INTRODUCTION TO SCIENTIFIC & ENG. COMPUTING
BIL 108E, CRN 44448

Week.9_ Polynomials Examples
Week.10_ Application of curve fitting : Approximation & Inregration

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TENTATIVE SCHEDULE

Wk	Date	Topics
1	Feb. 11	Introduction to Scientific and Engineering Computing
2	Feb. 18	Introduction to Program Computing Environment
3	Feb. 25	Variables, Operations and Simple Plot
4	Mar. 04	Algorithms and Logic Operators
5	Mar. 11	Flow Control, Errors and Source of Errors
6	Mar. 18	Functions & Linear Algebra
7	Mar. 25	Arrays
8	Apr. 01	Solving of Simple Equations
9	Apr. 08 -15	Polynomials Examples Exam 1
10	Apr. 15 -22	Applications of Curve Fitting
11	Apr. 22	Applications of Interpolation
12	Apr. 29	Applications of Numerical Integration
13	May.06	Symbolic Mathematics
14	May.13	Ord Dif.Equations (ODE) solution with Built-in Functions

Week 10

- LECTURE # 10

1 NUMERICAL APPROXIMATION
   1 NUMERICAL DIFFERENTIATION
   2 FORWARD FINITE DIFFERENCE
   3 BACKWARD FINITE DIFFERENCE
   4 CENTERED FINITE DIFFERENCE

2 NUMERICAL INTEGRATION
   1 MIDPOINT QUADRATURE
   2 TRAPEZOIDAL QUADRATURE
   3 SIMPSON QUADRATURE
   4 GAUß-LEGENDRE FORMULA
   5 ADAPTIVE SIMPSON FORMULA

NUMERICAL APPROXIMATION

NUMERICAL INTEGRATION AND DIFFERENTIATION

- To integrate a generic function, it is not possible to find a closed form of the primitive function.
- When a primitive is known, its use might not be easy.

$$f(x) = cos(4x)\, cos(3sin(x))$$

$$\int_0^{\pi} f(x)\, dx = \pi(\frac{3}{2}) \sum_{k=p}^{\infty} \frac{(-9/4)^k}{k!(k+4)!}$$

- Calculation on experimental measurements.
- **Use numerical methods to approximate the differentiation or integration**.

APPROXIMATION OF FUNCTION DERIVATIVES

- Consider a function f : [a, b] → R
- Find an approximation of the first derivative (f′) of *f* at a generic point x in interval (a, b).

$$\Delta f^{+}(\bar{x}) = \frac{f(\bar{x}+h) - f(\bar{x})}{h}$$

- is an approximation of ***f′(x)***, for h sufficiently small and positive.
- The above approximation is defined as **FORWARD FINITE DIFFERENCE**.

APPROXIMATION OF FUNCTION DERIVATIVES

- To estimate the error, check the difference between the real value and approximation
- With using Taylor series

$$f(\bar{x}+h) = f(\bar{x}) + hf'(\bar{x}) + \frac{h^2}{2}f''(\xi)$$

Here ξ is in the interval $(\bar{x}, \bar{x}+h)$

- Then the forward finite difference is

$$\Delta f^{+}(\bar{x}) = f'(\bar{x}) + \frac{h}{2}f''(\xi)$$

- $\Delta f^{+}(\bar{x})$ is a **first order approximation** of $f'(\bar{x})$

APPROXIMATION OF FUNCTION DERIVATIVES

- With a similar procedure for a sufficiently small and negative h .

$$\Delta f^{-}(\bar{x}) = \frac{f(\bar{x}) - f(\bar{x}-h)}{h}$$

- This is called **BACKWARD FINITE DIFFERENCE**

APPROXIMATION OF FUNCTION DERIVATIVES

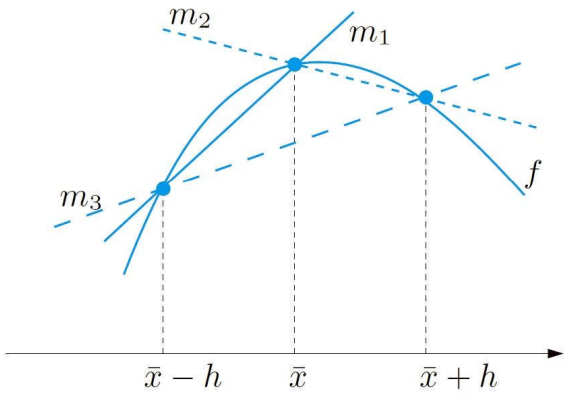
- CENTERED FINITE DIFFERENCE

$$\Delta f(\bar{x}) = \frac{f(\bar{x}+h) - f(\bar{x}-h)}{2h}$$

- This formula provides **second –order approximation**
- Error estimation

$$f'(\bar{x}) - \Delta f(\bar{x}) = \frac{h^2}{12}(f'''(\xi) + f'''(\eta))$$

APPROXIMATION OF FUNCTION DERIVATIVES



- When $x = x_i$ and $x_i = x_0 + i\,h$ with $h > 0$, $f'(x_i)$ is approximated with;

  ✓FORWARD FINITE DIFFERENCE
  ✓BACKWARD FINITE DIFFERENCE
  ✓CENTERED FINITE DIFFERENCE

Note: With the centered finite difference approximation, the centered formula cannot be used at beginning and ending points of interval. For this points use;

$1 / 2h\,[-3f(x_0) + 4f(x_1) - f(x_2)]$ at x_0
$1 / 2h\,[3f(x_n) - 4f(x_{n-1}) + f(x_{n-2})]$ at x_n

EXAMPLE:

akışkan

- The height *q(t)* reached at time *t* by a fluid in a straight cylinder of radius *R = 1m* with a circular hole of radius *r =0.1m* on the bottom, has been measured every 5 seconds yielding the following values;

t	0.0	5.0	10.0	15.0	20.0
q(t)	0.6350	0.5336	0.4410	0.3572	0.2822

- We want to compute an approximation of the emptying velocity *q(t)* of the cylinder, then compare with the one predicted by Torricelli's law: $q'(t) = -\gamma\,(r/R)^2\sqrt{g*q(t)}$, where g is the gravitational acceleration and $\gamma = 0.6$ is a correction factor.

EXAMPLE:

t	0.0	5.0	10.0	15.0	20.0
q(t)	0.6350	0.5336	0.4410	0.3572	0.2822
$q'(t)$	-0.0212	-0.0194	-0.0176	-0.0159	-0.0141
Δq^+	-0.0203	-0.0185	-0.0168	-0.0150	
Δq^-		-0.0203	-0.0185	-0.0168	-0.0150
Δq		-0.0194	-0.0176	-0.0159	

MATLAB FUNCTIONS

`diff`

`diff(y) ./ diff(x)`

```
>> help diff
 DIFF Difference and approximate derivative.
    DIFF(X), for a vector X, is [X(2)-X(1)  X(3)-X(2) ... X(n)-X(n-1)].
    DIFF(X), for a matrix X, is the matrix of row differences,
       [X(2:n,:) - X(1:n-1,:)].
    DIFF(X), for an N-D array X, is the difference along the first
       non-singleton dimension of X.
    DIFF(X,N) is the N-th order difference along the first non-singleton
       dimension (denote it by DIM). If N >= size(X,DIM), DIFF takes
       successive differences along the next non-singleton dimension.
    DIFF(X,N,DIM) is the Nth difference function along dimension DIM.
       If N >= size(X,DIM), DIFF returns an empty array.

    Examples:
       h = .001; x = 0:h:pi;
       diff(sin(x.^2))/h is an approximation to 2*cos(x.^2).*x
       diff((1:10).^2) is 3:2:19

       If X = [3 7 5
```


EXAMPLE (`diff`)

- Y = diff(X,n) applies diff recursively n times, resulting in the n th difference. Thus, **diff(X,2)** is the same as **diff(diff(X))**.

- Y = diff(X, n, dim) is the **n th** difference function calculated along the dimension specified by scalar **dim**. If order n equals or exceeds the length of **dim**, diff returns an empty array.

