# FF505 <br> Computational Science 

## Matrix Calculus

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- MATLAB, numerical computing vs symbolic computing
- MATLAB Desktop
- Script files
- 1D and 2D arrays
- Plot
- Interacting with matlab
- Matrix vs array operations
- Car market assignment

Other topics:

- matrices and vectors
- solving linear systems
- determinants
- linear transformation
- eigenvalues and eigenvectors
- diagonalization?


## Outline

1. Vectors and Matrices

Linear Algebra
Array Operations

## 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 =
    10 1 1 1
    0}10111
    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 |

## 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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## Dot and Cross Products

$\operatorname{dot}(\mathrm{A}, \mathrm{B})$ inner or scalar product: computes the projection of a vector on the other. eg. $\operatorname{dot}(\mathrm{Fr}, \mathrm{r})$ computes component of force F along direction r

```
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')
```

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

## Electrical Networks



## Matrix Multiplication

$$
\begin{array}{r}
i_{1}-i_{2}+i_{3}=0 \\
-i_{1}+i_{2}-i_{3}=0 \\
4 i_{1}+2 i_{2}=8 \\
2 i_{2}+5 i_{3}=9
\end{array}
$$

$$
\left[\begin{array}{ccc}
1 & -1 & 1 \\
-1 & 1 & -1 \\
4 & 2 & 0 \\
0 & 2 & 5
\end{array}\right]\left[\begin{array}{l}
i_{1} \\
i_{2} \\
i_{3}
\end{array}\right]=\left[\begin{array}{l}
0 \\
0 \\
8 \\
9
\end{array}\right] \quad A \mathbf{x}=\mathbf{b}
$$

node A node $B$
top loop
bottom loop $A \mathrm{x}=\mathrm{b}$

## Chemical Equations

$$
x_{1} \mathrm{CO}_{2}+x_{2} \mathrm{H}_{2} \mathrm{O} \rightarrow x_{3} \mathrm{O}_{2}+x_{4} \mathrm{C}_{6} \mathrm{H}_{12} \mathrm{O}_{6}
$$

To balance the equation, we must choose $x_{1}, x_{2}, x_{3}, x_{4}$ so that the numbers of carbon, hydrogen, and oxygen atoms are the same on each side of the equation.

$$
\begin{aligned}
x_{1} & =6 x_{4} \\
2 x_{1}+x_{2} & =2 x_{3}+6 x_{4} \\
2 x_{2} & =12 x_{4}
\end{aligned}
$$

carbon atoms
oxygen
hydrogen

## Matrix Multiplication

$$
\begin{aligned}
x_{1} & =6 x_{4} \\
2 x_{1}+x_{2} & =2 x_{3}+6 x_{4} \\
2 x_{2} & =12 x_{4}
\end{aligned}
$$

$$
\left[\begin{array}{cccc}
1 & 0 & 0 & -6 \\
2 & 1 & 2 & 6 \\
0 & 2 & 0 & 12
\end{array}\right]\left[\begin{array}{l}
x_{1} \\
x_{2} \\
x_{3} \\
x_{4}
\end{array}\right]=\left[\begin{array}{l}
0 \\
0 \\
0
\end{array}\right] \quad A \mathbf{x}=\mathbf{0}
$$

## 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 $A B$ 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 =
    610
    104
    5 8
>> C=randi(10,2,3)*100
C =
        1000900400
        200700 200
>> A*C % matrix multiplication
ans =
    8000 12400 4400
    10800 11800 4800
    600 10100 3600
```

Exercise: create a small example to show that in general, $A B \neq B A$.

## Matrix Functions

Eigenvalues and eigenvectors:

```
A = ones(6)
trace(A)
A = A - tril(A)-triu(A,2)
eig(A)
diag(ones(3,1),-1)
[V,D]=eig(diag(1:4))
rank(A) % rank of A
orth(A) % orthonormal basis
```


## Visualizing Eigenvalues

```
A=[5/4,0;0,3/4];
eigshow(A) %effect of operator A on unit
    verctor
```


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## Matrix Operations

```
%% matrix operations
A * C % matrix multiplication
B}=[56;78;910]*100% same dims as 
A .* B % element-wise multiplcation
% A .* C or }A*B\mathrm{ 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 % - 1*v
v + ones(1,length(v))
%v+1% same
A' % (conjuate) transpose
```


## Matrix and Array Operations

- Matrix operations follow the rules of linear algebra (not compatible with multidimensional arrays).
- Array operations execute element-by-element operations and support multidimensional arrays.
- The period character (.) distinguishes the array operations from the matrix operations.
- Array operations work on corresponding elements of arrays with equal dimensions
- scalar expansion: scalars are expanded into an array of the same size as the other input


## Matrix vs 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
$\rightsquigarrow$ Remark:
the operation division by a matrix is not defined. In MatLab it is defined but it has other meanings.


## Array Operations (Element-by-Element)

| 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. $\backslash \mathrm{B}$ | $[2,5] . \backslash[4,8]=[2 \backslash 4,5 \backslash 8]$ |  |  |
| . | Array exponentiation | A. ${ }^{-B}$ | $[3,5] . \sim 2=[3 \sim 2,5 \sim 2]$ |
|  |  |  | 2. $\wedge[3,5]=[2 \sim 3,2 \sim 5]$ |
|  |  |  | $[3,5] . \sim[2,4]=\left[3^{\sim} 2,5^{\sim} 4\right]$ |

## Matrix Operations

* Matrix multiplication
$\mathrm{C}=\mathrm{A} * \mathrm{~B}$ is the linear algebraic product of the matrices A and B . The number of columns of $A$ must equal the number of rows of $B$.

Matrix left division (mldivide)
/ Matrix right division (mrdivide)

- Matrix power
, Complex conjugate transpose
$\mathrm{x}=\mathrm{A} \backslash \mathrm{B}$ is the solution to the equation $A x=B$. Matrices A and B must have the same number of rows.
$\mathrm{x}=\mathrm{B} / \mathrm{A}$ is the solution to the equation $x A=B$. Matrices A and B must have the same number of columns. In terms of the left division operator, $B / A=\left(A ' \backslash B^{\prime}\right)$ '.
$A^{\wedge} B$ is $A$ to the power $B$, if $B$ is a scalar. For other values of $B$, the calculation involves eigenvalues and eigenvectors.
A' is the linear algebraic transpose of A. For complex matrices, this is the complex conjugate transpose.


## Matrix division

Backslash or matrix left division $A \backslash B$ It is roughly like $\operatorname{INV}(A) * B$ except that it is computed in a different way: $X=A \backslash B$ is the solution to the equation $A * X=B$ computed by Gaussian elimination.

Slash or right matrix division $A / B$
$X=A / B$ is the solution to the equation $X * A=B$. It is the matrix division of $B$ into $A$, which is roughly the same as $A * \operatorname{INV}(B)$, except it is computed in a different way. More precisely, $A / B=\left(B^{\prime} \backslash A^{\prime}\right)^{\prime}$.

Algorithms:
http://www.maths.lth.se/na/courses/NUM115/NUM115-11/backslash.html

