Faculty of Civil Engineering Belgrade
Master Study COMPUTATIONAL ENGINEERING
Fall semester 2005/2006

ASSIGNMENTS

LESSON IX

Numerical Differentiation and Numerical Integration

1. Based on the data-set

i	0	1	2	3	4
x_i	1.2	1.3	1.4	1.5	1.6
$f(x_i)$	1.5095	1.6984	1.9043	2.1293	2.3756

compute approximately $f'(1.4)$ and $f''(1.4)$. The obtained results compare with exact ones, i.e. $f'(1.4) = ch(1.4) \cong 2.1509$ and $f''(1.4) = sh(11.4) \cong 1.9043$.

Hint: Use first Newton's interpolation polynomial, i.e.

$$P_4(x) = f_0 + p\Delta f_0 + \frac{p(p-1)}{2!}\Delta^2 f_0 + \frac{p(p-1)(p-2)}{3!}\Delta^3 f_0 + \frac{p(p-1)(p-2)(p-3)}{4!}\Delta^4 f_0,$$

where $p = \dfrac{x - x_0}{h}$. Taking $f \approx P_4(x)$, we have $P_4'(x) = \dfrac{dP_4}{dp}\dfrac{dp}{dx}$, and because

$$P_4(x) = f_0 + p\Delta f_0 + \frac{p^2 - p}{2}\Delta^2 f_0 + \frac{p^3 - 3p^2 + 2p}{6}\Delta^3 f_0 + \frac{p^4 - 6p^3 + 11p^2 - 6p}{24}\Delta^4 f_0,$$

$$P_4'(x) = \frac{1}{h}(\Delta f_0 + \frac{2p-1}{2}\Delta^2 f_0 + \frac{3p^2-6p+2}{6}\Delta^3 f_0 + \frac{4p^3-18p^2+22p-6}{24}\Delta^4 f_0),$$

and by further differentiation

$$P_4''(x) = \frac{1}{h^2}(\Delta^2 f_0 + (p-1)\Delta^3 f_0 + \frac{6p^2-18p+11}{12}\Delta^4 f_0).$$

Now, based on table of differences

k	x_k	f_k	Δf_k	$\Delta^2 f_k$	$\Delta^3 f_k$	$\Delta^4 f_k$
0	1.2	1.5095				
			0.1889			
1	1.3	1.6984		0.0170		
			0.2059		0.0021	
2	1.4	1.9043		0.0191		0.0001
			0.2250		0.0022	
3	1.5	2.1293		0.0213		
			0.2463			
4	1.6	2.3756				

and taking $x = x_2 = 1.4$, $p = \frac{x_2 - x_0}{h} = \frac{1.4-1.2}{0.1} = 2$,

$$f'(1.4) \cong P_4'(1.4) = \frac{1}{0.1}(0.1889 + \frac{3}{2}0.0170 + \frac{1}{3}0.0021 - \frac{1}{12}0.0001) \cong 2.1509$$

$$f''(1.4) \cong \frac{1}{h^2}(0.0170 + 0.0021 - \frac{1}{12}0.0001) \cong 1.9092.$$

2. Using data-set from the previous problem, compute $f'(1.4)$ and $f''(1.4)$ by approximating the function f by Newton's second polynomial and Gauss' polynomials of first and second kind. Compare the results.

3. Based on data table

x	2.1	2.2	2.3	2.4
$f(x)$	5.1519	5.6285	6.1229	6.6355

compute approximately $f'(2.4)$ and $f''(2.4)$. Compare the obtained results with exact values rounded to four digits, i.e. $f'(2.4) \cong 5.2167$, $f''(2.4) \cong 1.8264$. Use second Newton's polynomial of fourth degree.

In spite of not being convenient, use also first Newton's polynomial. Compare the results with exact one's and also with approximated by Newton's polynomial.

4. Based on approximation of data given in previous table, by Gauss' polynomials of first and second kind, find $f'(2.4)$ and $f''(2.4)$. Compare the obtained results with exact ones, and with each other.