If X = [3 7 5 0 9 2] then

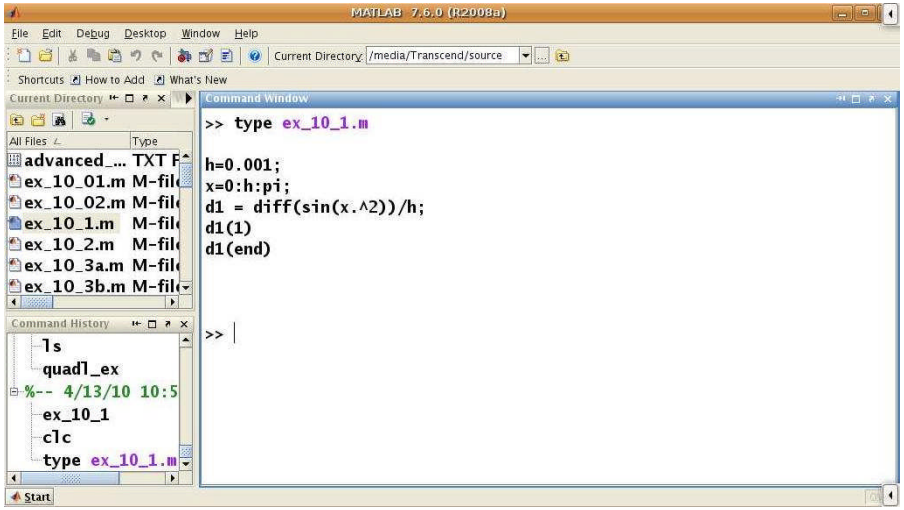
diff(X,1,1) is [-3 2 -3],

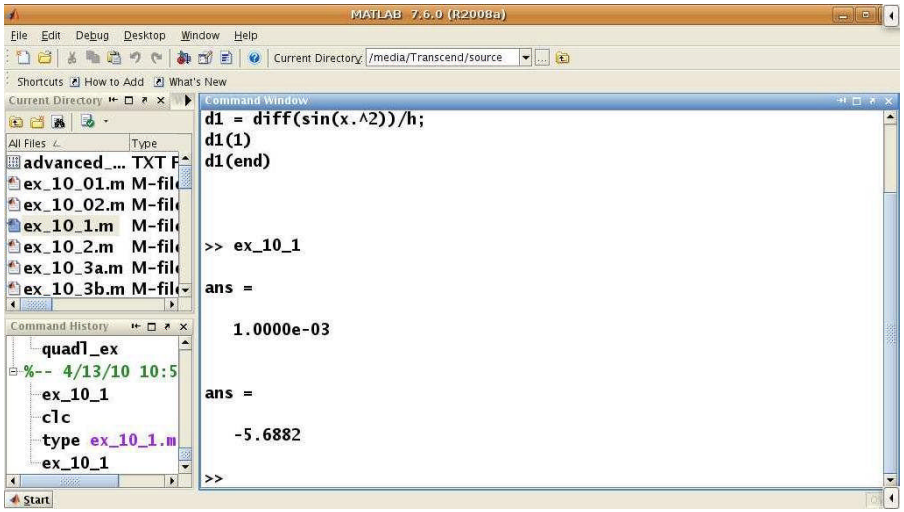
diff(X,1,2) is [4 -2 9 -7],

diff(X,2,2) is the 2nd order difference along the dimension 2, and

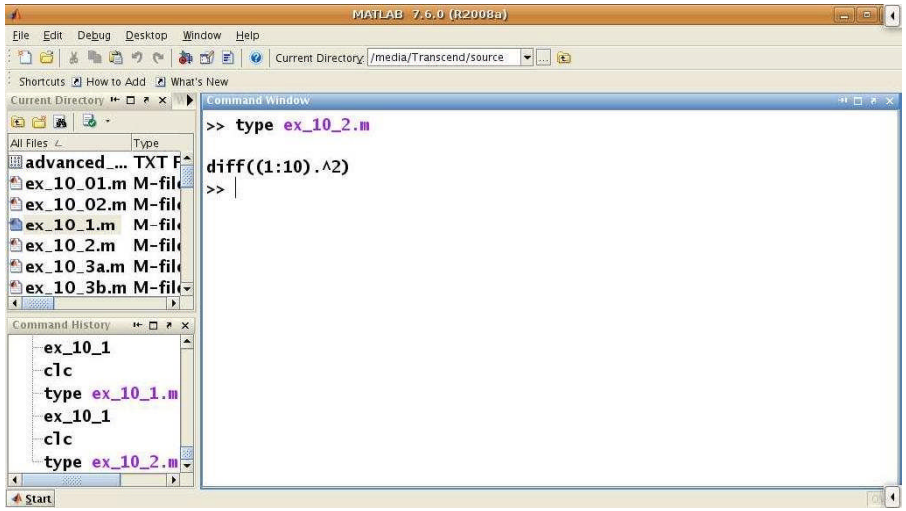
diff(X,3,2) is the empty matrix.

EXAMPLE (`diff`)

