Introduction to Scientific and Engineering Computing, BIL108E

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INTRODUCTION TO SCIENTIFIC & ENGINEERING COMPUTING BIL 108E, CRN24023

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Technical University of Istanbul

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Tentative Course Schedule, CRN 24023

Week	Date	Topics
1	Feb. 08	Introduction to Scientific and Engineering Computing
2	Feb. 15	Introduction to Program Computing Environment
3	Feb. 22	Variables, Operations and Simple Plot
4	Mar. 01	Algorithms and Logic Operators
5	Mar. 08	Flow Control, Errors and Source of Errors
6	Mar. 15	Functions
6	Mar. 20	Exam 1
7	Mar. 22	Arrays
8	Mar. 29	Solving of Simple Equations
9	Apr. 05	Polynomials Examples
10	Apr. 12	Applications of Curve Fitting
11	Apr. 19	Applications of Interpolation
11	**Apr. 18**	**Exam 2**
12	Apr. 26	Applications of Numerical Integration
13	May 03	Symbolic Mathematics
14	May 10	Ordinary Differential Equation (ODE) Solutions with Built-in Functions

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LECTURE # 10

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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.

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

$$\int_0^{\pi} f(x)\,dx = \pi\left(\frac{3}{2}\right)\sum_{k=0}^{\infty}\frac{(-9/4)^k}{k!(k+4)!}$$

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

APPROXIMATION OF FUNCTION DERIVATIVES

- Consider a function $f : [a, b] \longrightarrow \mathbb{R}$
- Find an approximation of the first derivative(f') of f at a generic point $\bar{x}$ in interval (a, b).

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

is an approximation of $f'(\bar{x})$, for h sufficiently small and positive h.

- The above approximation is defined as **FORWARD FINITE DIFFERENCE**.

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APPROXIMATION OF FUNCTION DERIVATIVES

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

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

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 $f'(\bar{x})$

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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**

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APPROXIMATION OF FUNCTION DERIVATIVES

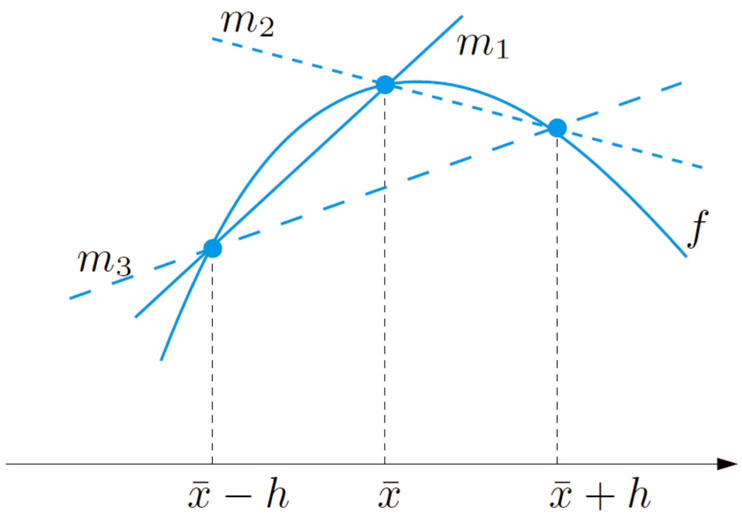
- CENTERED FINITE DIFFERENCE

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

- 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



APPROXIMATION OF FUNCTION DERIVATIVES

- When $\bar{x} = x_i$ 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

APPROXIMATION OF FUNCTION DERIVATIVES

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

  $\frac{1}{2h}[-3f(x_0) + 4f(x_1) - f(x_2)]$ at x_0

  $\frac{1}{2h}[3f(x_n) - 4f(x_{n-1}) + f(x_{n-2})]$ at x_n

EXAMPLE:

- 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 it 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.

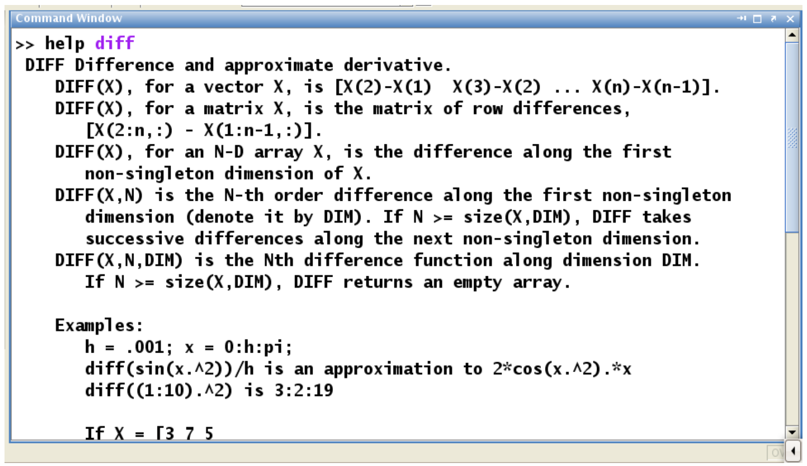
EXAMPLE:

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)`

MATLAB FUNCTIONS cont'd.

