Lecture 12

Numerical Differentiation and Integration

Numerical Integration-The Trapezoidal Rule

Ceng375 *Numerical Computations* at January 06, 2011

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Contents

Numerical Differentiation and Integration I

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- **Numerical Integration-The Trapezoidal Rule:**
  - Approximates, the integrand function with a *linear* interpolating polynomial to derive a very simple but important formula for numerically integrating functions between given limits.

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- However, integration involves only *addition*, so round-off is not problem.
- We cannot often find the true answer numerically because the analytical value is the limit of the sum of an infinite number of terms.
- We must be satisfied with approximations for both derivatives and integrals but, for most applications, the **numerical answer is adequate**.

Differentiation with a Computer I

- The derivative of a function, $f(x)$ at $x = a$, is defined as

$$\frac{df}{dx}\Big|_{x=a} = lim_{\Delta x \to 0} \frac{f(a + \Delta x) - f(a)}{\Delta x}$$

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$$\frac{df}{dx}\Big|_{x=a} = \frac{f(a + \Delta x) - f(a)}{\Delta x}$$

- Recalculating with smaller and smaller values of x starting from an initial value.
- What happens if the value is not small enough?

Differentiation with a Computer II

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- We find that the errors of the approximation decrease as Δx is reduced until about $\Delta x = 0.05/128$.

Differentiation with a Computer III

Δx	Approximation	Error	Ratio of errors
0.05	4.05010	−0.11528	
0.05/2	4.10955	−0.05583	2.06
0.05/4	4.13795	−0.02743	2.04
0.05/8	4.15176	−0.01362	2.01
0.05/16	4.15863	−0.00675	2.02
0.05/32	4.16199	−0.00389	1.99
0.05/64	4.16382	−0.00156	2.18
0.05/128	**4.16504**	**−0.00034**	**4.67***
0.05/256	4.16504	−0.00034	
0.05/512	4.16504	−0.00034	
0.05/1024	4.16992	0.00454	
0.05/2048	4.17969	0.01430	

Table: Forward-difference approximations for $f(x) = e^x sin(x)$.

Differentiation with a Computer IV

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- **Backward-difference** approximation.

$$\frac{df}{dx}\Big|_{x=a} = \frac{f(a) - f(a - \Delta x)}{\Delta x}$$

Differentiation with a Computer V

With MATLAB. **Analytical answer** to the function of Table 1.

```
format long;
syms x;
f='exp(x)*sin(x)';
df=diff(f,x)
exactvalue=subs(df,1.9,'x')
```

Differentiation with a Computer VI

With MATLAB. **Numerical answer** to the function of Table 1.

```
%%%Forward-Difference%%%%%
disp('Step        Del        Numerical           Error        Error')
disp('                       Derivative                       Ratio')
disp('----- ------------- ----------- ----------- ----------')
x=1.9;
delini=1;
error(1)=1;
for i=1:30
 del=delini/2;
 xplus=x+del;
 f=exp(x).*sin(x);
 fplus=exp(xplus).*sin(xplus);
 num=fplus-f;
 deriv=num/del;
 error(i+1)=deriv-exactvalue;
 [D]=sprintf('%2d %1.15f %12.10f %12.10f %f ',i,del,deriv,error(i),
                                               error(i)/error(i+1));
 disp(D);
 delini=del;
end
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$$f(x+h) = f(x) + f'(x) * h + f''(\xi) * h^2/2$$

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- If we repeat this but begin with the Taylor series for $f(x-h)$, it turns out that

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- If we add Eqs. 1 and 2, then divide by 2, we get the ***central-difference*** approximation to the derivative:

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- This shows that using a central-difference approximation is a much *preferred way* to estimate the derivative.
- Even though we use the same number of computations of the function at each step,
- we approach the answer **much more rapidly**.

Differentiation with a Computer IX

With MATLAB,

```
%%%Central-Difference%%%
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disp('                         Derivative                    Ratio')
disp('----- -------------- ------------ ------------ ----------')
x=1.9;
delini=0.1;
error(1)=1;
for i=1:20
 del=delini/2;
 xplus=x+del;
 xminus=x-del;
 fplus=exp(xplus).*sin(xplus);
 fminus=exp(xminus).*sin(xminus);
 num=fplus-fminus;
 deriv=num/(2*del);
 error(i+1)=deriv-exactvalue;
 [D]=sprintf('%2d %1.15f %12.10f %12.10f %f ',i,del,deriv,error(i),
                                                    error(i)/error(i+1));
 disp(D);
 delini=del;
end
```

Differentiation with a Computer X

Table 2 illustrates this, showing that errors decrease about four fold when Δx is halved (as Eq. 3 predicts) and that a more accurate value is obtained.

Δx	Approximation	Error	Ratio of errors
0.05	4.15831	−0.00708	
0.05/2	4.16361	−0.00177	4.00
0.05/4	4.16496	−0.00042	4.21
0.05/8	4.16527	−0.00011	3.80
0.05/16	**4.16534**	**−0.00004**	**2.75**
0.05/32	4.16534	−0.00004	
0.05/64	4.16565	−0.00027	

Table: Central-difference approximations for $f(x) = e^x sin(x)$.

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can be evaluated from the antiderivative.

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- Still, there are functions that do not have an antiderivative expressible in terms of ordinary functions.

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>> syms x
>> int(exp(x)/log(x))
Warning: Explicit integral could not be found.
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- Is there any way that the definite integral can be found when the antiderivative is unknown?

Numerical Integration - The Trapezoidal Rule II

- We can do it numerically by using the **composite trapezoidal rule**