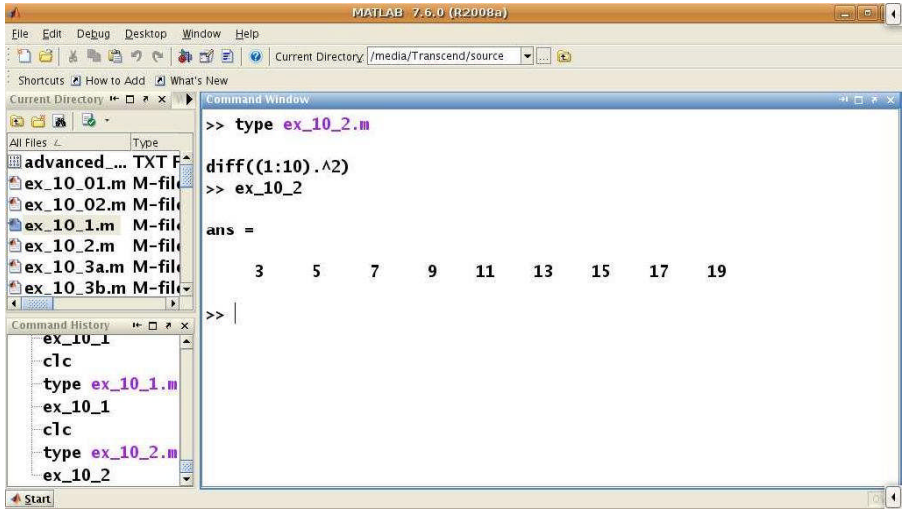




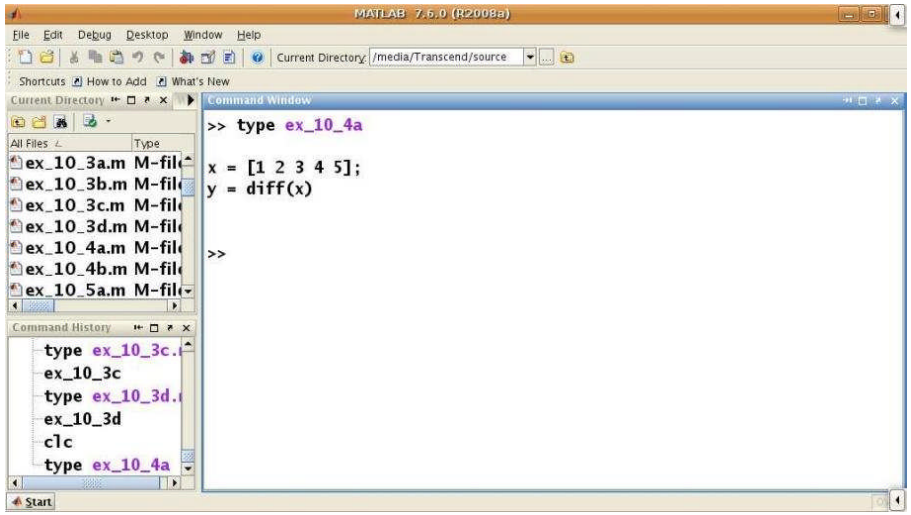
APPROXIMATION OF FUNCTION DERIVATIVES



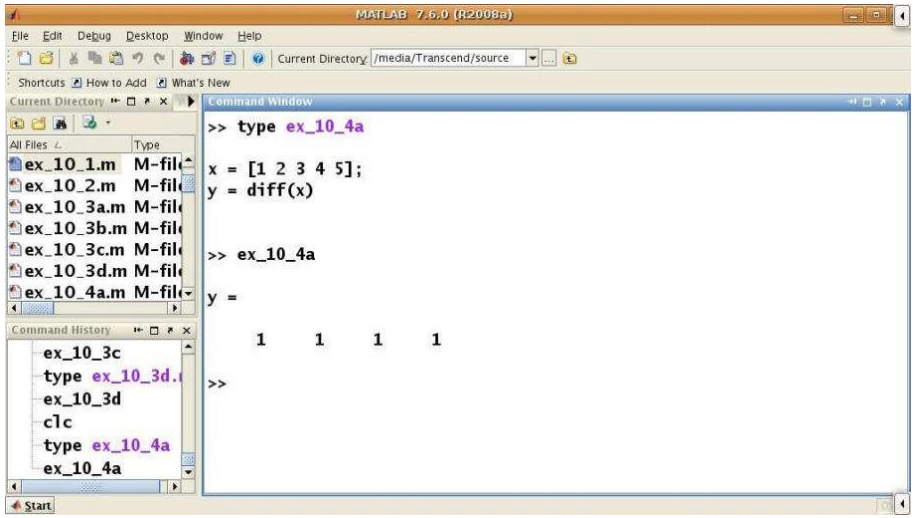
APPROXIMATION OF FUNCTION DERIVATIVES

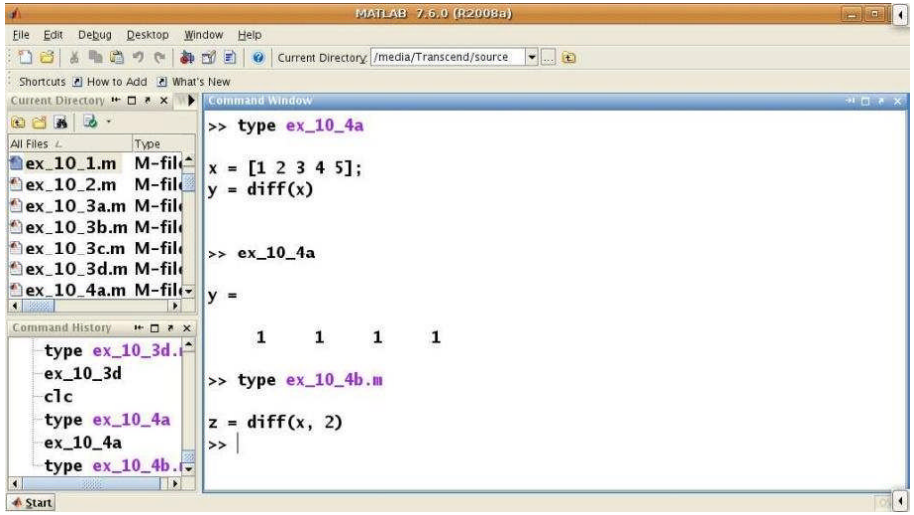


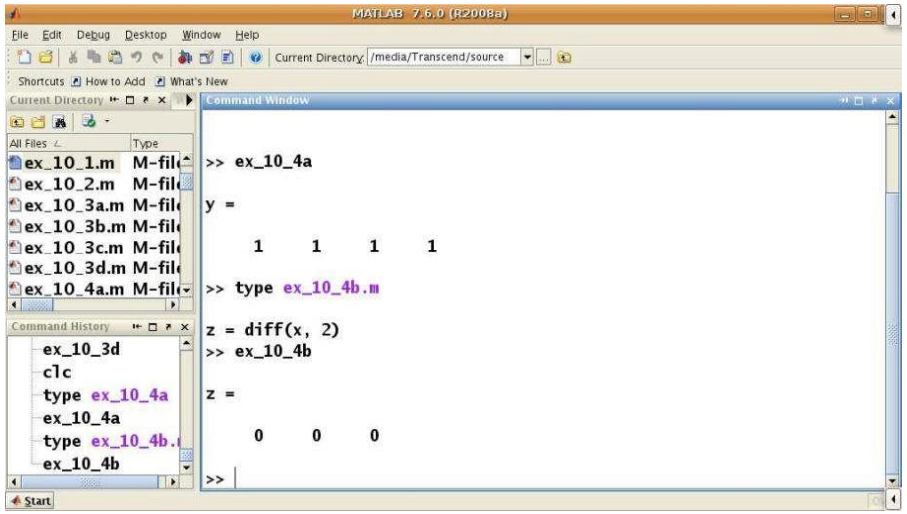
APPROXIMATION OF FUNCTION DERIVATIVES



APPROXIMATION OF FUNCTION DERIVATIVES

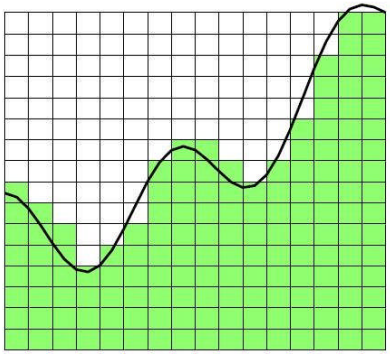






QUADRATURE

- The word "**quadrature**" reminds us an elementary technique for finding the area under the curve.
- Plot the function on graph paper and count the number of little squares that lie underneath the curve.



- Area under the curve is counted / calculated.

APPROXIMATION OF INTEGRALS

- Numerical Methods for approximating the integral

$$I(f) = \int_a^b f(x)\,dx$$

- Here *f* is an arbitrary continuous function

APPROXIMATION OF INTEGRALS

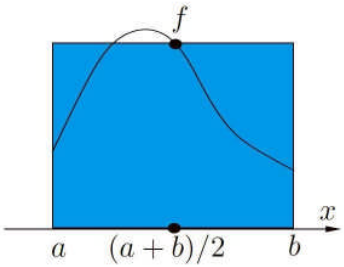
- Midpoint Quadrature
- Trapezoidal Quadrature
- Simpson Quadrature
- Gauß-Legendre Formula
- Adaptive Simpson Formula

APPROXIMATION OF INTEGRALS

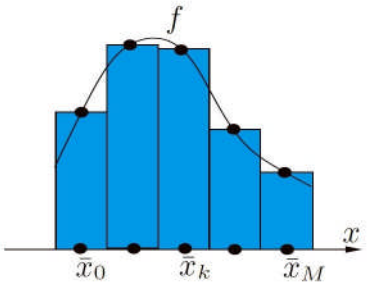
Newton-Cotes equation

- Define the function f (x) as an approximation with polynom P(x), and use it on an equally partitioned interval (a, b).
- Calculation with this method is also named as composite quadrature.