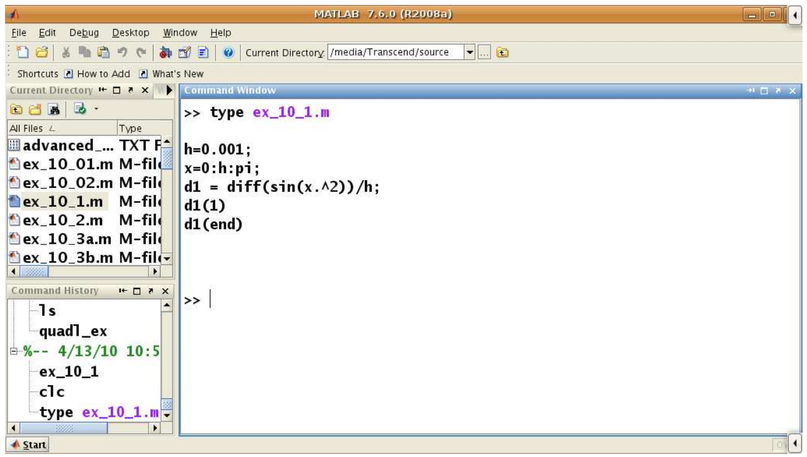


```
>> help diff
 DIFF Difference and approximate derivative.
    DIFF(X), for a vector X, is [X(2)-X(1)  X(3)-X(2) ... X(n)-X(n-1)].
    DIFF(X), for a matrix X, is the matrix of row differences,
       [X(2:n,:) - X(1:n-1,:)].
    DIFF(X), for an N-D array X, is the difference along the first
       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 :



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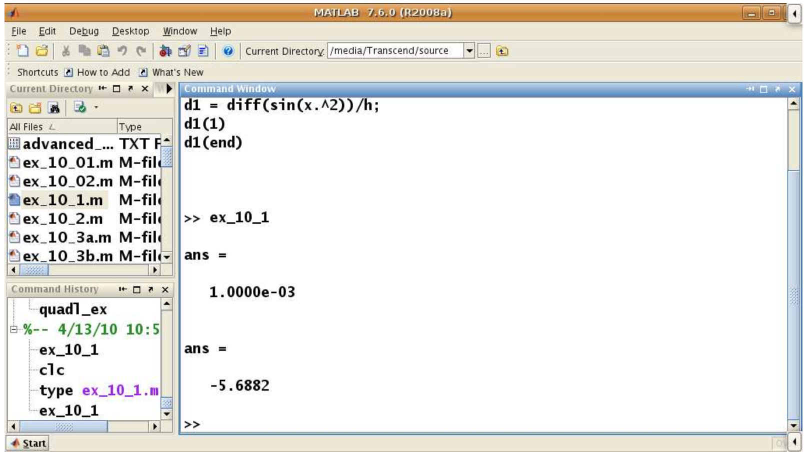
EXAMPLE :



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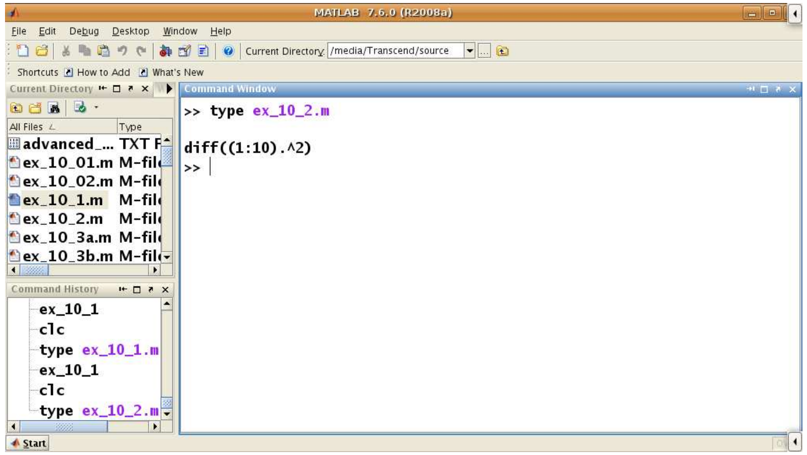

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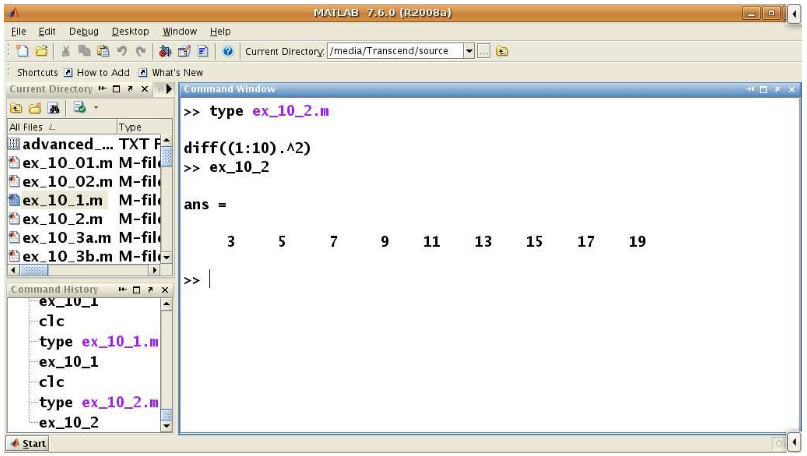

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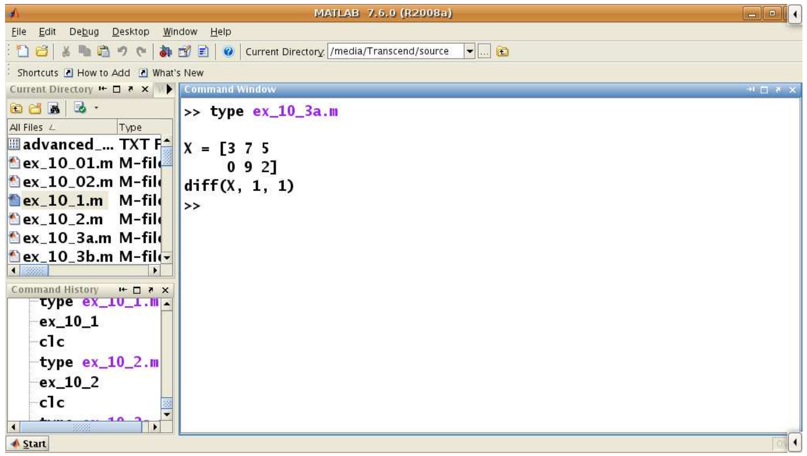

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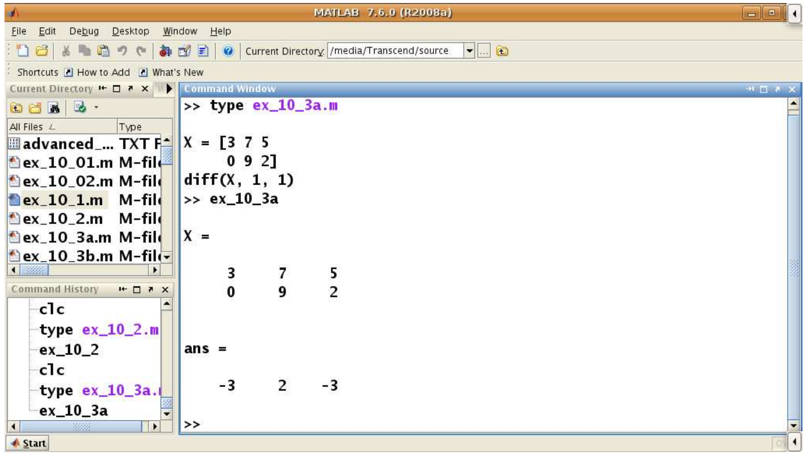

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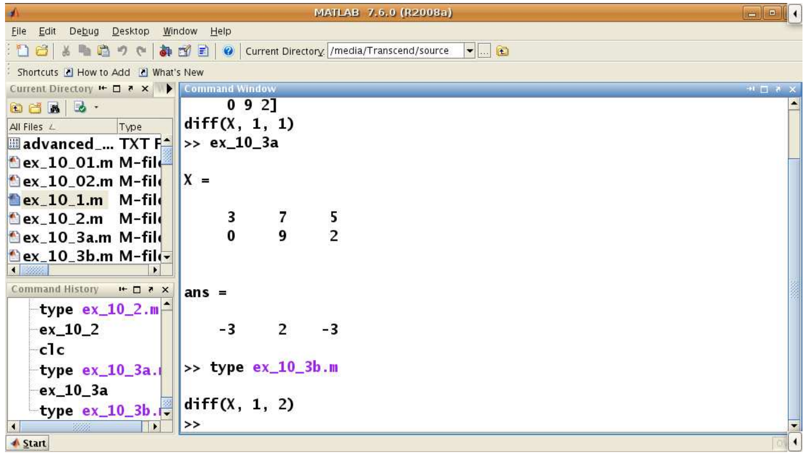

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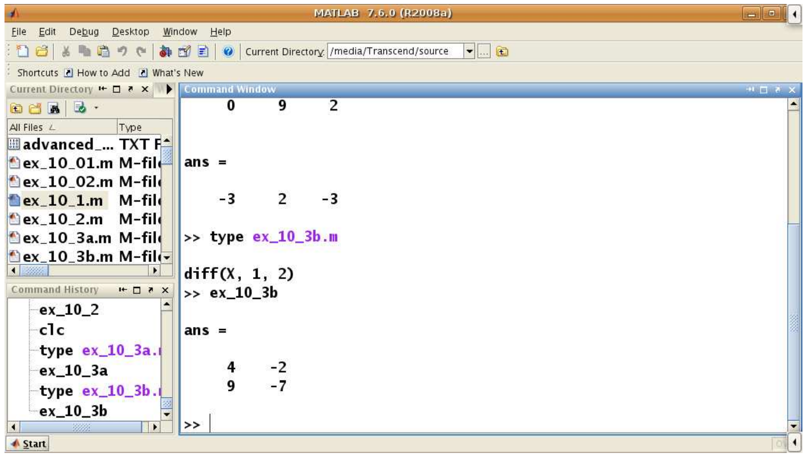

