FF505

Computational Science

Lecture 2

More on Matrix Calculations and Math Functions

Marco Chiarandini

Department of Mathematics & Computer Science
University of Southern Denmark

Outline

1. More on Matrix Calculations

2. Math Functions

3. Software Comparison

Resume

MATrix LABoratory

- MATLAB, numerical computing vs scientific computing, alternatives
- MATLAB Desktop
- Variables and Script files
- Vectors, matrices and arrays
- Solving systems of linear equations

Outline

1. More on Matrix Calculations

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Order of Operations

1. parenthesis, from innermost
2. exponentiation, from left to right
3. multiplication and division with equal precedence, from left to right
4. addition and subtraction with equal precedence, from left to right

```
>>4^2-12-8/4*2
ans =
     0
>>4^2-12-8/(4*2)
ans =
     3
>> 3*4^2 + 5
ans =
     53
>>(3*4)^2 + 5
ans =
     149
```

```
>>27^(1/3) + 32^(0.2)
ans =
     5
>>27^(1/3) + 32^0.2
ans =
     5
>>27^1/3 + 32^0.2
ans =
     11
```

Creating Matrices

```
eye(4) % identity matrix
zeros(4) % matrix of zero elements
ones(4) % matrix of one elements
```

```
A=rand(8)
triu(A) % upper triangular matrix
tril(A)
diag(A) % diagonal
```

```
>> [ eye(2), ones(2,3); zeros(2),
     [1:3;3:-1:1] ]

ans =

    1 0 1 1 1
    0 1 1 1 1
    0 0 1 2 3
    0 0 3 2 1
```

Can you create this matrix in one line of code?

```
-5     0     0     0     0     0     0     1     1     1     1
 0    -4     0     0     0     0     0     0     1     1     1
 0     0    -3     0     0     0     0     0     0     1     1
 0     0     0    -2     0     0     0     0     0     0     1
 0     0     0     0    -1     0     0     0     0     0     0
 0     0     0     0     0     0     0     0     0     0     0
 0     0     0     0     0     0     1     0     0     0     0
 1     0     0     0     0     0     0     2     0     0     0
 1     1     0     0     0     0     0     0     3     0     0
 1     1     1     0     0     0     0     0     0     4     0
 1     1     1     1     0     0     0     0     0     0     5
```

Matrix-Matrix Multiplication

In the product of two matrices A * B,
the number of columns in A must equal the number of rows in B.

The product AB has the same number of rows as A and the same number of columns as B. For example

```
>> A=randi(10,3,2) % returns a 3-by-2 matrix containing pseudorandom integer values
      drawn from the discrete uniform distribution on 1:10
A =
     6 10
    10 4
     5 8

>> C=randi(10,2,3)*100
C =
        1000 900 400
         200 700 200
>> A*C % matrix multiplication
ans =
        8000 12400 4400
       10800 11800 4800
        6600 10100 3600
```

Remark:
Matrix multiplication does not have the commutative property; that is, in general, $AB \neq BA$. Make a simple example to demonstrate this fact.

Matrix Operations

```
%% matrix operations
A * C % matrix multiplication
B = [5 6; 7 8; 9 10] * 100 % same dims as A
A .* B % element-wise multiplcation
% A .* C or A * B gives error - wrong dimensions
A .^ 2
1./B
log(B) % functions like this operate element-wise on vecs or matrices
exp(B) % overflow
abs(B)
v = [-3:3] % = [-3 -2 -1 0 1 2 3]
-v % -1*v

v + ones(1,length(v))
% v + 1 % same

A' % (conjuate) transpose
```

Multidimensional Arrays

Consist of two-dimensional matrices layered to produce a third dimension. Each layer is called a page.

```
cat(2,A,B) % is the same as [A,B].
cat(1,A,B) % is the same as [A;B].
```

```
>> A = magic(3); B = pascal(3);
>> C = cat(4,A,B) %concatenate matrices along DIM

C(:,:,1,1) =

     8 1 6
     3 5 7
     4 9 2

C(:,:,1,2) =
     1 1 1
     1 2 3
     1 3 6
```