5. Develop the formulas for first five derivatives of Newton's first and second approximation polynomials.
   Hint: Take

$$f_0 = f_0 + \binom{p}{1}\Delta f_0 + \binom{p}{2}\Delta^2 f_0 + \binom{p}{3}\Delta^3 f_0 + \cdots$$

$$f_p = f_0 + \binom{p}{1}\Delta f_{-1} + \binom{p+1}{2}\Delta^2 f_{-2} + \binom{p+2}{3}\Delta^3 f_{-3} + \cdots,$$

as first and second Newton's formula, where $p = \dfrac{x - x_0}{h}$.

6. Develop the formula for approximation of first five derivatives using Sterling's approximation polynomial.

7. Develop the formula for approximation of first five derivatives using Bessel's approximation polynomial.

8. Develop the generalized trapezoidal integration formula.

9. Using the data-set given in tabular form and containing values of $\sqrt{x}$, compute

$$\int_{1.00}^{1.30} \sqrt{x}\, dx.$$

x	1.0	1.05	1.10	1.15	1.20	1.25	1.30
$\sqrt{x}$	1.00000	1.02470	1.04881	1.07238	1.09544	1.11803	1.14017

Compare with exact result.

10. Using trapezoidal, Simpson's, and Newton-Cotes' formula with $n = 6$, compute $\int \sin x\, dx$ between 0 and $\pi/2$ based on values from the following table.

x	0.	$\pi/12$	$2\pi/12$	$3\pi/12$	$4\pi/12$	$5\pi/12$	$\pi/2$
$\sin x$	0.00000	0.25882	0.50000	0.70711	0.86603	0.96593	1.00000

Compare the results with exact value.

11. Apply the Simpson's integration rule to compute

$$\int_0^{\pi/2} \sin x\, dx$$

taking $h = \pi/8$ and halving it up to $\pi/2048$. Compare the results with exact one.

12. Apply the Romberg's integration rule to the previous problem.

13. Compute the integral of error-function

$$H(x) = \frac{2}{\sqrt{\pi}} \int_0^x e^{-t^2}\, dt$$

for $x = 0.5$ and $x = 1$, using Taylor's series.
Hint: Use series

$$e^{-t^2} = 1 - t^2 + \frac{t^4}{2} - \frac{t^6}{6} + \frac{t^8}{24} - \frac{t^{10}}{120} + \cdots,$$

i.e.

$$H(x) = \frac{2}{\sqrt{\pi}}[x - \frac{x^3}{3} + \frac{x^5}{10} - \frac{x^7}{42} + \frac{x^9}{216} - \frac{x^{11}}{1320} + \cdots].$$

14. Use different Newton-Cotes' formulas to compute the integral

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

of function given in tabular form

x	1.0	1.2	1.4	1.6	1.8	2.0
$f(x)$	1.0000	0.8333	0.7143	0.6250	0.5556	0.5000

with $a = 1,\ b = 2$. Compare the results with exact one, i.e.

$$\int_1^2 \frac{1}{x}\,dx = ln\ x\ \Big|_1^2 = ln\ 2 = 0.6931$$

15. The table in previous problem is accomplished with new values

x	1.1	1.3	1.5	1.7	1.9
$f(x)$	0.9091	0.7692	0.6667	0.5882	0.5263

Applying the trapezoidal formula to this set of data form the Romberg's integration rule and compare with exact result.

16. How long should be interval of integration h, so that the value of $ln\ 2$, as in Problem 14, would be computed with eight exact digits ?

