

Introduction to Scientific and Engineering Computing, BIL108E

INTRODUCTION TO SCIENTIFIC & ENGINEERING COMPUTING BIL 108E, CRN24023

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Tentative Course Schedule, CRN 24023

troduction Scientific and ngineering omputing, BII 108F	Week	Date	Topics
	1	Feb 08	Introduction to Scientific and Engineering Computing
Karaman	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

LECTURE # 10

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LECTURE # 10

NUMERICAL APPROXIMATION

- **1** NUMERICAL DIFFERENTIATION
 - **1** FORWARD FINITE DIFFERENCE
 - **2** BACKWARD FINITE DIFFERENCE
 - **3** CENTERED FINITE DIFFERENCE
- **2** NUMERICAL INTEGRATION
 - 1 MIDPOINT QUADRATURE
 - 2 TRAPEZOIDAL QUADRATURE
 - **3** SIMPSON QUADRATURE
 - 4 GAUB-LEGENDRE FORMULA
 - 5 ADAPTIVE SIMPSON FORMULA



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and

Engineering

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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.

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

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

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



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

Engineering

Computing,

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- 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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 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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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

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



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- 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

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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



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and

Computing,

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to Scientific Engineering

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.



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EXAMPLE:

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and

Engineering

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MATLAB FUNCTIONS cont'd.

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I	Command Window
	>> 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



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and

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Introduction

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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.



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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

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APPROXIMATION OF INTEGRALS

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

STANHILL SECTION

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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.



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MIDPOINT QUADRATURE





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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, ..., *M* into subintervals.

•
$$x_k = a + k H$$
, $k = 0, ..., M$ 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 \overline{f} on I_k
- $\bullet \ \bar{x_k} = \frac{x_{k-1} x_k}{2}$
- $I_{mp}^{c}(f) = H \sum_{k=1}^{M} f(\bar{x_k})$ This is called **COMPOSITE MIDPOINT QUADRATURE**
- Second –order approximate with respect to H



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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,

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



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TRAPEZOIDAL QUADRATURE





APPROXIMATION OF INTEGRALS

TRAPEZOIDAL QUADRATURE TRAPEZOIDAL QUADRATURE Karaman TRAPEZOIDAL QUADRATURE $x_{0} = a$ x_{k} $x_{M} = b$

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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).

$$I_{s}^{c}(f) = \frac{H}{6} \sum_{k=1}^{M} (f(x_{k-1}) + 4f(\bar{x_{k}}) + f(x_{k}))$$
$$I_{s}(f) = \frac{b-a}{6} (f(a) + 4f((a+b)/2) + f(b))$$



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INTERPOLATORY QUADRATURES GAUB-LEGENDRE FORMULA

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

- α_i : quadrature weights
- y_j: quadrature nodes

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MATLAB FUNCTIONS

- trapz : Uses areas of trapezoidals.
- cumtrapz : Uses composite trapezoidal quadrature
- quad : Uses the adaptive Simpson quadrature algorithm.
- quad1 : Uses Gauß–Legendre Formula



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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)).



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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.



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cumtrapz





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APPROXIMATION OF INTEGRALS

Introduction to Scientific

quad

>> help quad

QUAD Numerically evaluate integral, adaptive Simpson quadrature. Q = QUAD(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 recursive adaptive Simpson 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 = QUAD(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. The QUAD function in MATLAB 5.3 used a less reliable algorithm and a default tolerance of 1.e-3.

Q = QUAD(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.

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Introduction to Scientific

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APPROXIMATION OF INTEGRALS

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Computing, BIL108E 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.



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Introduction to Scientific



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EXAMPLES:

Evaluate the following integral with different methods.

Cosine is a built-in function in Matlab.

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



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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)



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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));



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SOURCE:

%

%

%

%

% %

%

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Introduction

to Scientific

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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
```



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SOURCE:

<pre>function [Isic]=simpsonc(a,b,M,f,varargin) %SIMPSONC Composite Simpson numerical integration.</pre>				
% ISIC = SIMPSONC(A,B,M,FUN) computes				
% an approximation of the in	ntegral			
% of the function FUN via th	ne Simpson method			
% (with M equispaced interva	als).			
% FUN accepts real scalar in	nput			
% x and returns a real scala	ar			
% value. FUN can also be an	inline object.			



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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



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Computing,

BIL108E

APPROXIMATION OF INTEGRALS

SOURCE:

```
Introduction
to Scientific
Engineering
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% %

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.



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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) \leq 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 = [];
```



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Computing,

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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
```



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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

Introduction to Scientific and Engineering Computing, BIL108E

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.