Array Operations

- **Addition/Subtraction**: trivial
- **Multiplication**:
  - of an array by a scalar is easily defined and easily carried out.
  - of two arrays is not so straightforward:
    MATLAB uses two definitions of multiplication:
    - array multiplication (also called element-by-element multiplication)
    - matrix multiplication
- **Division and exponentiation** MATLAB has two forms on arrays.
  - element-by-element operations
  - matrix operations

Element-by-Element Operations

Symbol	Operation	Form	Examples
+	Scalar-array addition	A + b	[6,3]+2=[8,5]
-	Scalar-array subtraction	A - b	[8,3]-5=[3,-2]
+	Array addition	A + B	[6,5]+[4,8]=[10,13]
-	Array subtraction	A - B	[6,5]-[4,8]=[2,-3]
.*	Array multiplication	A.*B	[3,5].*[4,8]=[12,40]
./	Array right division	A./B	[2,5]./[4,8]=[2/4,5/8]
.\	Array left division	A.\B	[2,5].\[4,8]=[2\4,5\8]
.^	Array exponentiation	A.^B	[3,5].^2=[3^2,5^2]
			2.^[3,5]=[2^3,2^5]
			[3,5].^[2,4]=[3^2,5^4]

Backslash or Matrix Left Division

`A\B` is roughly like `INV(A)*B` except that it is computed in a different way: `X = A\B` is the solution to the equation `A*X = B` computed by Gaussian elimination.

Slash or right matrix division:
`A/B` is the matrix division of `B` into `A`, which is roughly the same as `A*INV(B)`, except it is computed in a different way. More precisely, `A/B = (B'\A')'`.

`cross(A,B)` cross product: eg: moment $\mathbf{M} = \mathbf{r} \times \mathbf{F}$

`dot(A,B)` scalar product: computes the projection of a vector on the other.
eg. `dot(Fr,r)` computes component of force $\mathbf{F}$ along direction $\mathbf{r}$
Inner product, generalization of dot product

```
v=1:10
u=11:20
u*v' % inner or scalar product
ui=u+i
ui'
v*ui' % inner product of C^n
norm(v,2)
sqrt(v*v')
```

Useful Functions

```
% max (or min)
a = [1 15 2 0.5]
val = max(a)
[val,ind] = max(a)

% find
find(a < 3)
A = magic(3) %N-by-N matrix
      constructed from the integers 1
      through N^2 with equal row, column,
       and diagonal sums.
[r,c] = find(A>=7)

% sum, prod
sum(a)
prod(a)
floor(a) % or ceil(a)
max(rand(3),rand(3))
max(A,[],1)
min(A,[],2)
A = magic(9)
sum(A,1)
sum(A,2)
```

```
% pseudo-inverse
pinv(A) % inv(A'*A)*A'

% check empty e=[]
isempty(e)
numel(A)
size(A)
prod(size(A))
```

```
sort(4:-1:1)
sort(A) % sorts the columns
```

Useful Functions

Working with polynomials:

$$f(x) = a_1 x^n + a_2 x^{n-1} + a_3 x^{n-2} + \ldots + a_{n-1} x^2 + a_n x + a_{n+1}$$

is represented in MATLAB by the vector

$$[a_1, a_2, a_3, \ldots, a_{n-1}, a_n, a_{n+1}]$$

```
help polyfun
r=roots([1,-7,40,-34]) % x^3-7x^2+40x-34
poly(r) % returns the polynomial whose roots are r
roots(poly(1:20))
poly(A) % coefficients of the characteristic polynomial, det(lambda*EYE(SIZE(A)) - A)
```

Useful Functions

Product and division of polynomials:

$$f(x)g(x) = (9x^3 - 5x^2 + 3x + 7)(6x^2 - x + 2) =$$
$$= 54x^5 - 39x^4 + 41x^3 + 29x^2 - x + 14$$

$$\frac{f(x)}{g(x)} = \frac{9x^3 - 5x^2 + 3x + 7}{6x^2 - x + 2} = 1.5x - 0.5833$$

and a remainder of $-0.5833x + 8.1667$.

```
f = [9 -5 3 7];
g = [6 -1 2];
product = conv(f,g)
product =
    54 -39 41 29 -1 14

[quotient,remainder] = deconv(f,g)
quotient =
    1.5000 -0.5833
remainder =
         0 0 -0.5833 8.1667
```