17. Using different Newton-Cotes' formulas, compute $\int_0^2 y(x)\,dx$, based on data from the following table.

x	0.00	0.25	0.50	0.75	1.00	1.25	1.50	1.75	2.00
$y(x)$	1.000	1.284	1.649	2.117	2.718	3.490	4.482	5.755	7.389

Compare the results with exact result for $y(x) = e^x$,

$$\int_1^5 y(x)\,dx = e^2 - 1 = 6.389$$

18. Compute $\int_1^5 y(x)\,dx$ based on data-set given in the following table

x	1.0	1.5	2.0	2.5	3.0	3.5	4.0	4.5	5.0
$y(x)$	0.00	0.41	0.69	0.92	1.10	1.25	1.39	1.5	1.61

using Newton-Cotes' formulas with $n = 1(1)4$. The exact result is $(y(x) = \log\ x)$,

$$\int_0^5 \log x\,dx = x(\ln x - 1)\Big|_0^5 = 5(\ln 5 - 1) = 4.05$$

19. Compute $\int_1^5 \frac{dx}{1+x^2}$ by Newton-Cotes' formulas with $n = 3(1)6$, with seven digits of exactness. Exact result is $\pi/4$ or 0.7853982.

20. Compute $\int_2^{\pi/2} \sqrt{1 - \frac{1}{4}\sin^2 t}\ dt$ with exact four digits. This integral is of elliptic type, with exact result 1.4675. Use Romberg integration.

21. Compute the integral

$$\int_0^{\pi/2} \frac{dx}{\sin^2 x + \frac{1}{4}\cos^2 x}$$

using Newton-Cotes' formulas of degree $n = 1(1)4$ and $h = \frac{\pi}{4}(\frac{1}{4})\frac{\pi}{1024}$. Compare the obtained results with exact one, π.

22. Compute $\int\limits_0^1 e^{-x^3}\ dx$ with six exact digits using arbitrary method. Compare the result with one obtained by program Mathematica.

23. * Define the coefficients A_1, A_2, A_3 so that quadrature formula

$$\int\limits_a^b f(x)\ dx = A_1 \cdot f(x_1) + A_2 \cdot f(x_2) + A_3 f(x_3) + R_3(f)$$

is exact for all algebraic polynomials of degree $k \leq 2$, when

1. $(a,b) = (-1,1),\ x_1 = -1, x_2 = -\frac{1}{3}, x_3 = \frac{1}{3}$;
2. $(a,b) = (-1,1),\ x_1 = -\sqrt{\frac{3}{5}}, x_2 = 0, x_3 = \sqrt{\frac{3}{5}}$;
3. $(a,b) = (0,1),\ x_1 = -2, x_2 = -1, x_3 = 0$.

Hint: By putting $R_3(x^k) = 0$ $(k = 0,1,2)$, one gets the system

$$\begin{array}{ccccccc} A_1 & + & A_2 & + & A_3 & = & m_0 \\ A_1 x_1 & + & A_2 x_2 & + & A_3 x_3 & = & m_1 \\ A_1 x_1^2 & + & A_2 x_2^2 & + & A_3 x_3^2 & = & m_2 \end{array}$$

where

$$m_k = \int\limits_a^b x^k\ dx = \frac{1}{k+1}(b^{k+1} - a^{k+1}),$$

with solutions

$$A_1 = \frac{x_2 x_3 m_0 - (x_2 + x_3)m_1 + m_2}{(x_1 - x_2)(x_1 - x_3)},$$

$$A_2 = \frac{x_1 x_3 m_0 - (x_1 + x_3)m_1 + m_2}{(x_2 - x_1)(x_2 - x_3)},$$

$$A_3 = \frac{x_1 x_2 m_0 - (x_1 + x_2)m_1 + m_2}{(x_3 - x_1)(x_3 - x_2)},$$

By replacing values from 1., 2., 3., we get the integration formulas. Make a procedure for this type of integration formulas for arbitrary degree of exactness using program Mathematica.

24. Write a code in Mathematica for obtaining the coefficients A_k $(k = 1, 2, 3, 4)$ in quadrature formula

$$\int_{-1}^{1} f(x)\ dx = A_1 \cdot f(-1) + A_2 \cdot f(1) + A_3 f'(-1) + A_4 f'(1) + R(f)$$

with maximal possible algebraic degree of exactness.