MIDPOINT QUADRATURE



MIDPOINT QUADRATURE



- Approximate the integral I *(f)* for the interval [a, b]
- Divide the interval $I_k = [x_{k-1}, x_k]$ for $k = 1, \ldots, M$ into subintervals.
- $x_k = a + k\,H$, $k = 0, \ldots, M$ and $H = (b - a) / M$

$$I(f) = \sum_{k=1}^{M} \int_{I_k} f(x)\,dx$$

MIDPOINT QUADRATURE

- Approximate the function f with a polynomial $\bar{f}$ on I_k
- $\bar{x_k} = \frac{x_{k-1} - x_k}{2}$
- $I^c_{mp}(f) = H \sum_{k=1}^{M} f(\bar{x_k})$

- **This is called COMPOSITE MIDPOINT QUADRATURE**

  Second - order approximate with respect to *H*

CLASSIC MIDPOINT FORMULA

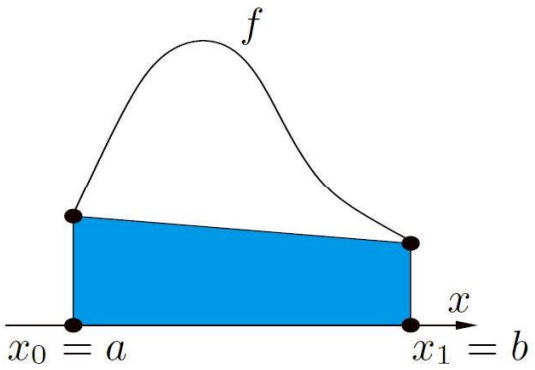
- Here the number of partitions M=1.

$$I_{mp}(f) = (b-a)\, f((a+b)/2)$$

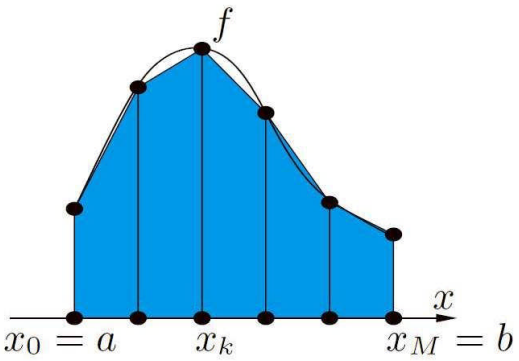
- Estimated error,

$$I(f) - I_{mp}(f) = \frac{(b-a)^3}{24} f''(\xi)$$

TRAPEZOIDAL QUADRATURE



TRAPEZOIDAL QUADRATURE



TRAPEZOIDAL QUADRATURE

- Calculation is done with the area of a trapezoidal.

$$I_t^c(f) = \frac{H}{2}\sum_{k=1}^{M}(f(x_k)+f(x_{k-1})) = \frac{H}{2}(f(a)+f(b))+H\sum_{k=1}^{M-1} f(x_k)$$

$$I_t(f) = \frac{b-a}{2}(f(a)+f(b))$$

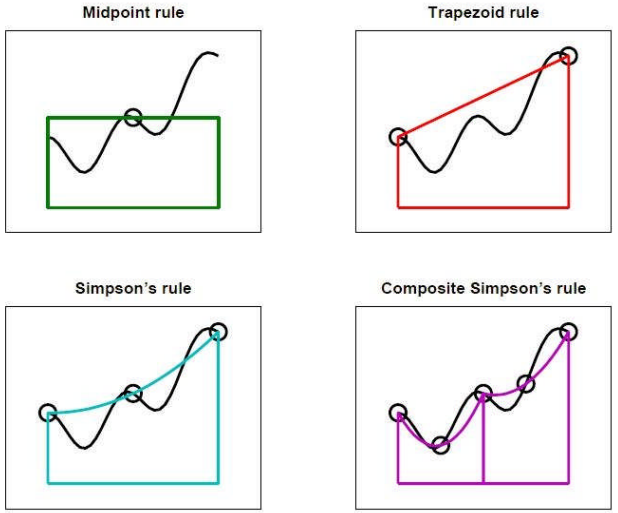
SIMPSON QUADRATURE

- Approximate the function by a parabola. This rule can be applied to the even number of segments (odd number of points).

$$I_s^c(f) = \frac{H}{6}\sum_{k=1}^{M}(f(x_{k-1}) + 4f(\bar{x_k}) + f(x_k))$$

$$I_s(f) = \frac{b-a}{6}(f(a) + 4f((a+b)/2) + f(b))$$

APPROXIMATION OF INTEGRALS



INTERPOLATORY QUADRATURES

GAUß-LEGENDRE FORMULA

$$I_{appr}(f) = \sum_{j=0}^{n} \alpha_j f(y_j)$$

- α_j : quadrature weights
- y_j : quadrature nodes

MATLAB FUNCTIONS

`trapz` : Uses areas of trapezoidals.
`cumtrapz` : Uses composite trapezoidal quadrature.
`quad` : Uses the adaptive Simpson quadrature algorithm.
`quadl` : Uses Gauß-Legendre Formula.

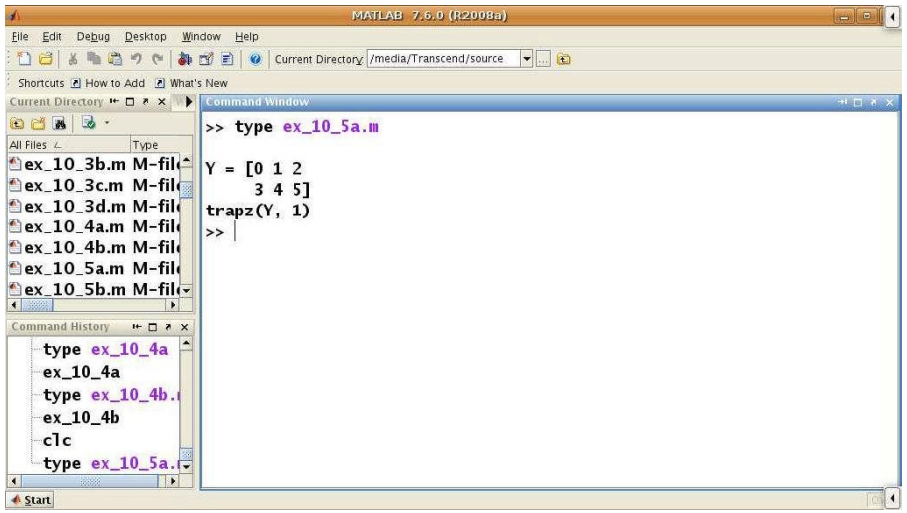
APPROXIMATION OF INTEGRALS

trapz

```
>> help trapz
 TRAPZ  Trapezoidal numerical integration.
    Z = TRAPZ(Y) computes an approximation of the integral of Y via
    the trapezoidal method (with unit spacing).  To compute the integral
    for spacing different from one, multiply Z by the spacing increment.

    For vectors, TRAPZ(Y) is the integral of Y. For matrices, TRAPZ(Y)
    is a row vector with the integral over each column. For N-D
    arrays, TRAPZ(Y) works across the first non-singleton dimension.

    Z = TRAPZ(X,Y) computes the integral of Y with respect to X using
    the trapezoidal method.  X and Y must be vectors of the same
    length, or X must be a column vector and Y an array whose first
    non-singleton dimension is length(X).  TRAPZ operates along this
    dimension.

    Z = TRAPZ(X,Y,DIM) or TRAPZ(Y,DIM) integrates across dimension DIM
    of Y. The length of X must be the same as size(Y,DIM)).
```