Reshaping

```
%% reshape and replication
A = magic(3) % magic square
A = [A [0;1;2]]
reshape(A,[4 3]) % columnwise
reshape(A,[2 6])
v = [100;0;0]
A+v
A + repmat(v,[1 4])
```

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Common Mathematical Functions

Exponential	
`exp(x)`	Exponential; e^x.
`sqrt(x)`	Square root; $\sqrt{x}$.
Logarithmic	
`log(x)`	Natural logarithm; $\ln x$.
`log10(x)`	Common (base-10) logarithm; $\log x = \log_{10} x$.
Complex	
`abs(x)`	Absolute value; x.
`angle(x)`	Angle of a complex number x.
`conj(x)`	Complex conjugate.
`imag(x)`	Imaginary part of a complex number x.
`real(x)`	Real part of a complex number x.
Numeric	
`ceil(x)`	Round to the nearest integer toward ∞.
`fix(x)`	Round to the nearest integer toward zero.
`floor(x)`	Round to the nearest integer toward $-\infty$.
`round(x)`	Round toward the nearest integer.
`sign(x)`	Signum function: $+1$ if $x > 0$; 0 if $x = 0$; -1 if $x < 0$.

Common Mathematical Functions

Trigonometric*	
`cos(x)`	Cosine; cos x.
`cot(x)`	Cotangent; cot x.
`csc(x)`	Cosecant; csc x.
`sec(x)`	Secant; sec x.
`sin(x)`	Sine; sin x.
`tan(x)`	Tangent; tan x.
Inverse trigonometric†	
`acos(x)`	Inverse cosine; arccos $x = \cos^{-1} x$.
`acot(x)`	Inverse cotangent; arccot $x = \cot^{-1} x$.
`acsc(x)`	Inverse cosecant; arccsc $x = \csc^{-1} x$.
`asec(x)`	Inverse secant; arcsec $x = \sec^{-1} x$.
`asin(x)`	Inverse sine; arcsin $x = \sin^{-1} x$.
`atan(x)`	Inverse tangent; arctan $x = \tan^{-1} x$.
`atan2(y,x)`	Four-quadrant inverse tangent.

*These functions accept x in radians.
†These functions return a value in radians.

Common Mathematical Functions

Hyperbolic	
`cosh(x)`	Hyperbolic cosine; $\cosh x = (e^x + e^{-x})/2$.
`coth(x)`	Hyperbolic cotangent; $\cosh x / \sinh x$.
`csch(x)`	Hyperbolic cosecant; $1/\sinh x$.
`sech(x)`	Hyperbolic secant; $1/\cosh x$.
`sinh(x)`	Hyperbolic sine; $\sinh x = (e^x - e^{-x})/2$.
`tanh(x)`	Hyperbolic tangent; $\sinh x / \cosh x$.
Inverse hyperbolic	
`acosh(x)`	Inverse hyperbolic cosine
`acoth(x)`	Inverse hyperbolic cotangent
`acsch(x)`	Inverse hyperbolic cosecant
`asech(x)`	Inverse hyperbolic secant
`asinh(x)`	Inverse hyperbolic sine
`atanh(x)`	Inverse hyperbolic tangent

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Why MATLAB?

1. You should learn first to do symbolic computations on paper.
   This will always be necessary to understand.

2. Matlab is much more efficient than Maple when computations become heavy

3. Matlab is more intuitive to program

4. Matlab is spread in the industry

(However, Maple could also be fine for the project)

Performance Comparison

Some advanced applications in mathematics and physics need to handle matrices of huge size, eg:

- discretization of (partial) differential equations
- finite element methods
- discrete laplacians.

Matrix storage

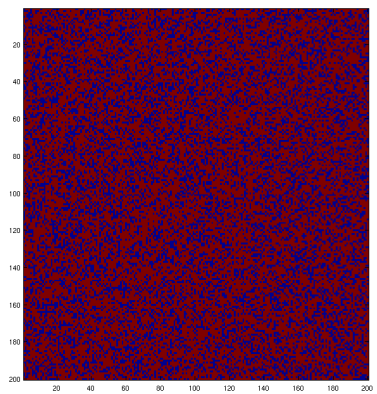
```
S = sparse((rand(5,5) < 2/3))
issparse(S)
M = full(S)
[i,j,k] = find(M);

save sparse i j k;
S=sparse(i,j,k);
```

```
M =
     1  0  1  1  1
     0  1  1  1  0
     1  1  1  1  1
     1  1  1  1  1
     0  1  0  1  1
```