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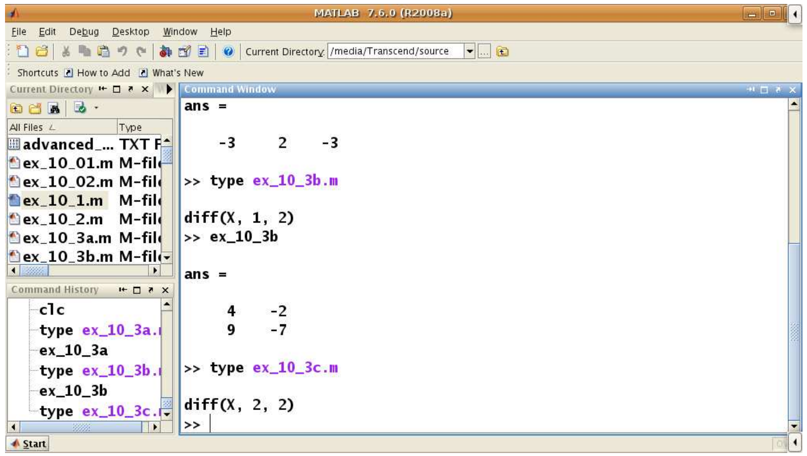

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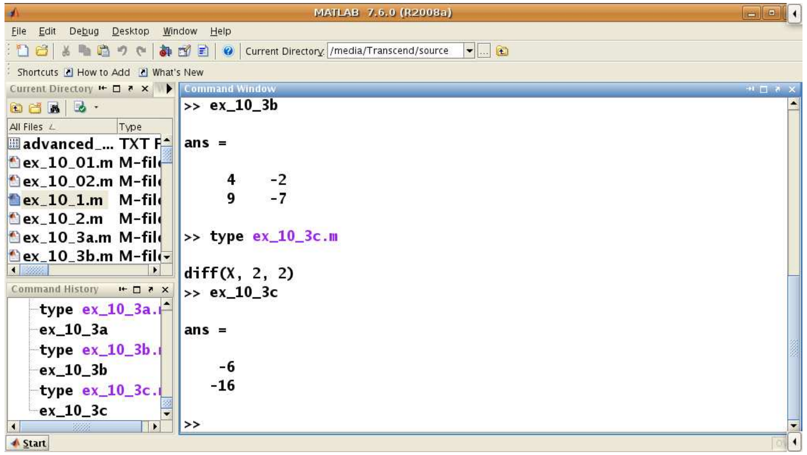

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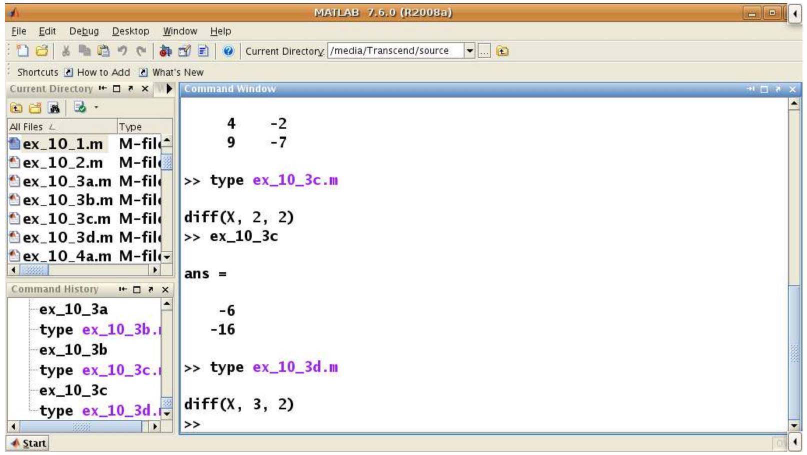

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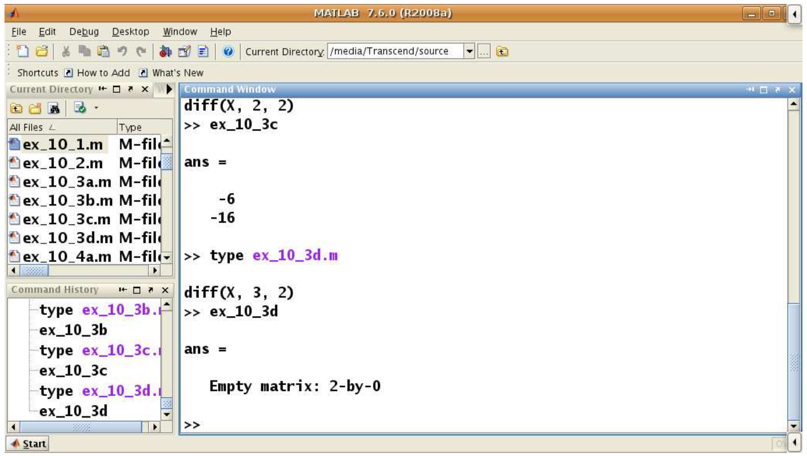

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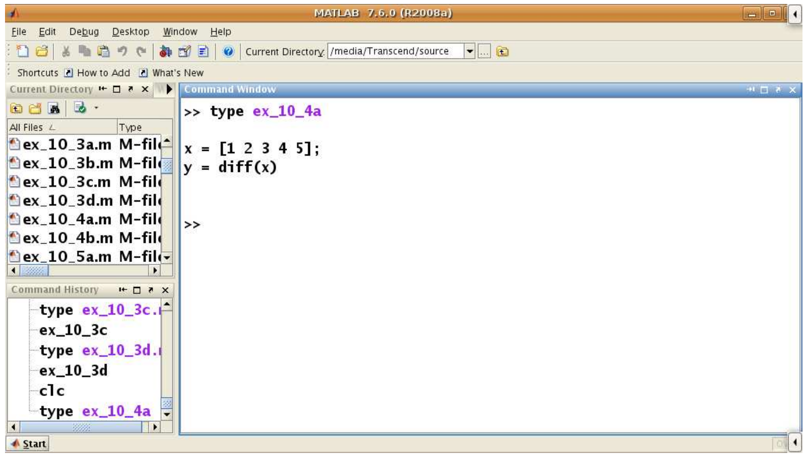

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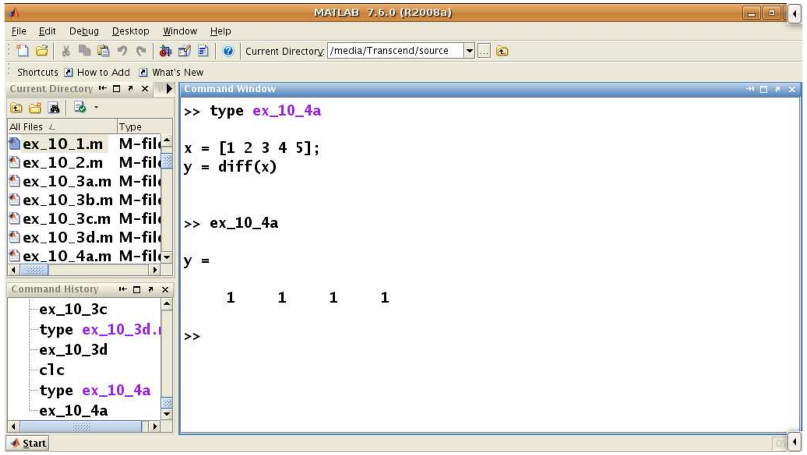

APPROXIMATION OF FUNCTION DERIVATIVES

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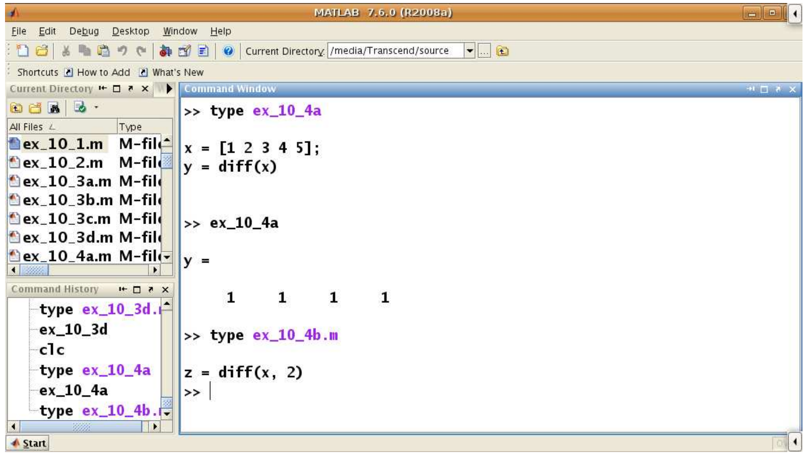

APPROXIMATION OF FUNCTION DERIVATIVES

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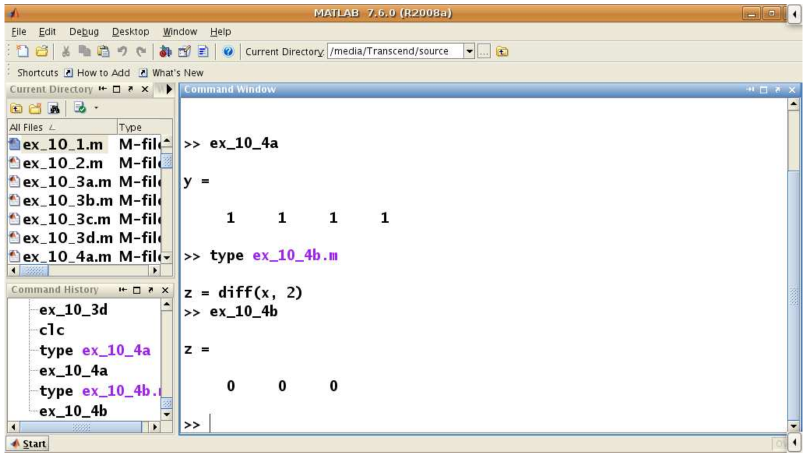
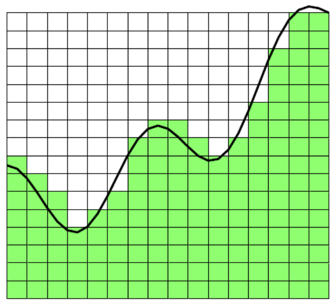


APPROXIMATION OF FUNCTION INTEGRALS

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

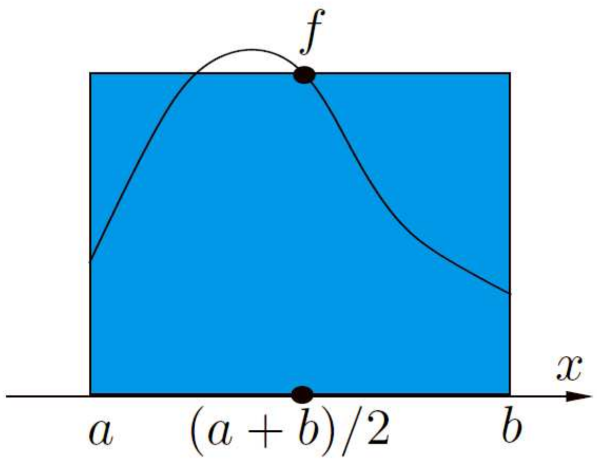
- Midpoint Quadrature
