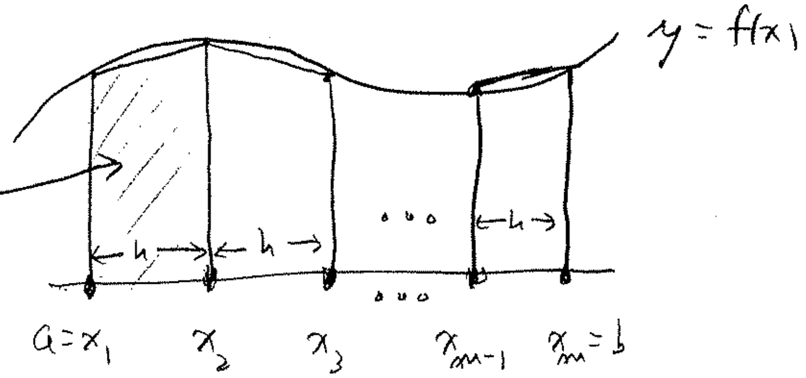
Suppl. Notes from book by C. Van Loan Intro. to Sci. Comput

Chapter 4 - Numerical Integration

Recall the trapezoidal rule from Calculus I

Area of trapezoid $= \dfrac{f(x_1)+f(x_2)}{2} \cdot h$



composite rule

$$x_k = a + \left(\frac{b-a}{m-1}\right)(k-1),\ k=1:m, \quad h = x_{k+1} - x_k = \frac{b-a}{m-1}$$

$$\int_a^b f(x)\,dx \approx \frac{f(x_1)+f(x_2)}{2}\cdot h + \frac{f(x_2)+f(x_3)}{2}\cdot h + \dots + \frac{f(x_{m-1})+f(x_m)}{2}\cdot h$$

$$= \frac{h}{2} f(x_1) + h f(x_2) + h f(x_3) + \dots + h f(x_{m-1}) + \frac{h}{2} f(x_m)$$

(familiar form) →
$$= \frac{h}{2}\left(f(x_1) + 2f(x_2) + 2f(x_3) + \dots + 2f(x_{m-1}) + f(x_m)\right)$$

$$= \frac{b-a}{2(m-1)}\left(f(x_1) + 2f(x_2) + \dots + 2f(x_{m-1}) + f(x_m)\right)$$

general form used in text →
$$= (b-a)\sum_{k=1}^{m} \omega_k f(x_k) = Q = \text{"quadrature rule"}$$

where
$$\omega_1 = \omega_m = \frac{1}{2(m-1)}$$
$$\omega_k = \frac{1}{m-1} \qquad k = 2:m-1$$

ω_k = "weights"

x_k = "abscissas"

m-point quadrature (integration) rule Q for

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

is

$$Q = (b-a)\sum_{k=1}^{m} w_k f(x_k)$$

where the abscissas x_k and weights w_k are chosen s.t. $Q \approx I$.

Efficiency depends of number of calculations of $f(x_k)$ needed.

Accuracy depends on rule + smoothness of $f(x)$.

Topics we'll cover:

4.1 Newton-Cotes Rules
(based on interpolating polynomials with equidistant x_k's)

4.2 Composite Rules
(based on partitioning of $[a,b]$)

4.3 Adaptive Quadrature
(based on adaptive (recursive) determination on partition in 4.2)

4.4 Special Topics
- Gauss Quadrature (better choice of x_k's)
- Spline Quadrature

(skip) → 4.5 Shared Memory Adaptive Quadrature
(parallel computing)

4.1 The Newton-Cotes (NC) Rule

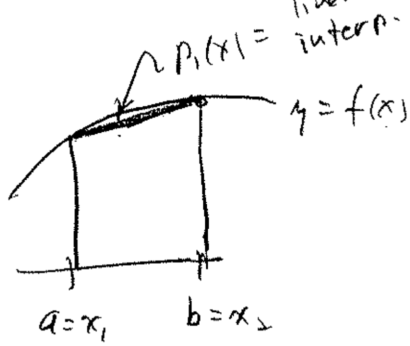
Idea: $f(x) \approx p(x) =$ polynomial interpolant of $f(x)$

