Fall 2006--Chem 330

Handout #2

Equations, derivatives, Integrals and fitting functions "spline"

Barrante 2-1: Equations of the second degree

2-i

$$x^2 + y^2 = 4 \qquad y = \sqrt{4 - x^2}$$

$x := -1$

$\text{root}\left[\left(x^2 - 4\right), x\right] = -2$

Gives $x^2 - 4 = 0$

$\text{Find}(x) = -2$

Place the blue editing line on the variable then use "Symbolics" scroll down to "variable" and then select "solve"

$x^2 - 4 = 0$ $\begin{pmatrix} 2 \\ -2 \end{pmatrix}$

Finally, open the Symbolic menu and select "solve" and type in the variable name.

$q^2 - 4 = 0 \text{ solve}, q \rightarrow \begin{pmatrix} 2 \\ -2 \end{pmatrix}$

Roots of a quadratic equation:

$$4 \cdot r^2 + r - 2 = 0$$

1. "root" function

$r := -1$

$\text{root}\left(4 \cdot r^2 + r - 2, r\right) = -0.843$

2. "given ...find " block function

$v := -1$

Given $4 \cdot v^2 + v - 2 = 0$

$\text{Find}(v) = -0.843$

3. Using "Symbolics", variable and solve

$4 \cdot x^2 + x - 2 = 0$ $\begin{pmatrix} \frac{-1}{8} + \frac{1}{8} \cdot 33^{\frac{1}{2}} \\ \frac{-1}{8} - \frac{1}{8} \cdot 33^{\frac{1}{2}} \end{pmatrix}$

$33^{\frac{1}{2}} \cdot \frac{1}{8} - \frac{1}{8} = 0.593$

$-33^{\frac{1}{2}} \cdot \frac{1}{8} - \frac{1}{8} = -0.843$

4. Using "solve, x"

$$4 \cdot y^2 + y - 2 = 0 \text{ solve, y} \rightarrow \begin{pmatrix} \frac{-1}{8} + \frac{1}{8} \cdot 33^{\frac{1}{2}} \\ \frac{-1}{8} - \frac{1}{8} \cdot 33^{\frac{1}{2}} \end{pmatrix}$$

5. high school algebra:

It has the form ax2+bx+c=0 and the roots are (-b+_ $(b^2-4ac)^{-2}$)/2a

a := 4 b := 1 c := −2

$$r1 := \frac{-b + \sqrt{b^2 - 4 \cdot a \cdot c}}{2 \cdot a} \qquad r2 := \frac{-b - \sqrt{b^2 - 4 \cdot a \cdot c}}{2 \cdot a}$$

r1 = 0.593 r2 = −0.843

2-j $(x1 - 2)^2 + (y1 + 4)^2 = 9$

$f(x1) := (x1 - 2)^2 + 4^2 - 9$

x1 := 2:

$\text{root}\left[(x1 - 2)^2 + 4^2 - 9, x1\right] = 2 + 2.646i$ OR $\text{root}(f(x1), x1) = 2 + 2.646i$

Solving a Nonlinear System of Equations

Solving a system of *n* equations in *n* unknowns using "Given .... Find" solve bolck.

Enter guess values for the n unknowns:

$x_2 := 1$ $y_2 := -1$ $z_2 := 0$

Enter the n equations:

Given

1. $2 \cdot x_2^3 - 2 \cdot y_2 = 7 - 2 \cdot z_2^4$
2. $y_2^3 + 4 \cdot z_2^2 = 4$

The symbolic equals sign **[Ctrl]=** should be used to define equations within the Solve Block.

3. $x_2 \cdot y_2 + z_2 \cdot \ln(x_2) = e^{z_2}$

$soln := Find(x_2, y_2, z_2)$

$$soln = \begin{pmatrix} 1.454 \\ 0.51 \\ -0.983 \end{pmatrix}$$

Barrante 4.1(d, l, n, r)
Differentiate the following functions.
(All the lowercase letters are the variable and All uppercase letters are constants.)

(d) $r = 3 \cdot \tan(2 \cdot \theta)$ <-- *Use* ***<cntrl>=*** *in equation. Set cursor* ***(blue editing line)*** *at θ, pull down* ***"Symbolic"*** *menu, select* ***"differentiate"*** *on variable.*

$$0 = 6 + 6 \cdot \tan(2 \cdot \theta)^2$$

(l) $s = \ln(t) \cdot e^{-3 \cdot t}$

$$0 = \frac{1}{t} \cdot \exp(-3 \cdot t) - 3 \cdot \ln(t) \cdot \exp(-3 \cdot t)$$

(r) $u = \frac{A}{r^{12}} - \frac{B}{r^6}$ $\qquad 0 = -12 \cdot \frac{A}{r^{13}} + 6 \cdot \frac{B}{r^7}$

Finall $d = 3 \cdot \cos(\theta)^2 - 1$

$$0 = -6 \cdot \cos(\theta) \cdot \sin(\theta)$$

$h = \sin(\theta)$

$$0 = \cos(\theta)$$

Derivatives and Integrals

Numerical evaluation of the derivative of a function for a set of values.

Enter a function h(x) you want to differentiate: $h(x) := 13 \cdot x^7$ $\qquad g(x) := x^2$

Enter points at which to compute derivative (as a range variable):

$i := 0..4$

$Dh(x) := \frac{d}{dx} h(x)$ $\qquad Dg(x) := \frac{d}{dx} g(x)$

h(i)
0
13
1664
28431
212992

Dh(i)
0
91
5824
66339
372736

g(i)	Dg(i)
0	0
1	2
4	4
9	6
16	8