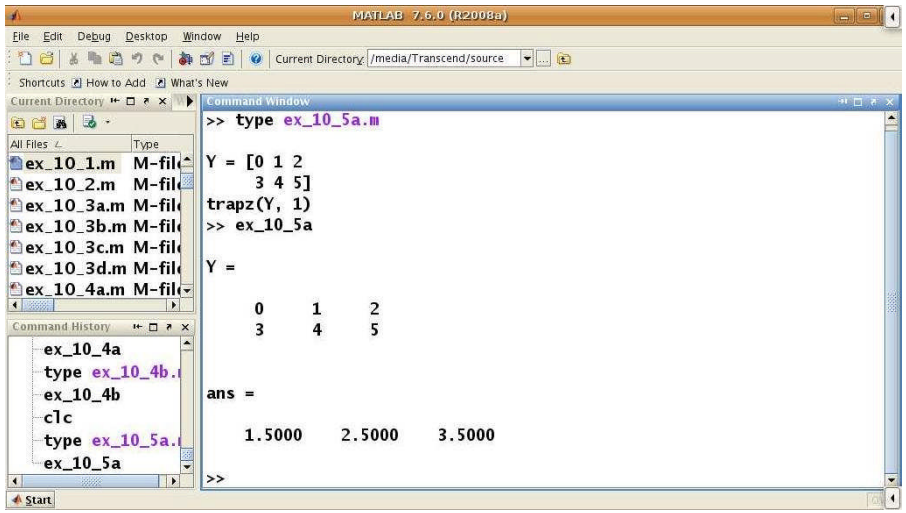

APPROXIMATION OF INTEGRALS

trapz



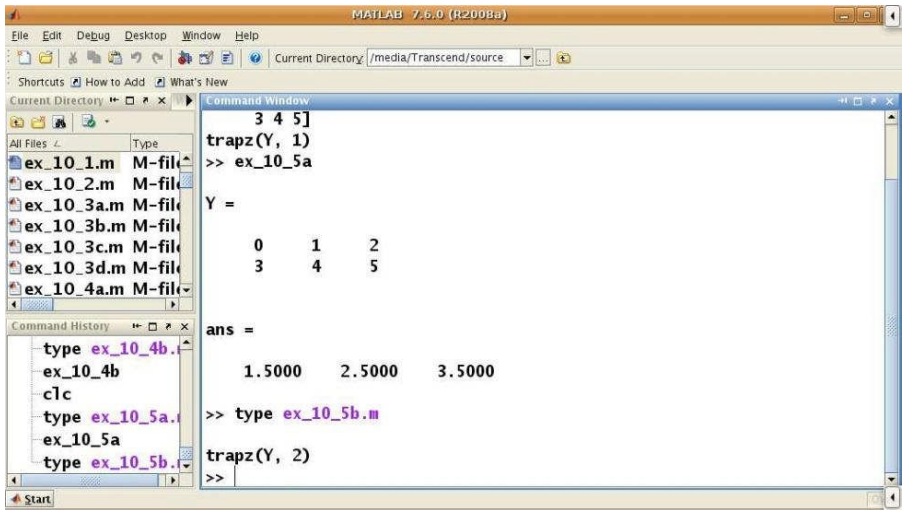
APPROXIMATION OF INTEGRALS

trapz

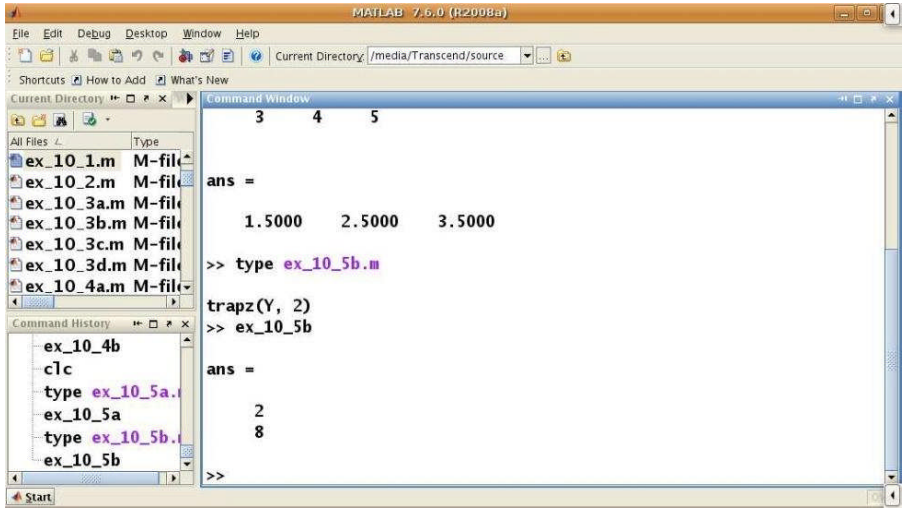


APPROXIMATION OF INTEGRALS

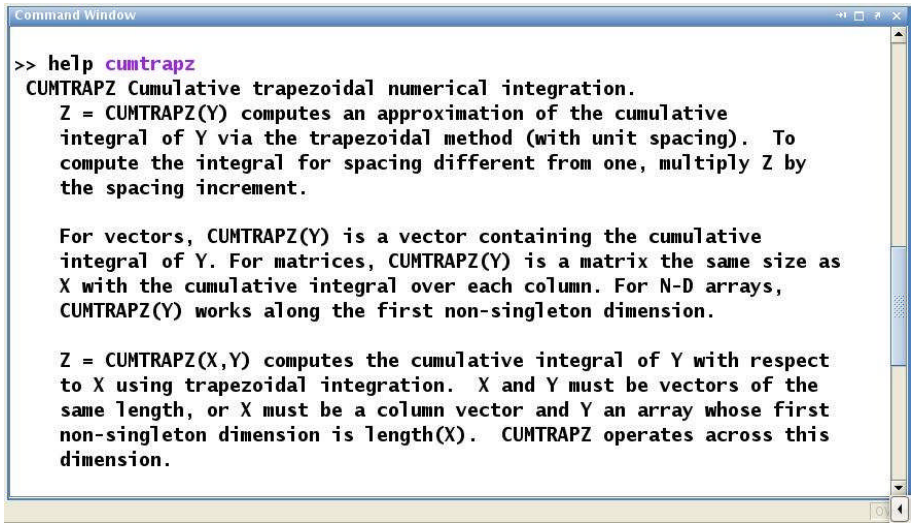
trapz



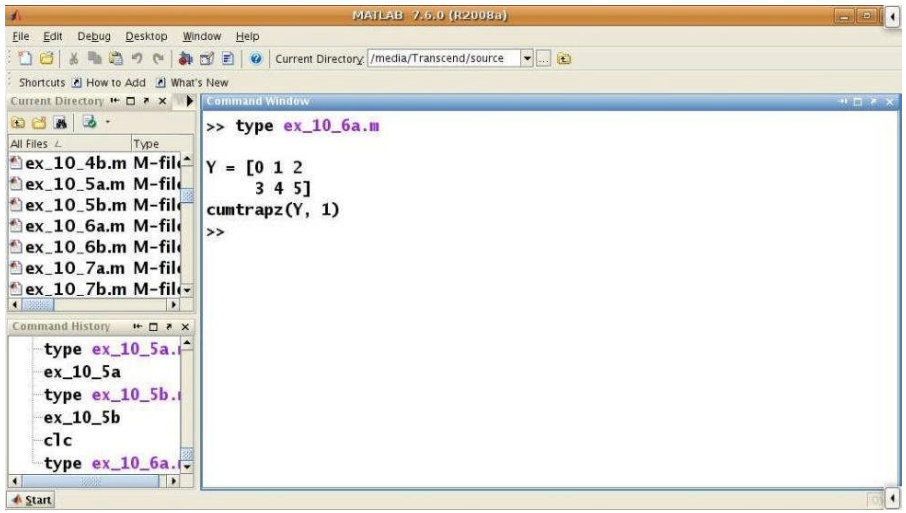
trapz



cumtrapz



cumtrapz



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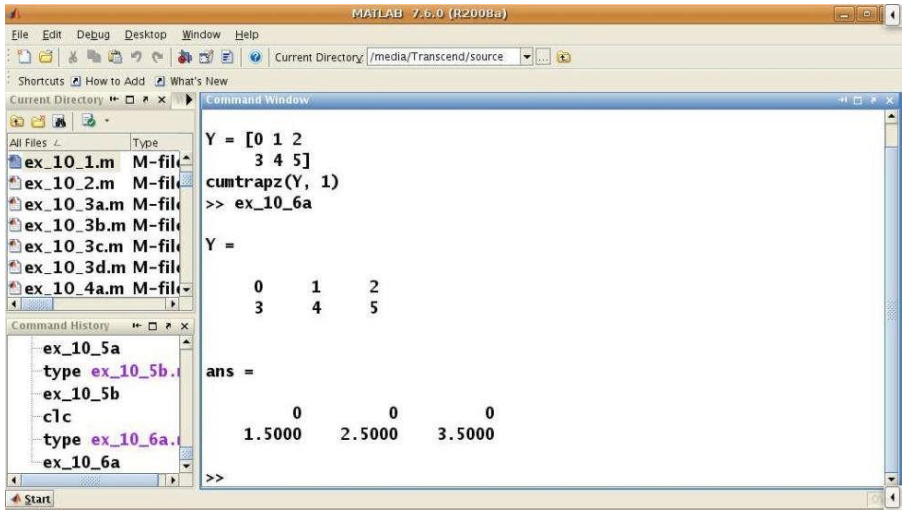