Hint: In order to obtain four unknown coefficients, we take $f(x) = 1, x, x^2, x^3$ and get the system

$$\begin{array}{ccccccccc} A_1 & + & A_2 & & & & & = & 2 \\ -A_1 & + & A_2 & + & A_3 & + & A_4 & = & 0 \\ A_1 & + & A_2 & + & -2A_3 & + & 2A_4 & = & \frac{2}{3} \\ A_1 & + & A_2 & + & 3A_3 & + & 3A_4 & = & 0 \end{array}$$

By solving previous system we get $A_1 = A_2 = 1,\ A_3 = -A_4 = \frac{1}{3}$, so that one gets a formula

$$\int_{-1}^{1} f(x)\ dx = f(-1) + f(1) - \frac{1}{3}(f'(1) - f'(-1)) + R(f)$$

This formula has an algebraic degree of exactness $p = 3$ $(R(x^4) = \dfrac{16}{15} \neq 0)$.

25. The integral

$$\int_{a}^{b} f(x)\ dx$$

is to be estimated by a quadratic-type rule, using three base points, $x_1,\ x_2$ and x_3, that are not necessarily equally spaced

and none of which necessarily coincides with a or b. Derive the appropriate integration formula and its associated error term. Check that the formula reduces to Simpson's rule when $x_1 = a$, $x_3 = b$, and $(x_2 - x_1) = (x_3 - x_2) = h$. Proceed the calculation by hand and by program Mathematica.
Hint: See problem 23.

26. (*) Consider the computation of the integral $\int_a^b f(x)\,dx$ using Simpson's rule

$$\int\limits_{x_0}^{x_2} f(x)\ dx = \frac{h}{3}[f(x_0) + 4f(x_1) + f(x_2)] - \frac{h^5}{90} f^{(IV)}(\xi)$$

repeatedly, each time halving the interval h. This is equivalent to the composite Simpson's rule

$$\int\limits_a^b f(x)\ dx = \frac{b-a}{6n}[f(a) + f(b) + 2\sum_{i=1}^{n-1} f(a + \frac{b-a}{n} i)$$
$$+ 4\sum_{\substack{i=1\\ \Delta i=2}}^{2n-1} f(a + \frac{b-a}{2n} i)] - \frac{(b-a)^5}{2880n^4} f^{(IV)}(\xi),$$
$$(a < \xi < b)$$

for $n = 1, 2, 4, 8, 16, \ldots$.

Let j be the number of interval halving operations. Then n and j are related by $n = 2^j$. Let I_j be the estimate of the integral for j repeated interval halving, and I_j^* be the improved estimate

$$I_j^* = \frac{16}{15} I_j - \frac{1}{15} I_{j-1},$$

using Richardson extrapolation, based on composite trapezoidal rule

$$I^* = I_{n1} + \frac{I_{n2} - I_{n1}}{1 - [\frac{n_1}{n_2}]^4}, \quad \text{for } n_2 = 2n_1,$$

write a function (or procedure) in Fortran/Mathematica named `SIMPRH (A,B,F,EPS,JMAX,J)`, where A and B are integration boundaries, `F` the name of integrated function, $f(x)$.

The procedure should obtain I_j^*, $(j = 0, 1, 2, \ldots)$ until $j >$`JMAX` or $|I_j^* - I_j| <$`EPS`.

Thus `EPS` may be considered to be tolerance on the estimated error. The number of interval-halving steps carried out should be stored in `J` upon exit.

27. (*) A semi-infinite medium ($x \geq 0$) has a thermal diffusivity α and a zero initial temperature at time $t = 0$. For $t > 0$ the surface at $x = 0$ is maintained at a temperature $T_s = T_s(t)$. By using the Duhamel's theorem (H.S. Carslaw and J.C. Jaeger, *Conduction of Heat in Solids*, 2nd ed., Oxford University Press, London, 1959, p.62), the subsequent temperature $T(x,t)$ inside the medium can be shown to be given by

$$T(x,t) = \frac{x}{2\sqrt{\pi\alpha}} \int_0^t T_s(\lambda) \frac{e^{-\dfrac{x^2}{4\alpha(t-\lambda)}}}{(t-\lambda)^{3/2}}\, d\lambda.$$

An alternative form of this integral can be obtained by introducing a new variable

$$\mu = \frac{x}{2\sqrt{\alpha(1-\lambda)}}.$$

Let T_s represent the period temperature in $^\circ F$ at a point on the earth surface, as a table of mean monthly air temperatures.