- Trapezoidal Quadrature
- Simpson Quadrature
- Gauß–Legendre Formula
- Adaptive Simpson Formula

APPROXIMATION OF INTEGRALS

Newton–Cotes equation

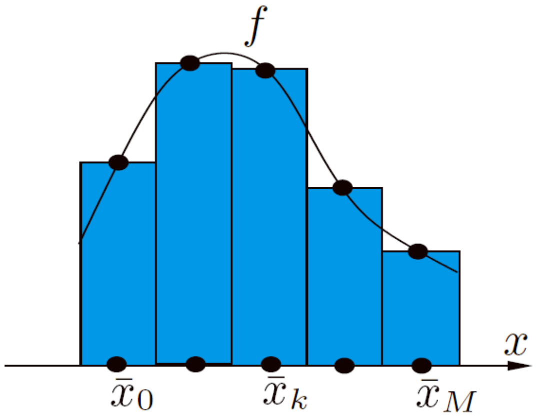
- Define the function $f(x)$ as an approximation with polynom $P(x)$, and use it on an equally partitioned interval (a, b).
- Calculation with this method is also named as **composite** quadrature.

MIDPOINT QUADRATURE



APPROXIMATION OF INTEGRALS

MIDPOINT QUADRATURE



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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 $H = (b-a)/M$

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

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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

APPROXIMATION OF INTEGRALS

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CLASSIC MIDPOINT FORMULA

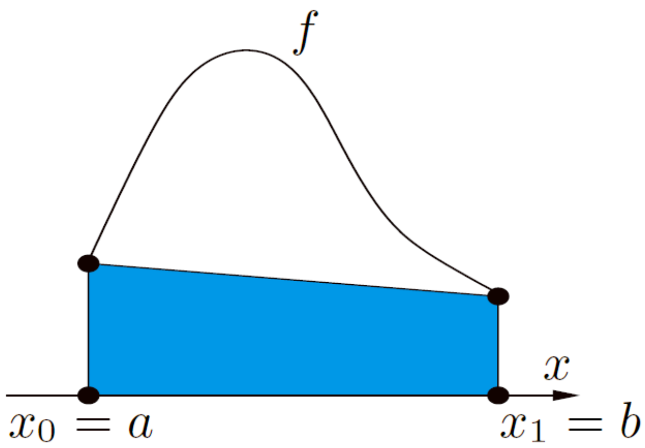
- Here the number of partitions M=1.

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

- Estimated error,

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

