EP375 Computational Physics

Topic 5

MATLAB TUTORIAL DIFFERENTIATION & INTEGRATION

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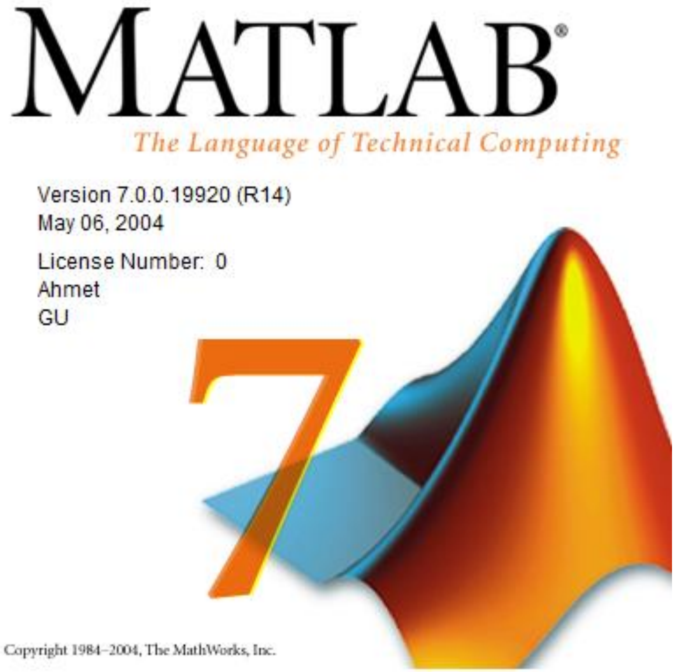


Introduction

- In engineering problems, we have mostly deal with the differentiation and integration of the functions of single- or multi-variables.

- In MATLAB there are some build-in functions to perform these operations:

`diff()`	to evaluate finite difference or derivative
`int()`	to evaluate the definite or indefinite integrals

Derivative

`diff(S)`

differentiates a symbolic expression S with respect to its free variable.

`diff(S,'v')` **or** `diff(S,sym('v'))`

differentiates S with respect to v.

`diff(S,n)`

for a positive integer n, differentiates S n times.

`diff(S,'v',n)` **and** `diff(S,n,'v')`

are also acceptable.

Example 1:

Find the first and second derivative of the function

f(x) = x^2 + exp(-x)

```
>> syms x
>> diff(x^2+exp(-x))    % first derivative
ans = 2*x-exp(-x)

>> diff(x^2+exp(-x),2) % second derivative
ans = 2+exp(-x)
```

Example 2:

Find the first derivative of the function $f(x) = x^2 + \exp(-x)$ at $x=3$.

```
>> syms x
>> d = diff(2*x^2);
>> x = 3;
>> eval(d)
ans = 12
```

Example 3:

Find the derivatives for the function $\partial f/\partial x$ and $\partial f/\partial y$

$f(x,y) = yx^2 + \exp(-x*y)$

```
>> syms x y
>> diff(y*x^2+exp(-x*y),'x')   % df/dx
ans = 2*x*y-y*exp(-x*y)

>> diff(y*x^2+exp(-x*y),'y')   % df/dy
ans = x^2-x*exp(-x*y)
```

Integration

`int(S)`

returns the indefinite integral of S with respect to its symbolic variable

`int(S,v)`

returns the indefinite integral of S with respect to the symbolic scalar variable v.

`int(S,a,b)`

returns the definite integral of S from a to b

Example 4:

Find the indefinite integral and definite for the range [1, 2] of the function f(x) = x^2 + exp(-x).

```
>> syms x
>> int(x^2+exp(-x))              % indefinite integral
ans = 1/3*x^3-exp(-x)

>> int(x^2+exp(-x),1,2)          % definite integral
ans = 7/3-exp(-2)+exp(-1)
```

Example 5:

Evaluate the integral: $$\int_0^4\int_{-1}^2 (x^2 + y^2)\,dx\,dy$$

```
>> syms x y
>> int( int(x^2+y^2,x,-1,2),y,0,4 )
ans = 76
```

Symbolic Expansion/Simplification

```
>> syms a b
>> expand((a+b)^3)
ans = a^3+3*a^2*b+3*a*b^2+b^3
```

```
>> syms x a b c
>> simplify(sin(x)^2 + cos(x)^2)
ans = 1

>> simplify(exp(c*log(sqrt(a+b))))
ans = (a+b)^(1/2*c)
```

HW1:

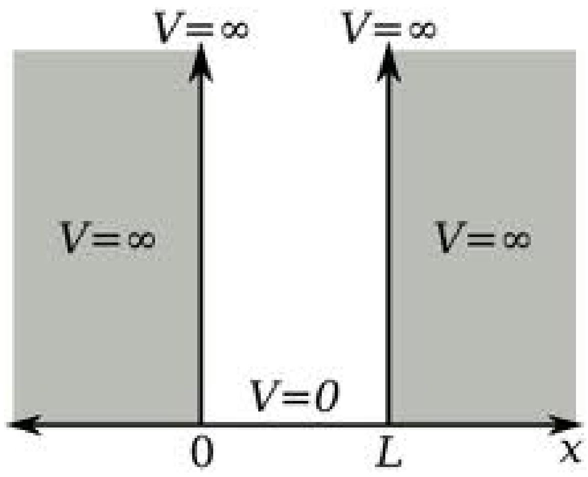
Find the partial derivatives $\partial f/\partial x$ and $\partial f/\partial y$ at x = y = 1 for the function f(x,y) = sin(x)/y + cos(y)/x

HW2:

Evaluate the integral: $$\int_0^3\int_0^\pi\int_0^{2\pi} r^2 \sin(\theta)\,d\phi\,d\theta\,dr$$

HW3:

Groud state wave function of a particle in an infinite quantum well as shown in figure is given by:



$$\Psi(x) = A\sin(\pi x / L)$$

Determine the normalization constant *A* in terms of *L*.

References:

[1]. http://www.mathworks.com/products/matlab

[2]. Numerical Methods in Engineering with MATLAB,
J. Kiusalaas, Cambridge University Press (2005)

[3]. Numerical Methods for Engineers, 6th Ed.
S.C. Chapra, Mc Graw Hill (2010)