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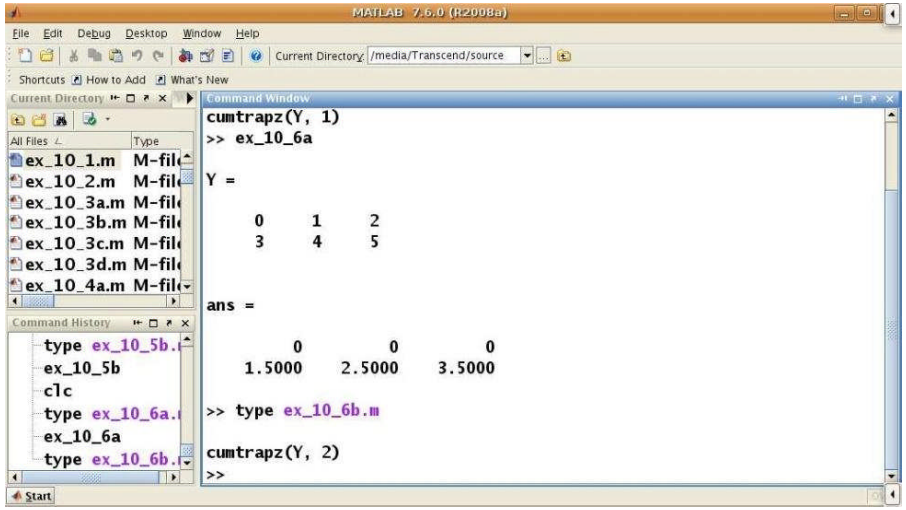
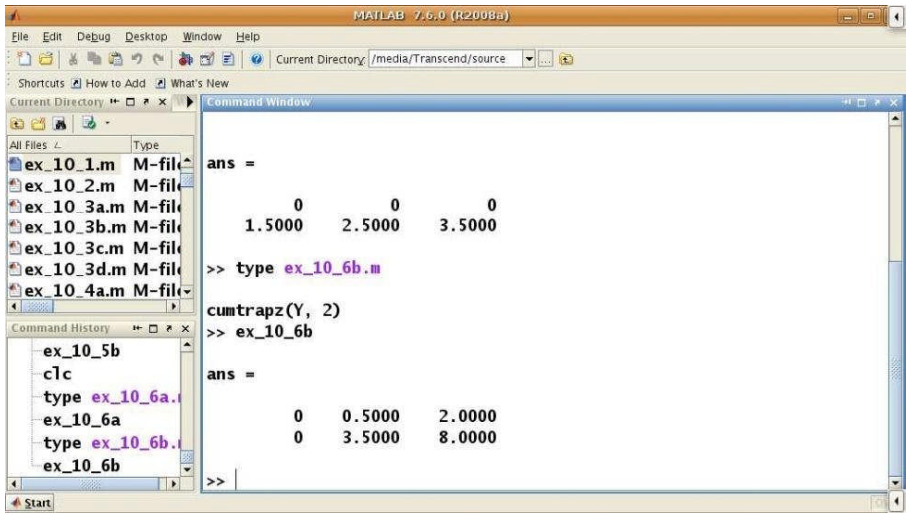
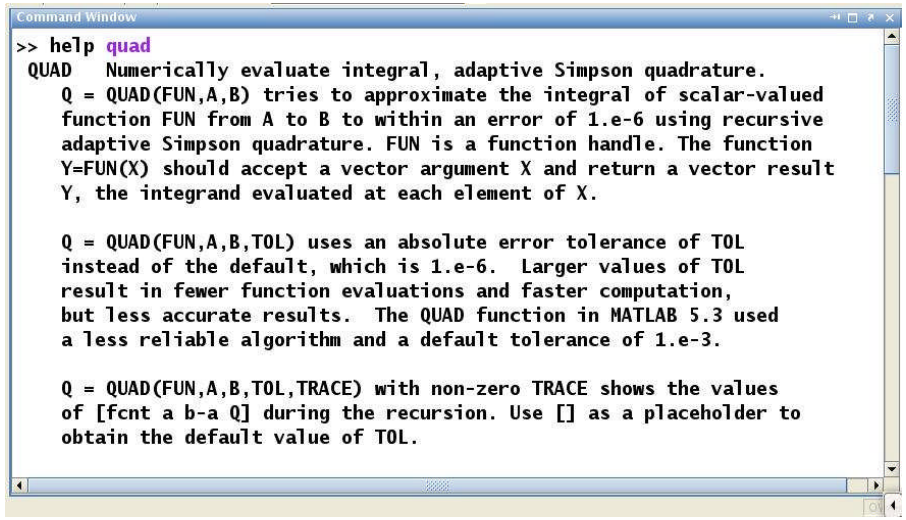