```
>> fx(i)=exp(x(i))/log(x(i))
>> x=linspace(2,3,10);
>> for i=1:10
fx(i)=exp(x(i))/log(x(i));
end
>> result=fx(1)+fx(10);
>> for i=2:9
result=result+2*fx(i);
end
>> result=(((3-2)/(10-1))/2)*result
%%%result=(0.1111/2)*result
result =   13.6904
```

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- That is the principle behind all numerical integration;
- We divide the distance from $x = a$ to $x = b$ into **vertical strips** and add the areas of these strips.
- The strips are often made equal in widths but that is not always required.

The Trapezoidal Rule I

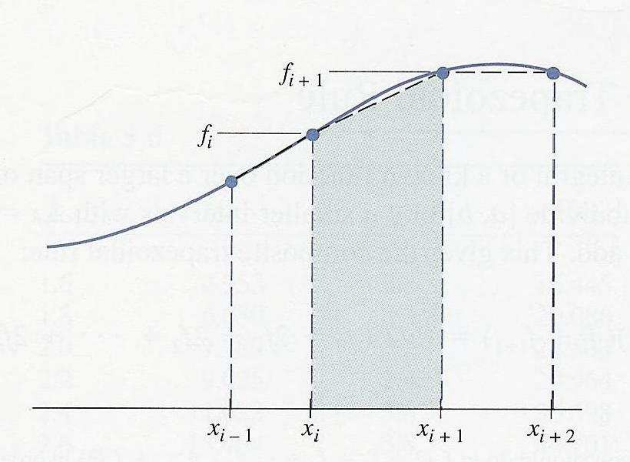

Figure: The trapezoidal rule.

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- It is clear that the area of the strip from x_i to x_{i+1} gives an approximation to the area under the curve:

$$\int_{x_i}^{x_{i+1}} f(x)dx \approx \frac{f_i + f_{i+1}}{2}(x_{i+1} - x_i)$$

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- We will usually write $h = (x_{i+1} - x_i)$ for the width of the interval.
- Error term for the trapezoidal integration is

$$Error = -(1/12)h^3 f''(\xi) = O(h^3)$$

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- We are approximating the curve with interpolating polynomials of degree-1.
- The gives us the ***trapezoidal rule***. Figure 1 illustrates this.
- It is clear that the area of the strip from x_i to x_{i+1} gives an approximation to the area under the curve:

$$\int_{x_i}^{x_{i+1}} f(x)dx \approx \frac{f_i + f_{i+1}}{2}(x_{i+1} - x_i)$$

- We will usually write $h = (x_{i+1} - x_i)$ for the width of the interval.
- Error term for the trapezoidal integration is

$$Error = -(1/12)h^3 f''(\xi) = O(h^3)$$

- What happens, if we are getting the integral of a known function over a larger span of x-values, say, from $x = a$ to $x = b$?

The Composite Trapezoidal Rule I

- We subdivide [a,b] into n smaller intervals with $\Delta x = h$, apply the rule to each subinterval, and add.

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- If $f''(x)$ is continuous in [a, b], there is some point within [a,b] at which the sum of the $f''(\xi_i)$ is equal to $nf''(\xi)$, where ξ in [a, b].
- We then see that, because $nh = (b-a)$,

$$Global\ error = (-1/12)h^3 nf''(\xi) = \frac{-(b-a)}{12}h^2 f''(\xi) = O(h^2)$$

The Composite Trapezoidal Rule II

- **Example:** Given the values for x and $f(x)$ in Table3.

x	$f(x)$	x	$f(x)$
1.6	4.953	2.8	16.445
1.8	6.050	3.0	20.086
2.0	7.389	3.2	24.533
2.2	9.025	3.4	29.964
2.4	11.023	3.6	36.598
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Table: Example for the trapezoidal rule.

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Table: Example for the trapezoidal rule.

- Use the trapezoidal rule to estimate the integral from $x = 1.8$ to $x = 3.4$.
- Applying the trapezoidal rule:

$$\begin{aligned}\int_{1.8}^{3.4} f(x)dx \quad &\approx \frac{0.2}{2}[6.050 + 2(7.389) + 2(9.025) + 2(11.023) \\ &+2(13.464) + 2(16.445) + 2(20.086) + 2(24.533) \\ &+29.964] = 23.9944\end{aligned}$$

The Composite Trapezoidal Rule III

- The data in Table 3 are for $f(x) = e^x$ and the true value is $e^{3.4} - e^{1.8} = 23.9144$.

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\begin{aligned}
Error &= -\frac{1}{12}h^3 n f''(\xi),\ 1.8 \le \xi \le 3.4 \\
&= -\frac{1}{12}(0.2)^3(8) * \left\{ \begin{array}{ll} e^{1.8} & (max) \\ e^{3.4} & (min) \end{array} \right\} = \left\{ \begin{array}{ll} -0.0323 & (max) \\ -0.1598 & (min) \end{array} \right\}
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- The actual error was -0.080. It is reasonable since the value is in the error bounds.

Last Words

Thanks for attending and listening.