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

m-pt NC $(m \geq 2)$:

$p_{m-1}(x) =$ poly. interpolant of $f(x)$ at m equally spaced points $x_k = a + \frac{k-1}{m-1}(b-a)$, $k = 1:m$

$$Q_{NC(m)} = \int_a^b p_{m-1}(x)\,dx$$



e.g. $m=2$ $\quad x_1 = a, \quad x_2 = b$

$$p_1(x) = f(a) + \frac{f(b)-f(a)}{b-a}(x-a)$$

$$= f[x_1] + f[x_1, x_2](x - x_1)$$

$$h = \frac{b-a}{2-1} = b-a$$

$$Q_{NC(2)} = \int_a^b p_1(x)\,dx$$

$$= \int_a^b \left(f(a) + \frac{f(b)-f(a)}{b-a}(x-a)\right)dx$$

$$= \left[f(a)\,x + \frac{f(b)-f(a)}{b-a}\frac{(x-a)^2}{2}\right]\Bigg|_{x=a}^{x=b}$$

$$= (b-a)\left[f(a) + \frac{f(b)-f(a)}{b-a}\left(\frac{b-a}{2}\right)\right]$$

$$= (b-a)\left[f(a) + \tfrac{1}{2}f(b) - \tfrac{1}{2}f(a)\right]$$

$$= (b-a)\left(\tfrac{1}{2}f(a) + \tfrac{1}{2}f(b)\right) =$$ 2 pt trapezoidal rule $(w_1 = w_2 = \frac{1}{2})$

<u>m = 3</u> $\quad x_1 = a, \quad x_2 = a + \frac{1}{2}(b-a) = \frac{a+b}{2} =: c, \quad x_3 = b$

$$p_2(x) = f[a] + f[a,c](x-a) + f[a,c,b](x-a)(x-c)$$

$$= f(a) + \frac{f(c)-f(a)}{c-a}(x-a) + \frac{\frac{f(b)-f(c)}{b-c} - \frac{f(c)-f(a)}{c-a}}{b-a}(x-a)(x-c)$$

$$Q_{NC(3)} = \int_a^b p_2(x)\,dx \qquad \text{Note } c-a = b-c = \tfrac{1}{2}(b-a)$$

$$= \int_a^b \left(f(a) + \frac{f(c)-f(a)}{c-a}(x-a) + \frac{f(b)-f(c)-(f(c)-f(a))}{\frac{1}{2}(b-a)^2}(x-a)(x-c) \right) dx$$

$$= \int_a^b \left[f(a) + \frac{2(f(c)-f(a))}{b-a}(x-a) + \frac{2(f(b)-2f(c)+f(a))}{(b-a)^2}(x-a)(x-c) \right] dx$$

$$= f(a)(b-a) + \frac{2(f(c)-f(a))}{b-a}\frac{(b-a)^2}{2} + \frac{2(f(b)-2f(c)+f(a))}{(b-a)^2} \underbrace{\int_a^b (x-a)(x-c)\,dx}_{= \frac{(b-a)^3}{12}}$$

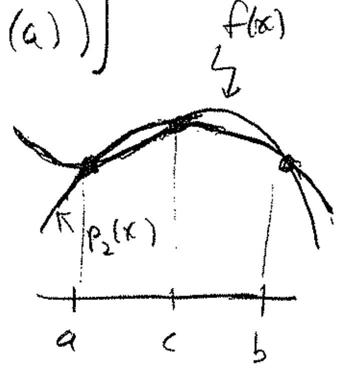
$$= (b-a)\left[\cancel{f(a)} + f(c) - \cancel{f(a)} + \frac{1}{6}\left(f(b) - 2f(c) + f(a)\right) \right]$$

$$= (b-a)\left[f(c) + \frac{1}{6}f(b) - \frac{2}{6}f(c) + \frac{1}{6}f(a) \right]$$

$$= (b-a)\left(\frac{1}{6}f(a) + \frac{4}{6}f(c) + \frac{1}{6}f(b) \right)$$

$$= \boxed{(b-a)\left(\frac{1}{6}f(a) + \frac{4}{6}f\left(\frac{a+b}{2}\right) + \frac{1}{6}f(a) \right) = Q_{NC(3)}}$$