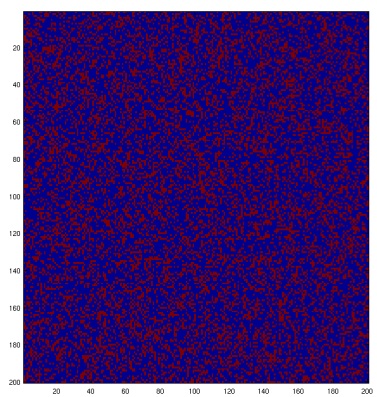
```
S =
   (1,1) 1
   (3,1) 1
   (4,1) 1
   (2,2) 1
   (3,2) 1
   (4,2) 1
   (5,2) 1
   (1,3) 1
   (2,3) 1
   (3,3) 1
   (4,3) 1
   (1,4) 1
   (2,4) 1
   ...
```

If X is an $m \times n$ matrix with nz nonzero elements then `full(X)` requires space to store $m \times n$ elements. On the other hand, `sparse(X)` requires space to store nz elements and $(nz + n + 1)$ integers.

```
S = sparse(+(rand(200,200) < 2/3));
A = full(S);
whos
Name Size Bytes Class
  A 200X200 320000 double array
  S 200X200 318432 double array (sparse)
imagesc(A) %pcolor(A)
```



```
S = sparse(+(rand(200,200) < 1/3));
A = full(S);
whos
  Name Size Bytes Class Attributes
  A 200x200 320000 double
  S 200x200 163272 double sparse
imagesc(A) %pcolor(A)
```



MATLAB and Octave

```
tic, load TestA;
load Testb; toc
tic, c=A\b; toc
```

```
>> whos
  Name Size Bytes Class Attributes
  A 1000000x1000000 51999956 double sparse
  b 1000000x1 8000000 double
  c 1000000x1 8000000 double
```

MATLAB

```
Elapsed time is 0.191414 seconds.
Elapsed time is 0.639878 seconds.
```

Octave

```
octave:1> comparison
Elapsed time is 0.276378 seconds.
Elapsed time is 0.618884 seconds.
```

Performance Comparison – MAPLE

```
> A:=ImportMatrix("TestA.mat",source=MATLAB);
memory used=72.8MB, alloc=72.9MB, time=0.51
memory used=122.8MB, alloc=122.8MB, time=0.59
memory used=192.4MB, alloc=192.2MB, time=1.57
memory used=262.6MB, alloc=224.3MB, time=2.44
memory used=300.7MB, alloc=224.3MB, time=3.24
...
memory used=1264.3MB, alloc=520.3MB, time=38.07
memory used=1325.2MB, alloc=568.3MB, time=43.73
memory used=1392.2MB, alloc=621.1MB, time=50.59
memory used=1465.8MB, alloc=679.2MB, time=58.95
memory used=1546.9MB, alloc=743.1MB, time=69.12
                                        [ 1000000 x 1000000 Matrix ]
                              A := ["A", [ Data Type: float[8] ]]
                                        [ Storage: sparse ]
                                        [ Order: Fortran_order ]
> b:=ImportMatrix("Testb.mat",source=MATLAB);
memory used=1621.2MB, alloc=743.1MB, time=76.11
                                          [ 1000000 x 1 Matrix ]
                                b := ["b", [ Data Type: float[8] ]]
                                          [ Storage: rectangular ]
                                          [ Order: Fortran_order ]
> with(LinearAlgebra):
> c:=LinearSolve(A,b);
Error, (in simplify/table) dimensions too large
```

Performance Comparison – R


```
library(R.matlab)
library(Matrix)
S<-readMat("sparse.mat")
b<-readMat("Testb.mat")

A <- sparseMatrix(S$i,S$j,S$k)

system.time(try(solve(A,b)))

Am <- as.(A,"matrix")
# fails
# Error in asMethod(object) :
# Cholmod error 'problem too large' at file ../Core/cholmod_dense.c, line 105
```

Resume

- Large sparse matrices and performance comparison
- Arrays
- Mathematical Functions

Next time:

- Programming, control structures
- Vectorization
- Advanced plotting
- random numbers generation