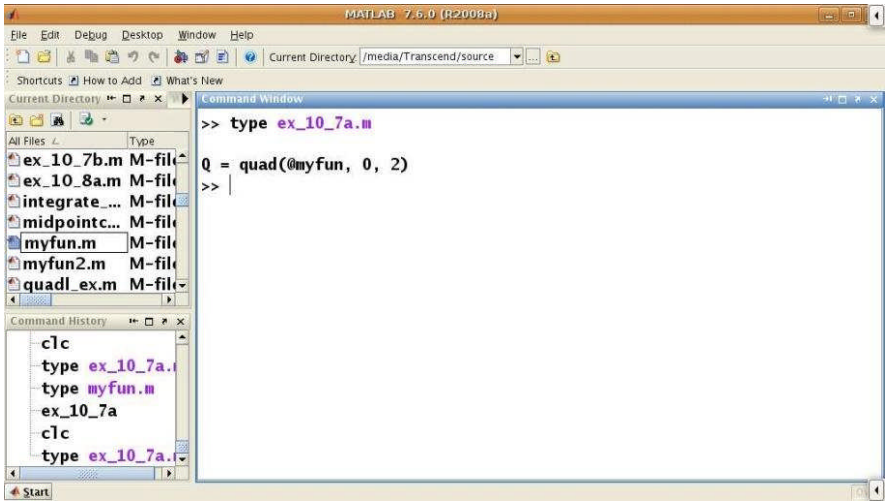
cumtrapz



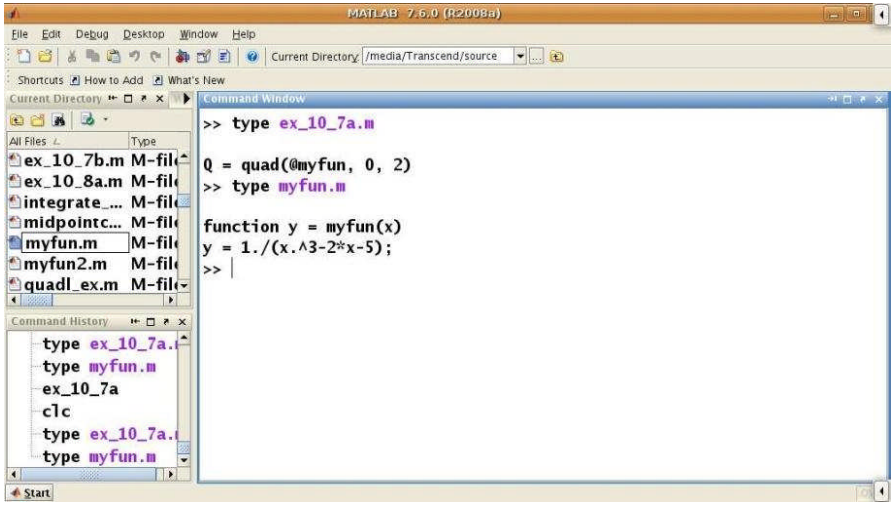
quad



quad



quad



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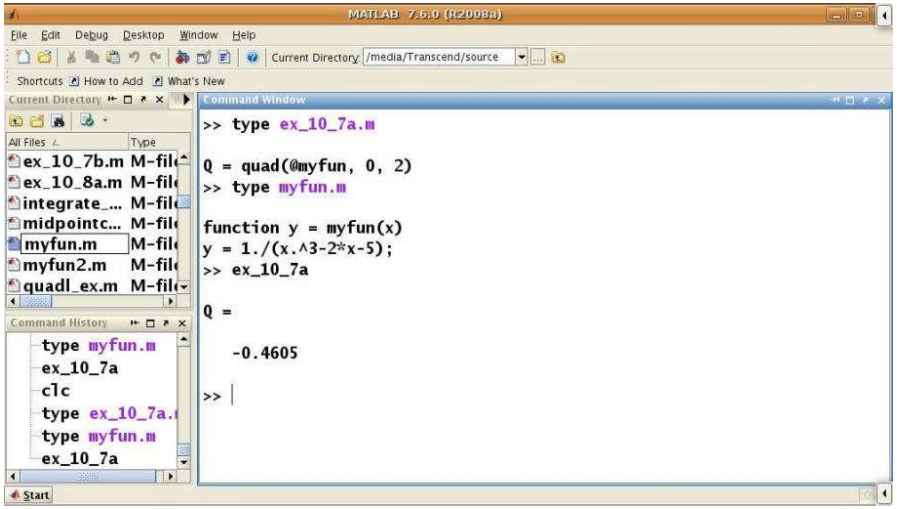

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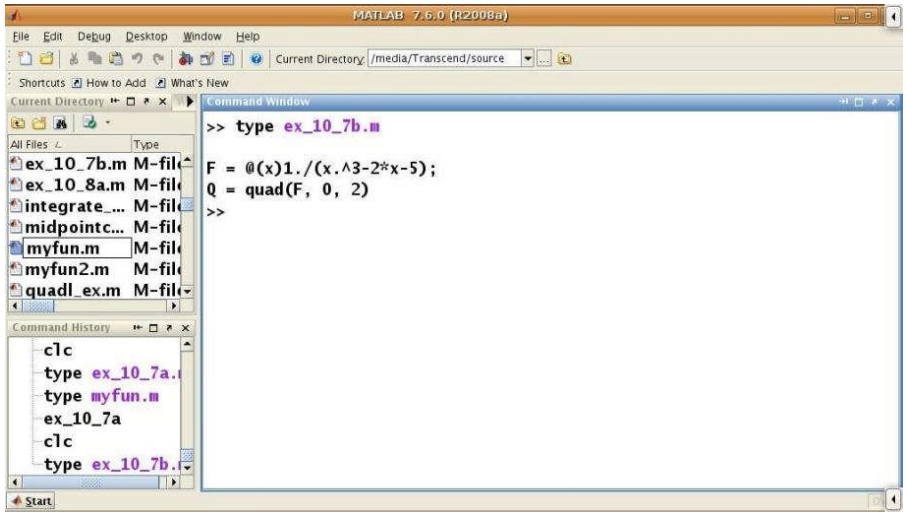
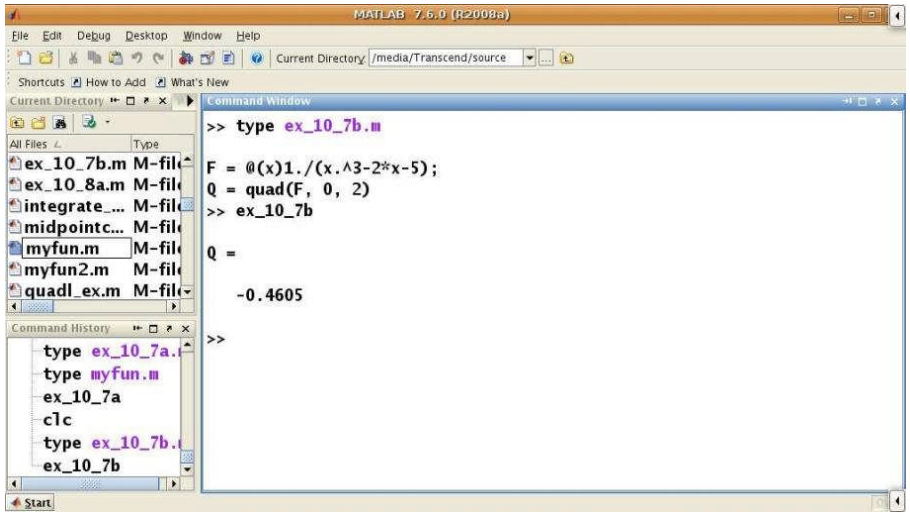


quad



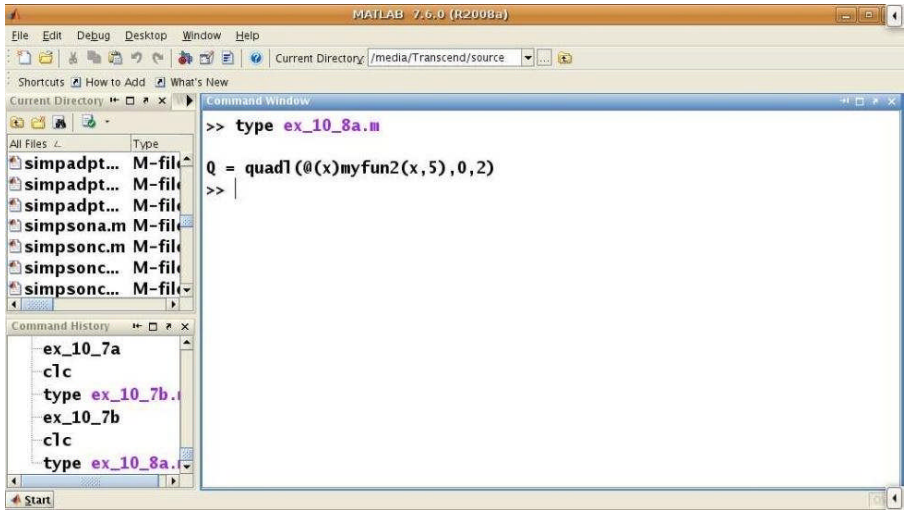
APPROXIMATION OF INTEGRALS

quadl

```
>> help quadl
 QUADL  Numerically evaluate integral, adaptive Lobatto quadrature.
    Q = QUADL(FUN,A,B) tries to approximate the integral of scalar-valued
    function FUN from A to B to within an error of 1.e-6 using high order
    recursive adaptive quadrature.  FUN is a function handle. The function
    Y=FUN(X) should accept a vector argument X and return a vector result
    Y, the integrand evaluated at each element of X.

    Q = QUADL(FUN,A,B,TOL) uses an absolute error tolerance of TOL
    instead of the default, which is 1.e-6.  Larger values of TOL
    result in fewer function evaluations and faster computation,
    but less accurate results.

    Q = QUADL(FUN,A,B,TOL,TRACE) with non-zero TRACE shows the values
    of [fcnt a b-a Q] during the recursion. Use [] as a placeholder to
    obtain the default value of TOL.

    [Q,FCNT] = QUADL(...) returns the number of function evaluations.
```

