

Indian Institute of Technology Roorkee

CHN-323

Computer Applications in Chemical Engineering

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Symbolic computing

- Evaluation of mathematical expressions in their exact form, without introducing numbers.
- MATLAB: numerical computing tool
- MAPLE, Mathematica, wolframalpha: symbolic computing tools
- MATLAB incorporated basic symbolic computing: calculus, linear algebra, solution of equations,...

Solving equation systems

➤ Example:

$$\begin{aligned}2x_1 + x_2 &= 0 \\ x_1 - x_2 &= 1\end{aligned}$$

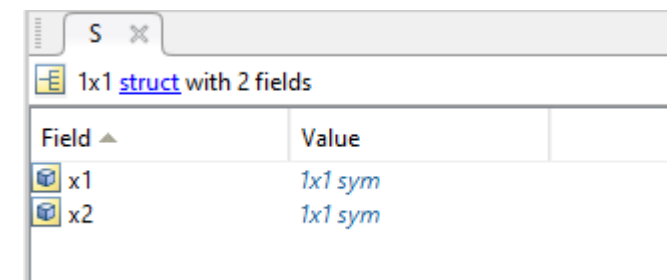
➤ MATLAB code

```
syms x1 x2  
eqns = [2*x1+x2==0, x1-x2==1];  
S = solve(eqns, [x1 x2])
```

```
S =  
struct with fields:  
x1: [1x1 sym]  
x2: [1x1 sym]
```

➤ Display the results

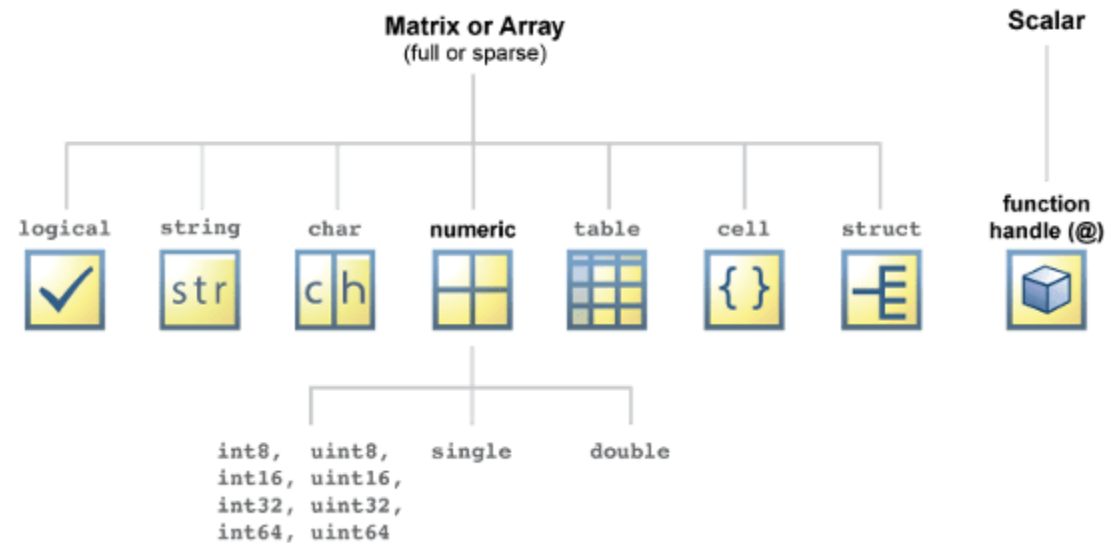
```
>> S.x1  
ans =  
1/3  
  
>> S.x2  
ans =  
-2/3
```



Field	Value
x1	1x1 sym
x2	1x1 sym

syms: a special data type

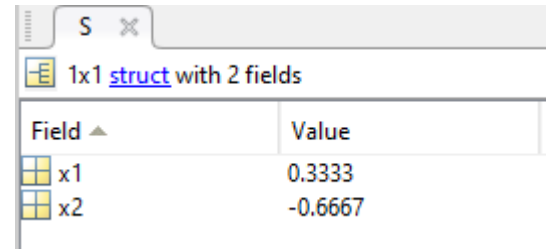
MATLAB Classes or data types



By default, MATLAB stores all numeric values as double-precision floating point.

Sym to double data type

```
>> S.x1=eval(S.x1);  
>> S.x2=eval(S.x2);
```



A screenshot of the MATLAB variable viewer window. The window title is 'S'. Below the title bar, it says '1x1 struct with 2 fields'. There is a table with two columns: 'Field' and 'Value'. The first row shows 'x1' with a value of '0.3333'. The second row shows 'x2' with a value of '-0.6667'.

Field	Value
x1	0.3333
x2	-0.6667

```
>> x1sol=S.x1
```

```
x1sol =
```

```
0.3333
```

```
>> x2sol=S.x2
```

```
x2sol =
```

```
-0.6667
```

```
x2single = single(x2sol);
```

Differentiation

➤ The "diff" command

```
>> syms x f  
>> f=diff(x^4)  
  
f =  
  
4*x^3
```

```
>> f=diff(x^4,1)  
  
f =  
  
4*x^3
```

```
>> f=diff(x^4,2)  
  
f =  
  
12*x^2
```

Differentiation: Multiple Variables

```
>> syms x y  
>> f=y/(y-x);  
>> dfx2=diff(f,2)
```

dfx2 =

$$-(2*y)/(x - y)^3$$

```
>> dfy3=diff(f,y,3)
```

dfy3 =

$$- 6/(x - y)^3 - (6*y)/(x - y)^4$$

Integration

- The "int" command
- Both indefinite and definite integration

```
>> syms x  
intx=int(x-(x^2));  
>> intx
```

```
intx =
```

```
-(x^2*(2*x - 3))/6
```

```
>> pretty(intx)
```

$$\frac{x^2 (2x - 3)}{6}$$

Definite integration

```
>> syms x
>> intx=int(x-(x^2),1,2)
intx =
-5/6
```

```
>> syms x
>> intx=int(x-(x^2));
>> val=subs(intx,2)-subs(intx,1)
val =
-0.8333
```

Solving differential equations

- The "dsolve" command
- Example 1: Consider the Equation

$$\frac{dy}{dx} + 6x^2 y = 2x^2 y^{1/2}$$

Search dsolve in MATLAB help and code it yourself.