# More Eigenanalysis (1)

There are a lot of extra features and functions
I haven't investigated, and it's not one of my areas

Matlab says eig has problems with sparse matrices There's another function, eigs, which may do better

You can get the Hessenberg and Schur forms

And then there's the question of whether to balance

# More Eigenanalysis (2)

- Real symmetric and complex Hermitian are easy You will be unlucky to have problems with those ones Mere numerical inaccuracy excepted, of course
- Otherwise: Be Very Careful Unsymmetric eigenanalysis is full of 'gotchas'
- Many experts say you shouldn't do it at all You should use Singular value decomposition

# Singular Values (1)

Singular value decomposition is called SVD A more robust extension of eigenanalysis

Gives the same results in the simple cases. The term for these is normal matrices

Also handles non-square matrices And ones with missing eigenvectors

If you don't know it, don't worry about it But it's an important technique in many fields

# Singular Values (2)

Try the following with a variety of matrices a

# Singular Values (3)

The trivial cases give exactly the same answers Matlab uses the reverse orders of eigenvalues

```
a = hilb (3)
eig (a)
    [ 0.0027; 0.1223; 1.4083]
svd (a)
    [ 1.4083; 0.1223; 0.0027]
```

# Singular Values (4)

But SVD handles the foul cases I used correctly

```
a = [1.0, 1.0; 0.0, 1.0]
[r, s, t] = svd(a)
r * s * †'
    1.0000 1.0000
    0.0000 1.0000
a = [0.0, 1.0; 0.0, 0.0]
[r, s, t] = svd(a)
r * s * t'
```

## Complex Numbers (1)

FFT and eigenalysis have produced these We have completely ignored them — why?

- Because there has been nothing to say!
   Really do use complex numbers just like real ones
   Their differences don't show up in linear algebra
- ⇒ There is only one critical warning Regard complex exceptions as pure poison That means mainly overflow and division by zero

See the course How Computers Handle Numbers

## Complex Numbers (2)

```
a = [4.2 + 2.2i, -3.9 + 9.3i, 0.1 + 0.0i;
    8.6 + 0.0i, 0.7 - 2.3i, 0.0 - 0.3i;
    8.4 - 5.9i, -8.1 + 9.6i, 3.8 - 0.8i]
b = [-6.8 + 2.3i ; 2.7 - 7.0i ; 2.0 + 0.0i]
linsolve (a,b)
     0.0362 - 0.5311i
     0.7195 + 0.6147i
     4.0269 + 1.5706i
eig (a)
    -3.2517 - 8.1715i
     7.9506 + 7.7844i
     4.0011 - 0.5129i
```

### A Bit of Numerical Analysis

Very roughly, the error in linear algebra is:

 $N \times cond. \, number \times epsilon$ 

Where *N* is the size of the matrix *Cond. number* is how 'nasty' the matrix is *epsilon* is the error in the values/arithmetic

- Almost always, the main error is in the input data
   Good linear algebra algorithms are very accurate
- ⇒ Rounding error isn't usually the problem

# Real vs Floating-Point

See "How Computers Handle Numbers"
Only significant problem is loss of accuracy

Not going to teach much numerical analysis
But it's well-understood for much of linear algebra

PLEASE don't use single precision
 And do watch out for growth of inaccuracy

# Solution of Equations (1)

Let's look at a classic numerically foul problem The Hilbert matrix is positive definite And horribly ill-conditioned ...

In Mathematica rational arithmetic, result is exact

### Solution of Equations (2)

```
{ -10,990,-23760,240240,-1261260,3783780, -6726720,7001280,-3938220,923780}
```

Now we do it in Matlab's floating-point

```
a = hilb (10)
b = ones (10, 1)
num2str (linsolve (a, b), 6)
-9.99803, 989.83, -23756.4, 240207,
-1.2611e+06, 3.78335e+06, -6.72601e+06,
7.0006e+06, -3.93786e+06, 923701
```

### Error Analysis

Traditionally, this is overall error analysis Usually in terms of norms etc. It is a well-understood area, with useful results

Use the formulae for it in books etc.

Sorry, but there is no time to go into it further

# Sparse Arrays (1)

Matlab has good support for sparse arrays You use them just like dense arrays – ha, ha!

Don't be fooled – this is a problem area
 It can be done very well, but don't just rush in

First problem is many operations cause infilling A 16 MB array can expand to 16 GB

Sparse algorithms are designed to minimise that

# Sparse Arrays (2)

Problem is that nothing comes for free

Very often the sacrifice is numerical robustness
 Some problems may give inaccurate answers, or fail
 I mentioned Matlab's warning about the eig function

So proceed cautiously with sparse arrays

Find out what best practice is before proceeding

But lots of people do it, very successfully

### **Esoteric Analyses**

The above are the basic methods of linear algebra

- Every field has its own specialised methods
   There are thousands of them and each field differs
- Matlab has a few, otherwise program them Almost always formulae in reference books
- The only warning is to watch out for errors
   Both algorithm failure and numerical inaccuracy

#### Practical Break

We shall now stop for some practical exercises These use the actual linear algebra functions

The same comments apply as before

But, before that, one more slide ...