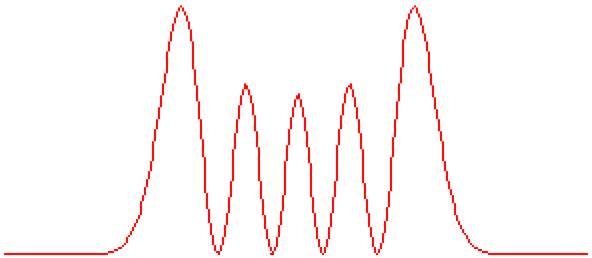
EP547 Computational Methods in QM

Topic 6

Numerical and Symbolic Differentiation & Integration



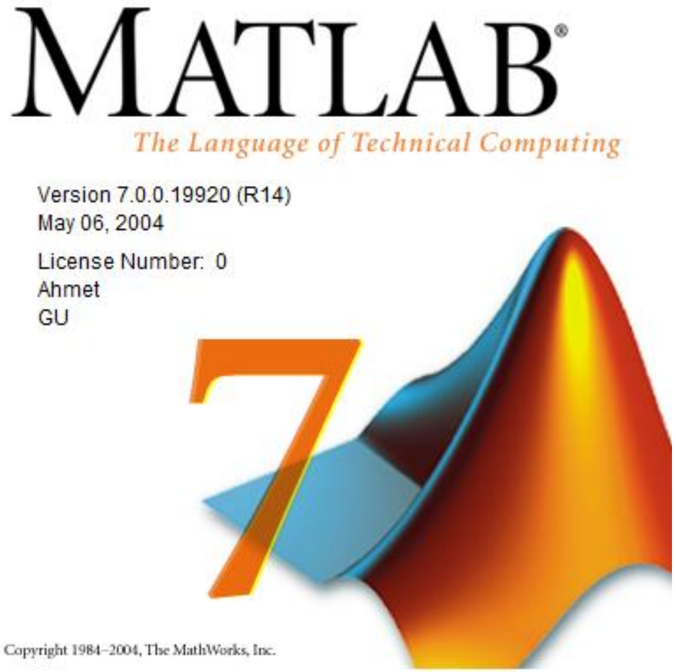
Department of
Engineering Physics

University of Gaziantep

Feb 2013

Content

1. **Introduction**
2. **Differentiation**
3. **Integration**



Introduction

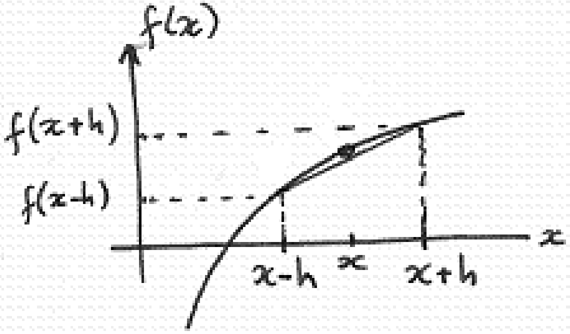
In engineering problems, we have mostly deal with the differentiation and integration of the functions of single- or multi-variables.

In this chapter,

- We will first consider numerical derivative and integration.

- Then we will use MATLAB built-in functions
  `diff()` to evaluate finite difference or derivative
  `int()` to evaluate the definite or indefinite integrals.

Numerical Derivatives



$$CDA = \frac{f(x+h) - f(x-h)}{2h} \approx f'(x)$$

Proof:

Taylor's expansion,

$$f(x+h) = f(x) + h\frac{f'(x)}{1!} + h^2\frac{f''(x)}{2!} + h^3\frac{f'''(x)}{3!} + \dots$$

$$f(x-h) = f(x) - h\frac{f'(x)}{1!} + h^2\frac{f''(x)}{2!} - h^3\frac{f'''(x)}{3!} + \dots$$

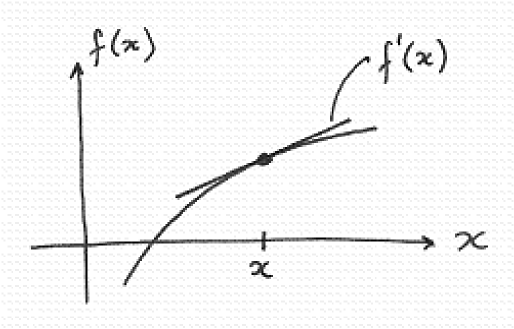
$$\Rightarrow CDA = f'(x) + \frac{h^2}{6} f'''(x) + O(h^4)$$

i.e $CDA \approx f'(x)$

the error $\approx \frac{h^2}{6} f'''(x)$.

Numerical Derivatives

- For a function f(x)



$$f'(x) \approx \frac{f(x+h) - f(x-h)}{2h}$$

$$f''(x) \approx \frac{f(x+h) - 2f(x) + f(x-h)}{h^2}$$

- Partial derivatives for a function f(x, y, z)

$$\frac{\partial f}{\partial x} \approx \frac{f(x+h,y,z) - f(x-h,y,z)}{2h}$$

$$\frac{\partial^2 f}{\partial x^2} \approx \frac{f(x+h,y,z) - 2f(x,y,z) + f(x-h,y,z)}{h^2}$$

$$\frac{\partial^2 f}{\partial x \partial y} \approx \frac{f(x+h,y+h,z) - f(x-h,y+h,z) - f(x+h,y-h,z) + f(x-h,y-h,z)}{4h^2}$$

Example 1:

Find the first and second derivative of the function

$f(x) = x^2 + \exp(-x)$ at $x = 3$ for $h = 0.01$.

```
>> edit derivative.m
```

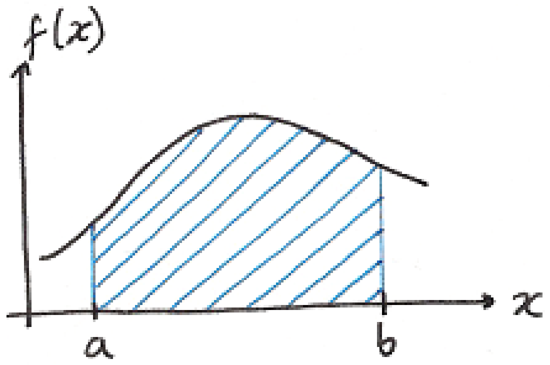
```
function [d1 d2] = derivative(x,h)
  d1 = (f(x+h)-f(x-h))/(2*h);
  d2 = (f(x+h)+f(x-h)-2*f(x))/h^2;
end

function y = f(x)
  y = x^2 + exp(-x);
end
```

```
>> [d1 d2] = derivative(3, 0.01)
d1 = 5.9502
d2 = 2.0498
```

Numerical Integration

- The integral of a function *f(x)* between the limits *a* and *b* is simply the area under the curve between *a* and *b*.

$$Area = \int_a^b f(x)dx$$

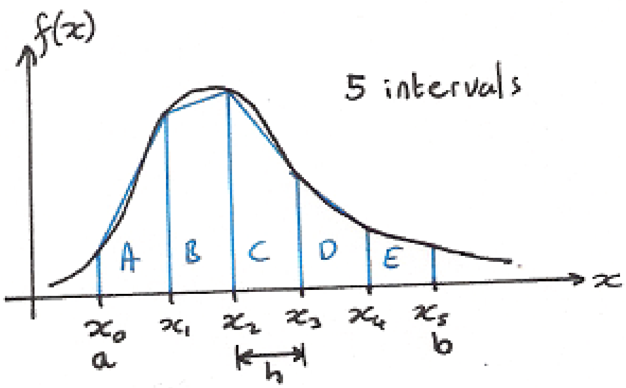


- Sometimes, finding the integral analytically can be difficult or *impossible*.
- So a numerical solution may be necessary or simply convenient.

Trapezoidal Method

We want the integral $\int_a^b f(x)\,dx$.

First consider approximating with five trapezoids:



$A = \frac{h}{2}\left(f(x_0) + f(x_1)\right)$ $\qquad h = \frac{x_5 - x_0}{5}$

$B = \frac{h}{2}\left(f(x_1) + f(x_2)\right)$ $\qquad = \frac{b-a}{5}$

$C = \frac{h}{2}\left(f(x_2) + f(x_3)\right)$

$D = \frac{h}{2}\left(f(x_3) + f(x_4)\right)$ $\qquad$ let $f_i = f(x_i)$

$E = \frac{h}{2}\left(f(x_4) + f(x_5)\right)$

$A+B+C+D+E$ = Extended Trapezoidal Formula (ETF).

$h\left(f_0/2 + f_1 + f_2 + f_3 + f_4 + f_5/2\right)$

For n intervals

$ETF = h\left(\frac{f_0}{2} + f_1 + f_2 + f_3 + \cdots + f_{n-1} + \frac{f_n}{2}\right)$

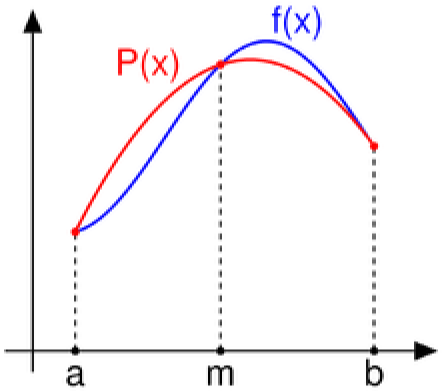
with $h = \frac{b-a}{n}$ $\quad x_i = a + ih, \quad i = 0, 1, 2, \ldots, n$

$$\int_a^b f(x)dx \approx h\left(\frac{f(a)+f(b)}{2} + \sum_{i=1}^{n-1} f(a+ih)\right)$$

$$h = \frac{b-a}{n}$$

Simpson's Method

Trapezoids are replaced by the quadratic polynomials!



Suppose that the interval $[a, b]$ is split up in n subintervals, with n an even number. Then, the composite Simpson's rule is given by

$$\int_a^b f(x)\,dx \approx \frac{h}{3}\left[f(x_0) + 2\sum_{j=1}^{n/2-1} f(x_{2j}) + 4\sum_{j=1}^{n/2} f(x_{2j-1}) + f(x_n)\right],$$

where $x_j = a + jh$ for $j = 0, 1, ..., n-1, n$ with $h = (b-a)/n$; in particular, $x_0 = a$ and $x_n = b$.

Example 2:

Evaluate the integral $\int_0^3 \sqrt{x}\,dx$ for n = 100 parts

```
>> edit integral.m
```

```
function integ = integral(a,b,n)
  h = (b-a)/n;
  s = (f(a)+f(b))/2.0;
  for i=1:n-1
      s = s + f(a+i*h);
  end
  integ = h*s;
end

function y = f(x)
  y = sqrt(x);
end
```

```
>> integral(0,3,100)
ans = 3.4630
```

Symbolic 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 3:

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 4:

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

```
>> syms x
>> d = diff(x^2+exp(-x));
>> x = 3;
>> eval(d)
ans = 5.9502
```

Example 5:

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)
```

Symbolic 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 6:

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 7:

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

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

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)

[4]. http://en.wikipedia.org/wiki/Trapezoidal_rule

[5]. http://en.wikipedia.org/wiki/Simpson%27s_rule