$=$ <u>Simpson's rule</u> $\quad \boxed{w_1 = w_3 = \frac{1}{6}, \; w_2 = \frac{4}{6}}$



4.1.1 Derivation general m

$$p_{m-1}(x) = \sum_{k=1}^{m} \left(c_k \prod_{i=1}^{k-1} (x - x_i) \right)$$

$$x_i = a + (i-1)h, \quad h = \frac{b-a}{m-1}$$

equally spaced abscissa

$$c_k = f[x_1, x_2, \ldots, x_k]$$

change variables:

$$x\Big|_a^b = a + sh\Big|_{s=0}^{m-1}$$

$$dx = h\, ds$$

$$x - x_i = (s - (i-1))h$$

$$Q_{NC(m)} = \int_a^b p_{m-1}(x)\,dx$$

$$= h \int_0^{m-1} p_{m-1}(a+sh)\,ds$$

$$= h \int_0^{m-1} \sum_{k=1}^{m} c_k \prod_{i=1}^{k-1} \left[(s-i+1)h\right] ds$$

$$= \sum_{k=1}^{m} c_k h^k \underbrace{\int_0^{m-1} \prod_{i=1}^{k-1} (s-i+1)\,ds}_{=:}$$

$$= \sum_{k=1}^{m} c_k h^k S_{mk}$$

(Note $\prod_{i=1}^{k-1} (s-i+1) = s(s-1)(s-2)\cdots(s-k+2)$)

$\underline{k=1}$ $\quad \prod_{i=1}^{k-1} (s-i+1) := 1$

$\underline{k=2}$ $\quad \prod_{i=1}^{2-1} (s-i+1) = s$

$\underline{k=3}$ $\quad \prod_{i=1}^{3-1} (s-i+1) = s(s-1) \quad \ldots$

<u>Denote</u> $f_i := f(x_i)$ $\quad (h = x_{i+1} - x_i \text{ for all } i)$

$$c_1 = f[x_1] = f_1$$

$$c_2 = f[x_1, x_2] = \frac{f(x_2) - f(x_1)}{x_2 - x_1} = \frac{f_2 - f_1}{h}$$

$$c_3 = f[x_1, x_2, x_3] = \frac{\frac{f(x_3) - f(x_2)}{x_3 - x_2} - \frac{f(x_2) - f(x_1)}{x_2 - x_1}}{x_3 - x_1} = \frac{\frac{f_3 - f_2}{h} - \frac{f_2 - f_1}{h}}{2h}$$

$$= \frac{f_3 - 2f_2 + f_1}{2h^2}$$

similarly

$$c_4 = f[x_1, x_2, x_3, x_4] = \frac{f_4 - 3f_3 + 3f_2 - f_1}{3!\,h^3}$$

...

<u>Recipes for S_{mk}</u> $\quad 1 \le k \le m$

$$S_{m1} = \int_0^{m-1} 1 \cdot ds = m - 1$$

$$S_{m2} = \int_0^{m-1} s\, ds = \frac{s^2}{2}\Big|_0^{m-1} = \boxed{\frac{(m-1)^2}{2}}$$

$$S_{m3} = \int_0^{m-1} s(s-1)ds = \int_0^{m-1} (s^2 - s)ds = \frac{s^3}{3} - \frac{s^2}{2}\Big|_0^{m-1}$$

$$= \frac{(m-1)^3}{3} - \frac{(m-1)^2}{2} = (m-1)^2\left(\frac{1}{3}(m-1) - \frac{1}{2}\right)$$

$$= \frac{(m-1)^2(m-1-\frac{3}{2})}{3} = \boxed{\frac{(m-1)^2(m-\frac{5}{2})}{3}}$$

$$S_{m4} = \int_0^{m-1} s(s-1)(s-2)\, ds = \ldots = (m-1)^2(m-3)^2/4$$

...