TRAPEZOIDAL QUADRATURE



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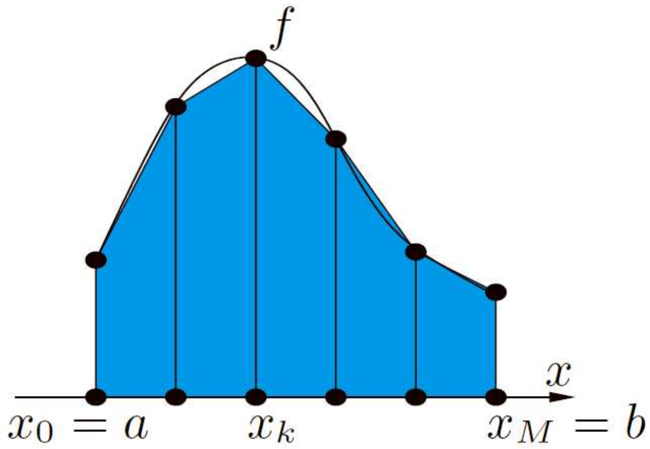
TRAPEZOIDAL QUADRATURE



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TRAPEZOIDAL QUADRATURE

Calculation is done with the area of a trapezoidal.

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

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

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SIMPSON QUADRATURE

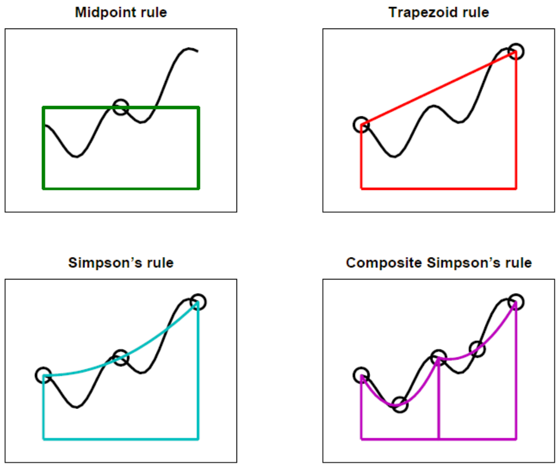
Approximate the function by a parabola. This rule can be applied to the even number of segments (odd number of points).

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

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

APPROXIMATION OF INTEGRALS

APPROXIMATION OF INTEGRALS



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

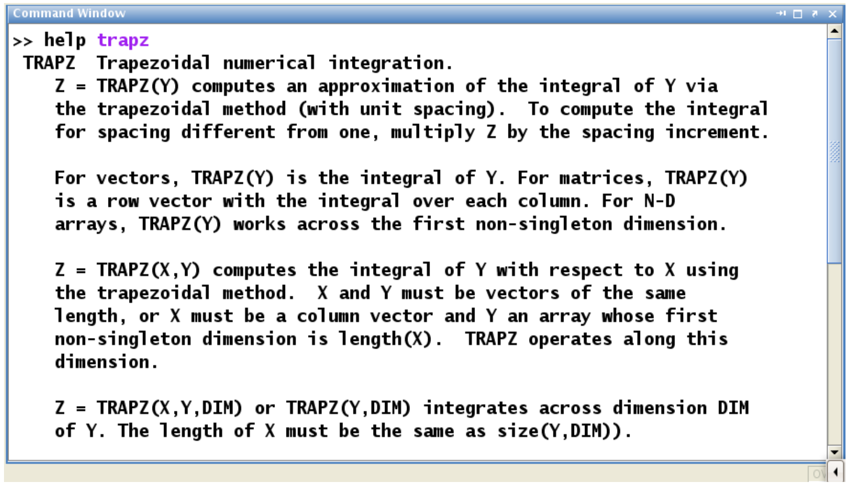
APPROXIMATION OF INTEGRALS

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

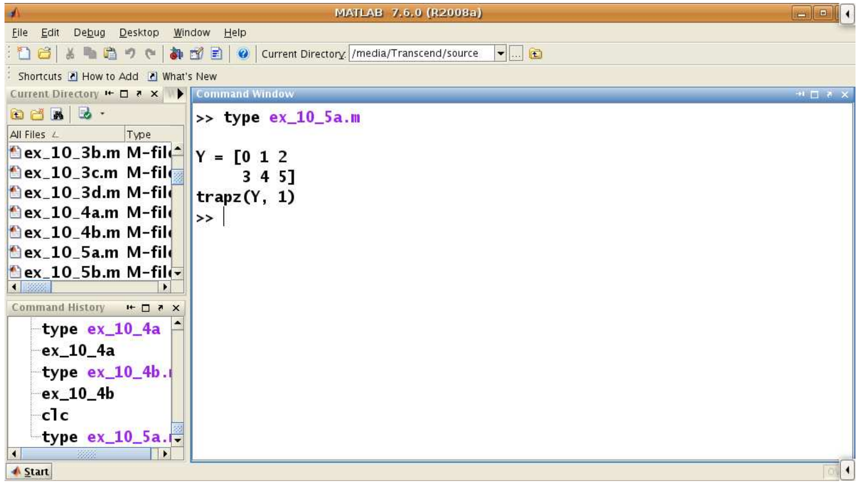
`trapz`


Command Window