	Subot.	*N.Sad*	*Bg.*	*Krag.*	*Nis*	*Vranje*	*Knjaz.*
Jan							
Feb							
Mar							
Apr							
May							
Jun							
Jul							
Aug							
Sep							
Oct							
Nov							
Dec							

Compute the likely mean monthly ground temperatures at $5, 10, 20, 50$ feet below the earth surface at each of the given locations. Plot these computed temperatures to show their relation to the corresponding surface temperatures. In each case, assume:

(a) Dry ground with $\alpha = 0.0926 sq.ft/hr$;

(b) The mean monthly ground and air temperatures at the surface are approximately equal;

(c) The pattern of air temperatures repeats itself indefinitely from one year to the next.

28. (*) Suppose that $(m+1)(n+1)$ functional values $f(x_i, y_i)$ are available for all combinations of $m+1$ levels of x_i, $i = 0, 1, \ldots, m$ and $n+1$ levels of y_j, $j = 0, 1, \ldots, n$. Define La-

grangian interpolation coefficients as follows:

$$X_{m,i} = \prod_{\substack{k=0 \\ k\neq i}}^{m} \frac{x - x_k}{x_i - x_k}, \qquad i = 0, 1, \ldots, m,$$

$$Y_{n,j} = \prod_{\substack{k=0 \\ k\neq j}}^{m} \frac{y - y_k}{y_j - y_k}, \qquad j = 0, 1, \ldots, n.$$

Show that

$$P_{m,n}(x, y) = \sum_{i=0}^{m} \sum_{j=0}^{n} X_{m,i}(x) Y_{n,j}(y) f(x_i, y_j)$$

is a two-dimensional polynomial of degree m in x and degree n in y of the form

$$P_{m,n}(x, y) = \sum_{i=0}^{m} \sum_{j=0}^{n} a_{i,j} x^i y^j,$$

and satisfies the $(m+1)(n+1)$ conditions

$$P_{m,n}(x_i, y_j) = f(x_i, y_j) \quad i = 0, 1, \ldots, m, \quad j = 0, 1, \ldots, n,$$

and therefore that $P_{m,n}(x, y)$ may be viewed as a two-dimensional interpolating polynomial passing through the $(m+1)(n+1)$ points $(x_i, y_i, f(x_i, y_i))$, $i = 0, 1, \ldots, m$, $j = 0, 1, \ldots, n$.

29. (*) Find a three-dimensional interpolating polynomial of degree m in x, n in y, and q in z of the form

$$P(m, n, q)(x, y, z) = \sum_{i=0}^{m} \sum_{j=0}^{n} \sum_{k=0}^{q} a_{i,j,k}\, x^i y^j z^k,$$

that satisfies $(m+1)(n+1)(q+1)$ conditions

$$P_{m,n,q}(x_i, y_j, z_k) = f(x_i, y_j, z_k) \quad i = 0, 1, \ldots, m, \quad j = 0, 1, \ldots, n, \quad k = 0, 1, \ldots, q.$$

Develop a comparable interpolating polynomial for any number of independent variables. Use any algorithmic (Fortran, Pascal, C) and symbolic (Mathematica)programming language.

30. Write subprograms (procedures) for calculation of approximate values of definite integrals by trapezoidal (`TRAP`) and Simpson's (`SIMPSON`) formulas.