Check i) Trapezoidal rule $\quad m=2$

$$Q_{NC(2)} = \sum_{k=1}^{2} c_k h^k S_{2k} = c_1 h S_{21} + c_2 h^2 S_{22}$$

$$= f_1 h(2-1) + \frac{f_2 - f_1}{h} h^2 \frac{(2-1)^2}{2}$$

$$= f_1 h + (f_2 - f_1) h \cdot \frac{1}{2} = h\left(\frac{1}{2} f_1 + \frac{1}{2} f_2\right) = (b-a)\left(\frac{1}{2} f_1 + \frac{1}{2} f_2\right)$$

ii) Simpson's rule $\quad m=3$

$$Q_{NC(3)} = \sum_{k=1}^{3} c_k h^k S_{3k} = c_1 h S_{31} + c_2 h^2 S_{32} + c_3 h^3 S_{33}$$

$$= f_1 h(3-1) + \frac{f_2 - f_1}{h} h^2 \frac{(3-1)^2}{2} + \frac{f_3 - 2f_2 + f_1}{2h^2} h^3 \frac{(3-1)^2 (3-\frac{5}{2})}{3}$$

$$= h\left(2f_1 + (f_2 - f_1) 2 + \frac{f_3 - 2f_2 + f_1}{2} \frac{2^2 \cdot \frac{1}{2}}{3}\right)$$

$$= h\left(2f_1 + 2f_2 - 2f_1 + \frac{1}{3} f_3 - \frac{2}{3} f_2 + \frac{1}{3} f_1\right)$$

$$= h\left(\frac{1}{3} f_1 + \frac{4}{3} f_2 + \frac{1}{3} f_3\right)$$

$$= (b-a)\left(\frac{1}{6} f_1 + \frac{4}{6} f_2 + \frac{1}{6} f_3\right) \qquad \left(h = \frac{b-a}{2}\right)$$

$$Q_{NC(4)} = (b-a)(f_1 + 3f_2 + 3f_3 + f_4)/8$$ ← see text

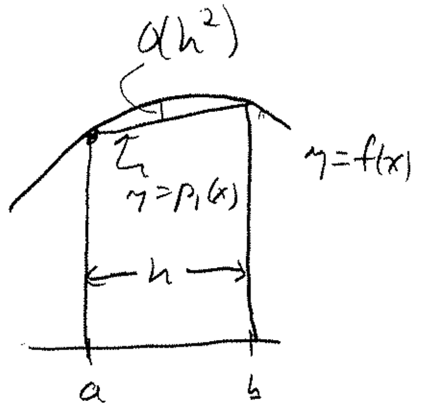
Note: The weights w_k can be computed once + for all and saved!

We expect Error $= \left| Q_{NC(m)} - \int_a^b f(x)dx \right| = O(h^{m+?}) \ldots ??$

for $f \in C^{m+??}[a,b] \ldots$

4.1.3 Newton-Cotes Error

Error for trapezoidal rule



$$\text{error} = \left| \int_a^b f(x)\,dx - Q_{NC(2)} \right| \overset{\text{expect}}{=} O(h \cdot h^2)$$
$$= O(h^3)$$

$h = \frac{b-a}{2-1} = b-a$

Let $p_1(x) = f(a) + f[a,b](x-a)$
$= 1^{st}$ degree poly. interpolant of f at a, b.

$$Q_{NC(2)} = \int_a^b p_1(x)\,dx = \int_a^b \left(f(a) + f[a,b](x-a)\right) dx$$

$$\underline{\text{Thm2}} \Rightarrow f(x) - p_1(x) = \frac{f^{(2)}(\eta_x)}{2!}(x-a)(x-b) \quad \text{for some } \eta_x \in [a,x]$$
$f \in C^2[a,b]$

$$\therefore \underline{\text{error}} = \left| \int_a^b f(x)\,dx - Q_{NC(2)} \right| = \left| \int_a^b \frac{f^{(2)}(\eta_x)}{2!}(x-a)(x-b)\,dx \right|$$

$$\leq \frac{M_2}{2} \left| \int_a^b (x-a)(x-b)\,dx \right|, \quad |f^{(2)}(x)| \leq M_2,\ x \in [a,b]$$