```
>> 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)).
```

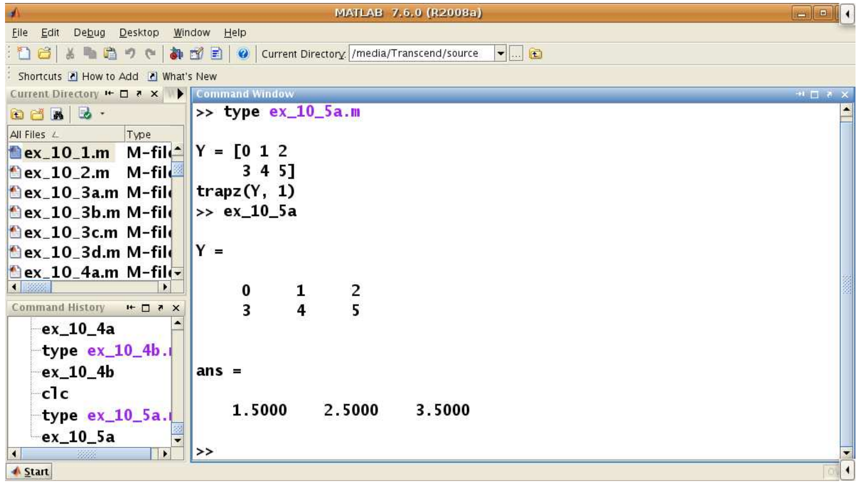
APPROXIMATION OF INTEGRALS

trapz



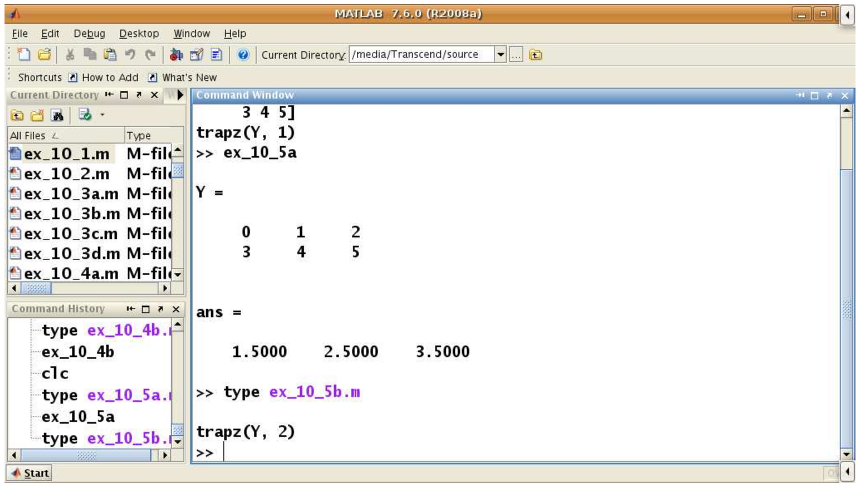
APPROXIMATION OF INTEGRALS

trapz



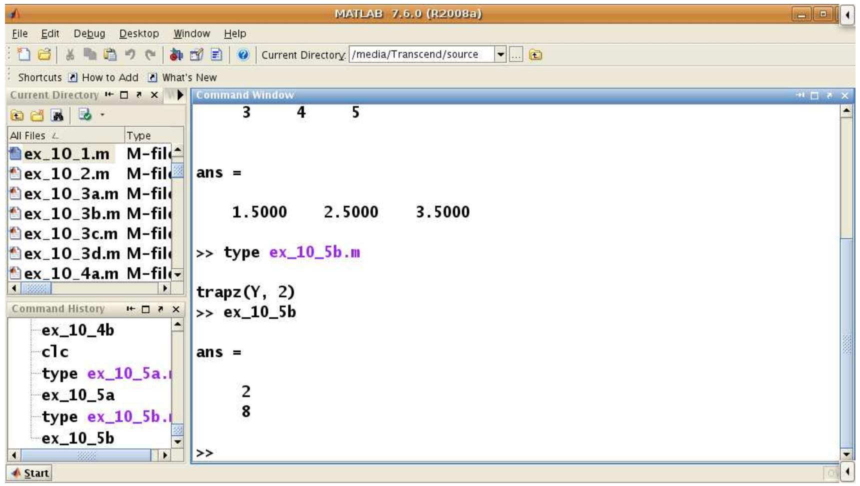
APPROXIMATION OF INTEGRALS

trapz



APPROXIMATION OF INTEGRALS

trapz



cumtrapz