Integral function should be given by function procedure or subprogram. Test example is

$$\int_0^1 \frac{\sqrt{x}\sin x}{1+e^x}\,dx, \quad h = 0.01$$

Hint: Generalized trapezoidal and Simpson's formula are, respectively:

$$\int_a^b f(x)\ dx \cong h[\frac{f(a)+f(b)}{2} + f(a+h) + f(a+2h) + \cdots + f(b-h)]$$

$$\int_a^b f(x)\ dx \cong \frac{h}{3}[f(a) + 4f(a+h) + 2f(a+2h) + 4f(a+3h) + \cdots$$

$$+ 4f(b-h) + f(b)].$$

31. According to quadrature formula

$$\int_{-1}^1 \sqrt{1-x^2}\ f(x)\ dx \cong \frac{\pi}{m+1}\sum_{k=1}^{m} \sin^2\frac{k\cdot\pi}{m+1}\cdot f(\cos\frac{k\cdot\pi}{m+1})$$

write a procedure (subprogram) for calculation of integral of form

$$\int_{-1}^1 \sqrt{1-x^2}\ f(x)\ dx.$$

List of subprogram parameters should include m, function, and (on output) integral value. Test the program with $f(x) = \cos\ x$.

32. Write a program (procedure) in any procedural and symbolic language for obtaining a value of integral

$$I(a) = \int_0^\infty e^{-x^2} \sin ax\ dx$$

for $a = 0.0(0.1)1.0$, using formula

$$I(a) = \int_0^\infty e^{-x^2} \sin ax\ dx = \frac{1}{2} \sum_{n=0}^{\infty} \frac{(-1)^n n!}{(2n+1)!}\ a^{2n+1}.$$

Summation has to be stopped when general summation member is by module less than 10^{-8}.

33. Write a program (procedure) in any procedural and symbolic language for obtaining a value of integral using Gauss' formula through three points of form

$$\int_a^b f(x)\, dx = h[\frac{5}{18} \sum_{i=0}^{n-1} f(p_i) + \frac{4}{9} \sum_{i=0}^{n-1} f(q_i) + \frac{5}{18} \sum_{i=0}^{n-1} f(r_i)],$$

where

$$h = \frac{b-a}{n};$$
$$p_i = a + 0.112701666 \cdot h + i \cdot h;$$
$$q_i = a + 0.5 \cdot h + i \cdot h;$$
$$r_i = a + 0.887298334 \cdot h + i \cdot h.$$

Test the program with the following integrals:

$$\int_{0.8}^{1.762} \sqrt{1+x^3}\, dx; \quad \int_{1.3}^{2.624} \frac{dx}{\sqrt{x^3-1}}; \quad \int_{0.6}^{1.724} \sqrt{x(1+x^2)}\, dx;$$

$$\int_{0.}^{1.234} \frac{\sin^2 x}{\sqrt{1+x^3}}\,dx; \quad \int_{0.}^{1.047} \frac{e^{\frac{x}{2}}}{\sqrt{x+1}}\,dx.$$

Input parameters are n, integral boundaries, and functions to be integrated.

34. According to formula

$$\int_{-1}^{1} \frac{1}{\sqrt{1-x^2}} f(x)\,dx \cong \frac{\pi}{m}\sum_{k=1}^{m} f(\cos\frac{\pi}{2m}(2k-1))$$

write a corresponding program in any algorithmic or symbolic language. Input parameter list should contain m and function to be integrated. Output parameter is integral value.
Test the program with function $f(x) = \cos x,\ m = 10.$

35. For approximative calculation of integral using formula

$$\int_{-1}^{1} \sqrt{1-x^2} f(x)\,dx \cong \sum_{k=1}^{n} A_k\, f(x_k),$$

where

$$x_k = \cos\frac{k\pi}{n+1}, \qquad A_k = \frac{\pi}{n+1}\sin^2\frac{k\pi}{n+1} \qquad (k = 1, 2, \ldots, n),$$

write a corresponding (sub)program in any algorithmic or symbolic language. Input parameter is n and on output is integral value. Function to be integrated should be given in arbitrary way.
Test the program with function $f(x) = e^x$ for $n = 5(1)15$.