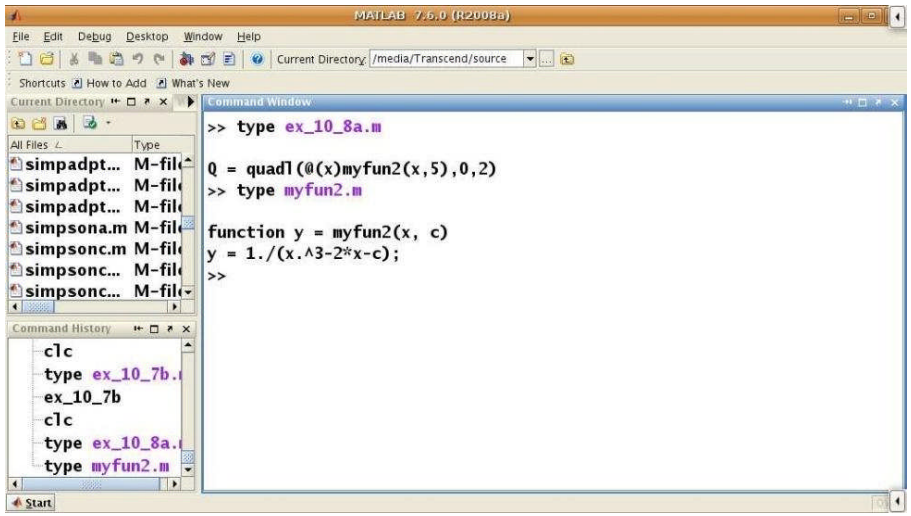

APPROXIMATION OF INTEGRALS

quadl



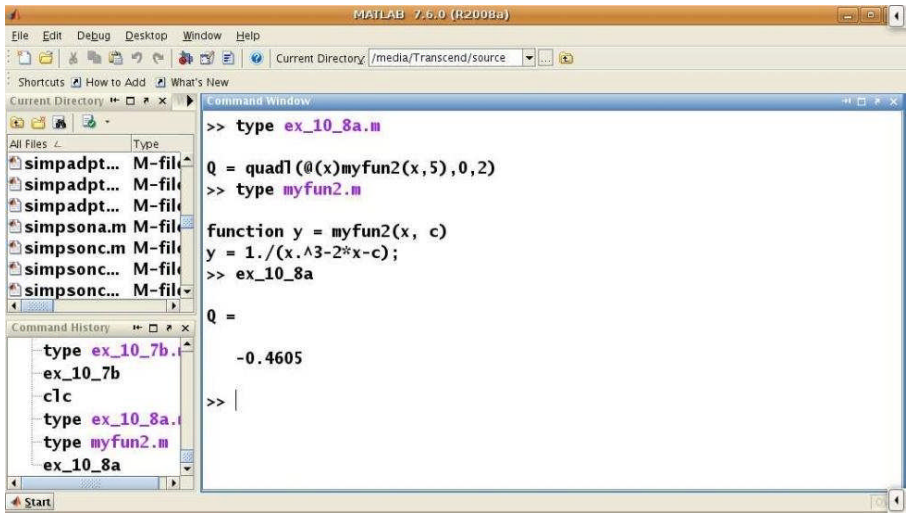
APPROXIMATION OF INTEGRALS

quadl



APPROXIMATION OF INTEGRALS

quadl



APPROXIMATION OF INTEGRALS

- EXAMPLES:
- Evaluate the following integral with different methods.

$$\int_0^{3\pi/2} \cos(x)\,dx$$

- Cosine is a built-in function in Matlab.

```
y= quad ('cos',0,3*pi/2)
y= quadl('cos',0,3*pi/2)
```


APPROXIMATION OF INTEGRALS

- EXAMPLES:
- Evaluate the following integral with different methods.

$$\int_0^{8} (x\, e^{-x^{0.8}} + 0.2)\,dx$$

```
quad ('x.*exp(-x.^0.8)+0.2', 0,8)
quadl('x.*exp(-x.^0.8)+0.2', 0,8)
```


APPROXIMATION OF INTEGRALS

- *SOURCE:* trapezoid

```
function I=trapezoid(fun,a,b,npanel)
n=npanel+1;          %total number of nodes (düğüm nok)
h=(b-a)/(n-1);       %stepsize
x=a:h:b;             %divide the interval
f=feval(fun,x);      %evaluate the integral
I=h*(0.5*f(1)+sum(f(2:n-1))+0.5*f(n));
```


APPROXIMATION OF INTEGRALS

- *SOURCE:* midpointc

```
function Imp=midpointc(a,b,M,f)
% MIDPOINTC Composite midpoint numerical integration.
% IMP = MIDPOINTC(A,B,M,FUN) computes
%  an approximation of the integral
%  of the function FUN via the midpoint
%  method (with M equispaced intervals).
%  FUN accepts real scalar input x and
%  returns a real scalar
%  value. FUN can also be an inline object.
H=(b-a)/M;
x = linspace(a+H/2,b-H/2,M); fmp=feval(f,x);
Imp=H*sum(fmp);
return
```

APPROXIMATION OF INTEGRALS

- *SOURCE:* simpsonc

```
function [Isic]=simpsonc(a,b,M,f,varargin)
% SIMPSONC Composite Simpson numerical integration.
% ISIC = SIMPSONC(A,B,M,FUN) computes
% an approximation of the integral
% of the function FUN via the Simpson method
% (with M equispaced intervals).
% FUN accepts real scalar input
% x and returns a real scalar
% value. FUN can also be an inline object.
```


APPROXIMATION OF INTEGRALS

- *SOURCE cont'd.:*

```
H=(b-a)/M;
x=linspace(a,b,M+1);
fpm=feval(f,x,varargin{:});
fpm(2:end-1) = 2*fpm(2:end-1);
Isic=H*sum(fpm)/6;
x=linspace(a+H/2,b-H/2,M);
fpm=feval(f,x,varargin{:});
Isic = Isic+2*H*sum(fpm)/3;
return
```


APPROXIMATION OF INTEGRALS

- *SOURCE:* simpadpt
- function [JSf,nodes]=simpadpt(f,a,b,tol,hmin)

```
% SIMPADPT  Numerically evaluate integral,
% adaptive Simpson quadrature.
%  JSF = SIMPADPT(FUN,A,B,TOL,HMIN)
%  tries to approximate the integral of function
%  FUN from A to B to within an error
%  of TOL using recursive
%  adaptive Simpson quadrature.
%  The inline function Y = FUN(V) should
%  accept a vector argument V and return a vector result Y,
%  the integrand evaluated at each element of X.
%
% [JSF,NODES] = SIMPADPT(...) returns the distribution of nodes.
```


APPROXIMATION OF INTEGRALS

- *SOURCE cont'd.:*

```
A=[a,b]; N=[]; S=[]; JSf = 0; ba = b - a; nodes=[];
while ~isempty(A),
   [deltaI,ISc]=caldeltai(A,f);
   if abs(deltaI) <= 15*tol*(A(2)-A(1))/ba;
         JSf = JSf + ISc;
   S = union(S,A);
   nodes = [nodes, A(1) (A(1)+A(2))*0.5 A(2)];
   S = [S(1), S(end)]; A = N; N = [];
```

APPROXIMATION OF INTEGRALS

- *SOURCE cont'd.:*

```
    elseif A(2)-A(1) < hmin
        JSf=JSf+ISc;
        S = union(S,A);
        S = [S(1), S(end)]; A=N; N=[];
        warning('Too small step-length');
    else
        Am = (A(1)+A(2))*0.5; A = [A(1) Am];
        N = [Am, b];
    end
end
```


APPROXIMATION OF INTEGRALS

- *SOURCE cont'd.:*

```
nodes=unique(nodes);
return
function [deltaI,ISc]=caldeltai(A,f)
L=A(2)-A(1);
t=[0; 0.25; 0.5; 0.5; 0.75; 1];
x=L*t+A(1);
L=L/6;
w=[1; 4; 1];
fx=feval(f,x);
IS=L*sum(fx([1 3 6]).*w); ISc=0.5*L*sum(fx.*[w;w]);
deltaI=IS-ISc;
return
```


References for Week 10

1 Alfio Quarteroni, Fausto Saleri, Scientific Computing with Matlab and Octave, Springer, 2006.

2 Moler C, NumericalComputing with Matlab, Mathworks Inc., 2004 (http://www.mathworks.com/moler).

3 Thomas Huckle, Stefan Schneider, Numerische Methoden, Springer, 2006.

4 http://www.mathworks.com/help/techdoc/ref/diff.html

Have a nice Week End