```
>> help cumtrapz
 CUMTRAPZ Cumulative trapezoidal numerical integration.
    Z = CUMTRAPZ(Y) computes an approximation of the cumulative
    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, CUMTRAPZ(Y) is a vector containing the cumulative
    integral of Y. For matrices, CUMTRAPZ(Y) is a matrix the same size as
    X with the cumulative integral over each column. For N-D arrays,
    CUMTRAPZ(Y) works along the first non-singleton dimension.

    Z = CUMTRAPZ(X,Y) computes the cumulative integral of Y with respect
    to X using trapezoidal integration.  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).  CUMTRAPZ operates across this
    dimension.
```

APPROXIMATION OF INTEGRALS

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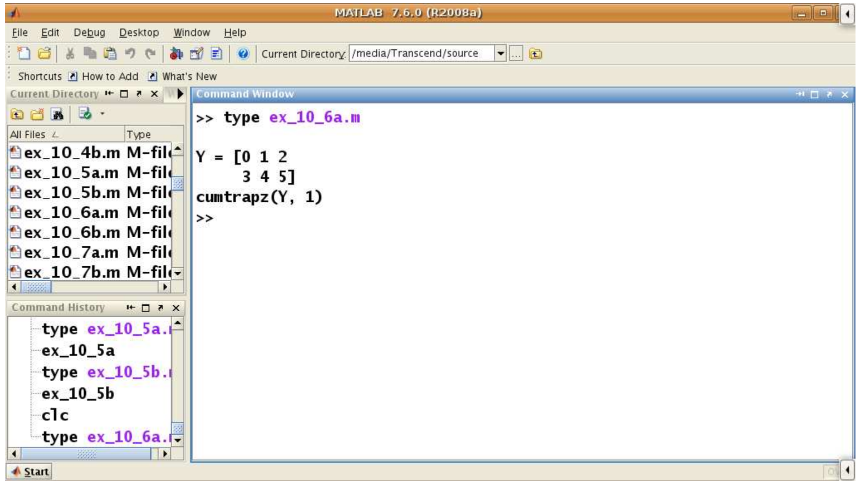
cumtrapz



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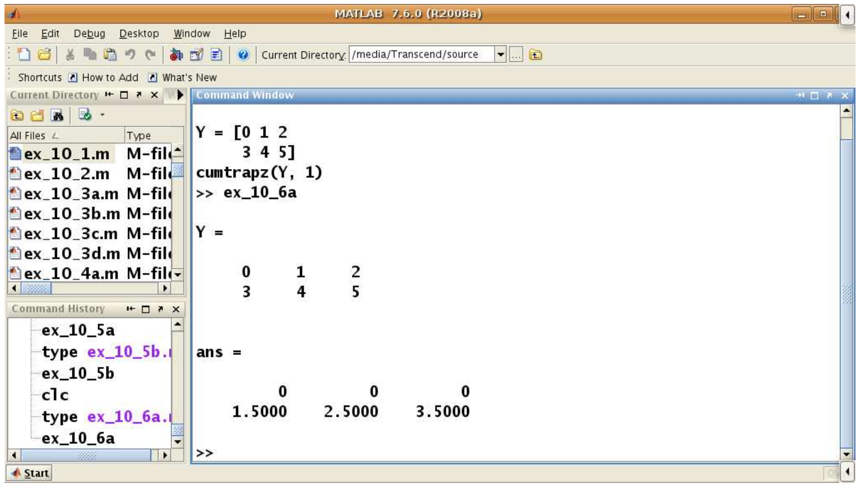
cumtrapz



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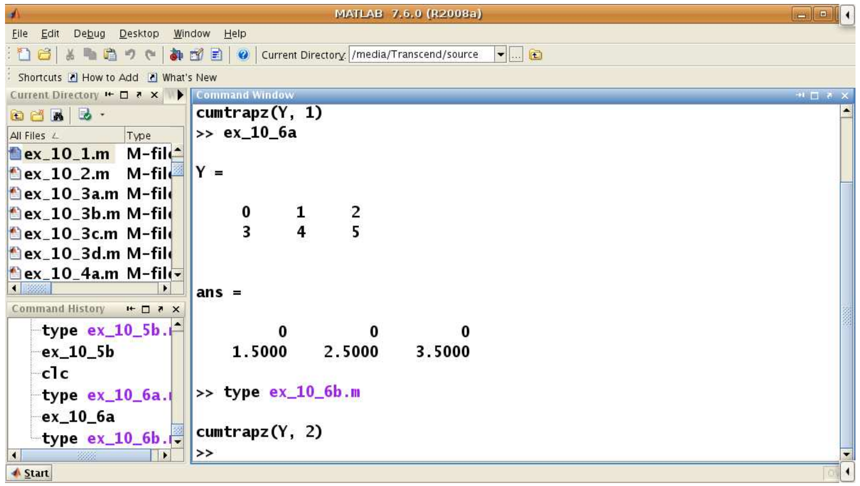
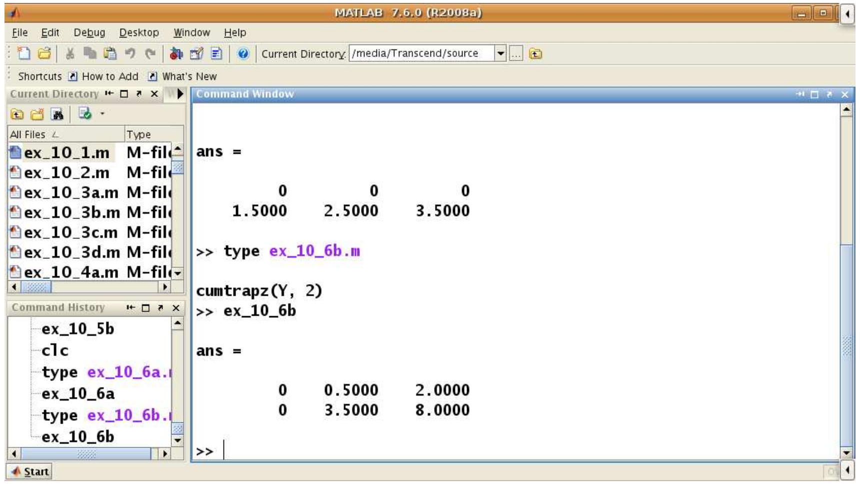
cumtrapz



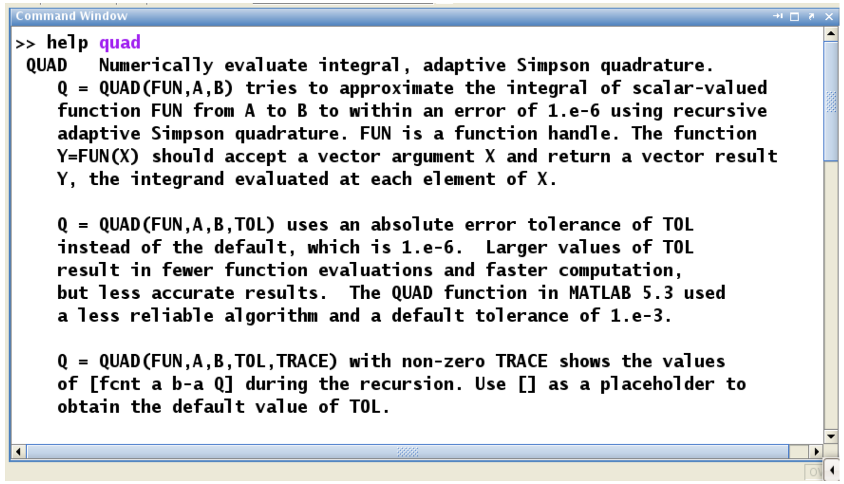
APPROXIMATION OF INTEGRALS

cumtrapz



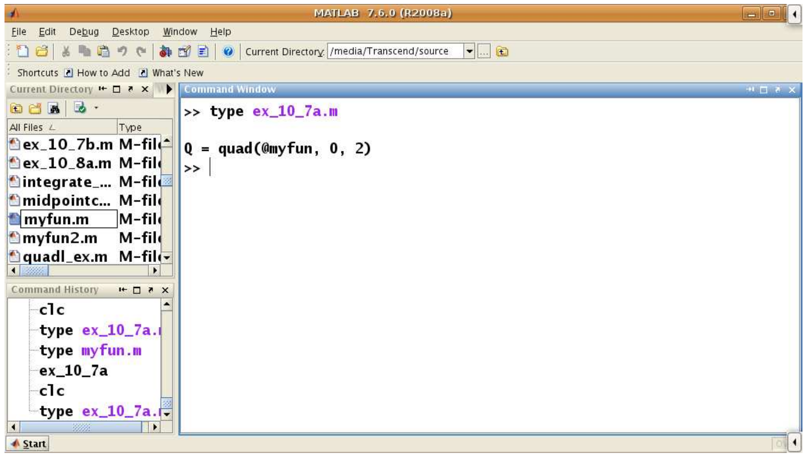
APPROXIMATION OF INTEGRALS

quad



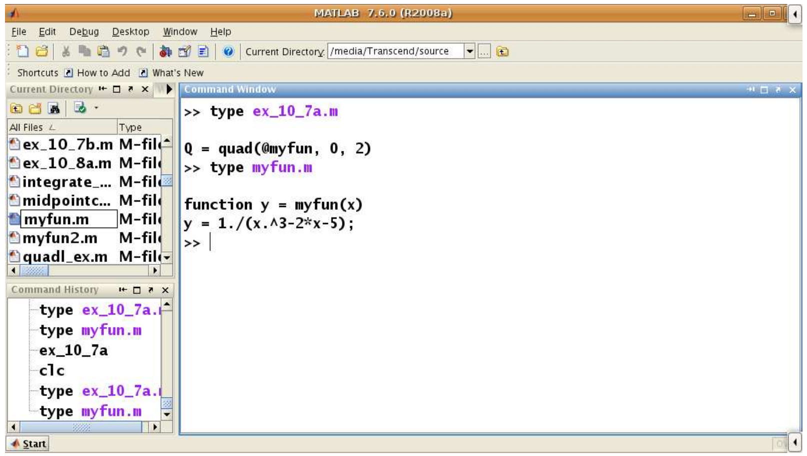
APPROXIMATION OF INTEGRALS

quad



APPROXIMATION OF INTEGRALS

quad



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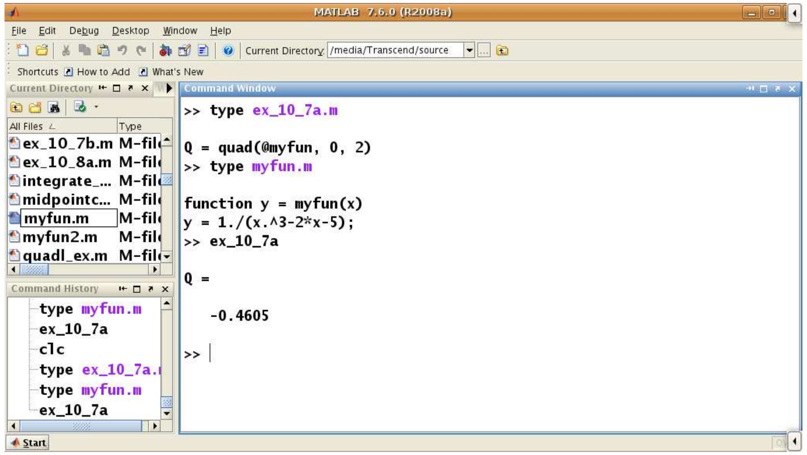
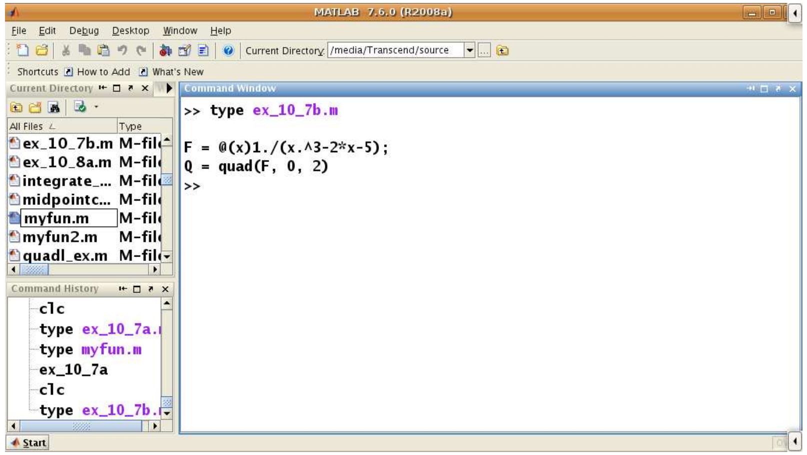
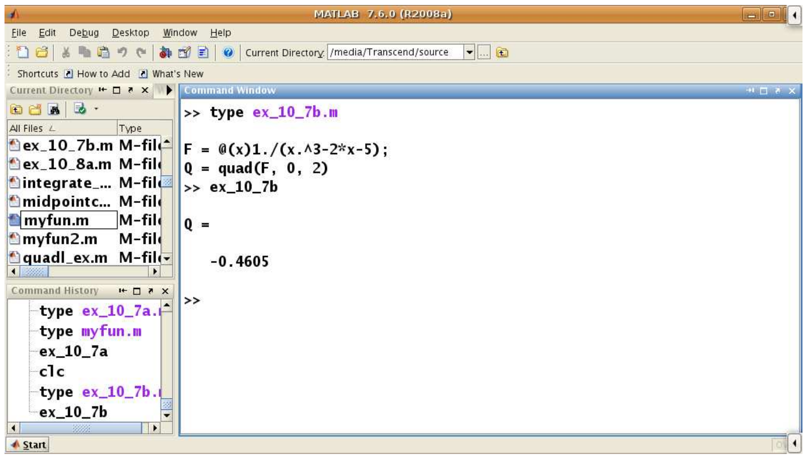


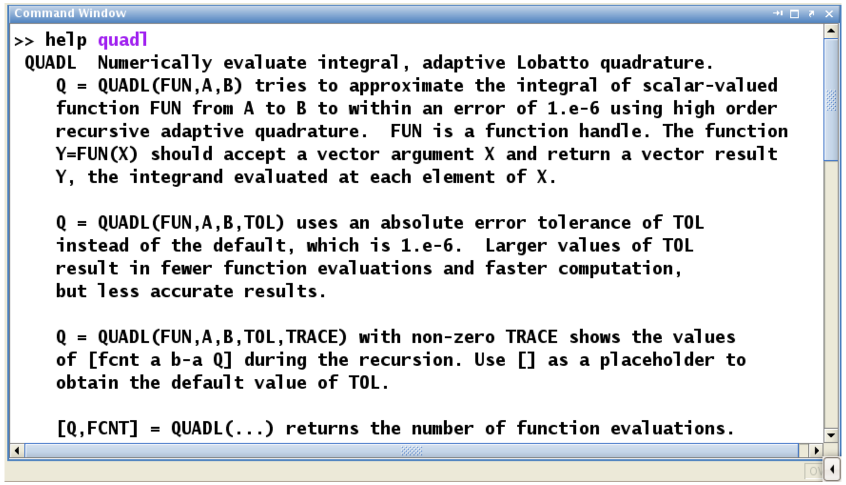
quad



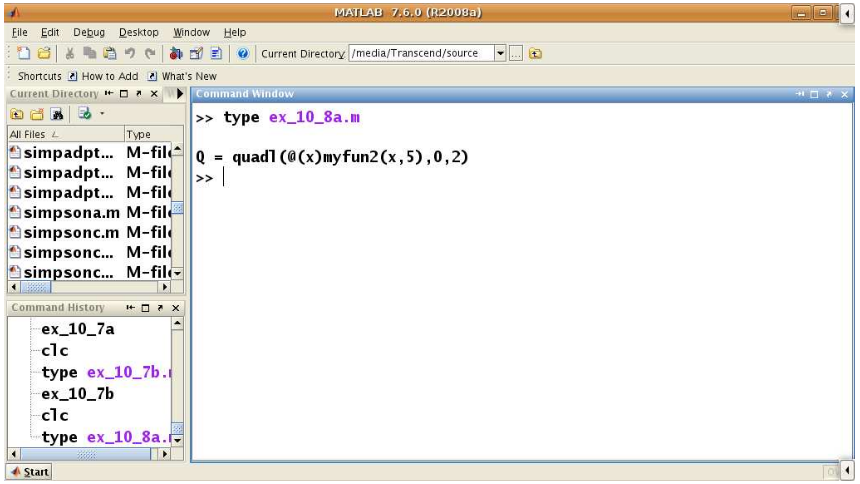
quad



quadl



quadl



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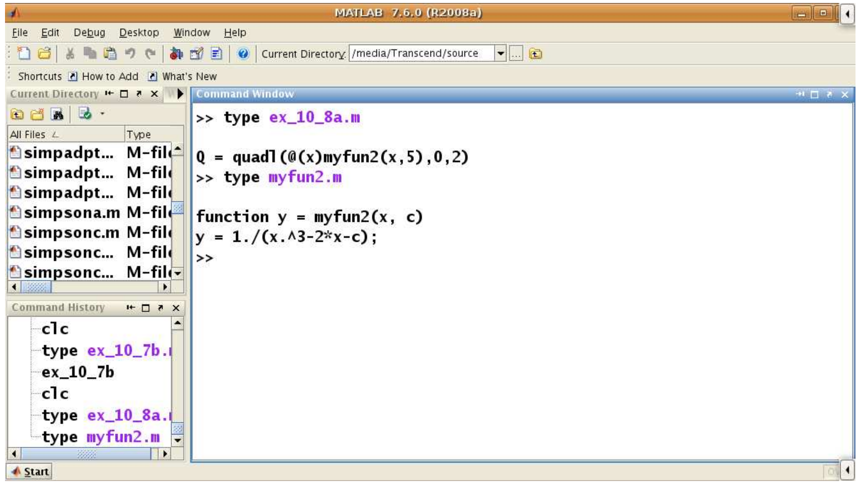
quadl



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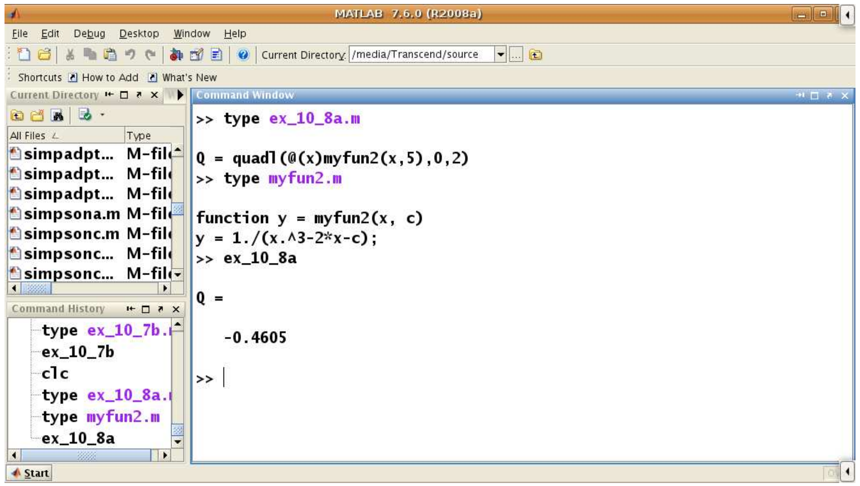
quadl



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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)
```

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)
```


SOURCE:

```
function I=trapezoid(fun,a,b,npanel)
n=npanel+1; %total number of nodes
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));
```


SOURCE:

```
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
```


SOURCE:

```
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.
```

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
```


SOURCE:

```
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.
```


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 = [];
```


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

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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.