substitute
$x = a + sh$
$h = b - a$
$dx = s\,dh$

$$= \frac{M_2}{2} \left| \int_0^1 sh(1-s)h \cdot h\,ds \right|$$

$$= \frac{M_2}{2} h^3 \left| \int_0^1 s(1-s)\,ds \right|$$

$$= \frac{M_2}{2} h^3 \int_0^1 s - s^3\,ds$$

$$= \frac{M_2}{2} h^3 \left(\frac{s^2}{2} - \frac{s^3}{3} \right) \Big|_0^1 = \frac{M_2}{2} h^3 \underbrace{\left(\frac{1}{2} - \frac{1}{3} \right)}_{\frac{1}{6}}$$

$$= \frac{M_2}{12} h^3 = \frac{M_2}{12}(b-a)^3 = O(h^3)$$

(Note If $f(x)$ is a 1^{st} degree poly., $f(x) \equiv p_1(x)$ and M_2 can be taken as 0, so error $\equiv 0$)

Another sample error estimate for

$Q_{NC(3)}$ = <u>Simpson's rule</u> :

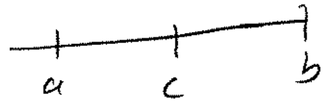
<u>Thm 4</u> If $f \in C^4[a,b]$ then

$$\text{error} = \left| \int_a^b f(x)\,dx - Q_{NC(3)} \right| \le \frac{(b-a)^5}{2880} M_4$$

where $\max\limits_{x \in [a,b]} |f^{(4)}(x)| \le M_4$.

<u>Pf:</u> Let $p(x) = c_1 + c_2(x-a) + c_3(x-a)(x-b) + c_4(x-a)(x-b)(x-c)$

interpolate $f(x)$ at a, b, c, d



d unspecified for now.

$c = \frac{a+b}{2}$ = midpt of $[a,b]$

Note $c_1 = f[a]$, $c_2 = f[a,b]$, $c_3 = f[a,b,c]$

$\therefore$ $q(x) = c_1 + c_2(x-a) + c_3(x-a)(x-b)$

is the 2nd degree interpolating poly of f

at $(a, f(a))$, $(b, f(b))$, $(c, f(c))$, i.e. $q(x) = p_2(x)$

$$\therefore\ Q_{NC(3)} = \int_a^b q(x)\,dx = \int_a^b c_1 + c_2(x-a) + c_3(x-a)(x-b)\,dx$$

<u>Note</u>
$$\int_a^b p(x)\,dx = \int_a^b q(x)\,dx + c_4 \int_a^b (x-a)(x-b)(x-c)\,dx$$

$$= Q_{NC(3)} + c_4 \underbrace{\int_a^b (x-a)(x-b)(x-c)\,dx}_{=0 \text{ (next page)}}$$

Now note since $c = \frac{a+b}{2}$, $h = \frac{b-a}{2} = b-c = c-a$

change of variables:

$x\Big|_a^b = c + s\Big|_{-1}^{1} h$, $dx = h\,ds$

$x - a = c + sh - a$

$= (c-a) + sh = (s+1)h$

$x - b = c + sh - b$

$= c - b + sh$

$= -h + sh$

$= (s-1)h$

$$\int_a^b (x-a)(x-b)(x-c)\,dx$$

$$= \int_{-1}^{1} (s+1)h(s-1)h\,sh \cdot h\,ds$$

$$= h^4 \int_{-1}^{1} (s+1)(s-1)s\,ds$$

$$= h^4 \int_{-1}^{1} s(s^2-1)\,ds$$

$$= h^4 \int_{-1}^{1} \underbrace{s^3 - s}_{\text{odd function of } s}\,ds =$$

$$= h^4 \cdot 0 = \underline{\underline{0}}$$

$$\therefore \int_a^b p(x)\,dx = Q_{NC(3)}$$

Recall Thm 2 $\Rightarrow$ $f(x) - p(x) = \frac{f^{(4)}(n_x)}{4!}(x-a)(x-b)(x-c)(x-d)$

$$\therefore \int_a^b f(x)\,dx - Q_{NC(3)} = \int_a^b (f(x) - p(x))\,dx$$

(note x-dependence)

$$= \int_a^b \frac{f^{(4)}(n_x)}{24}(x-a)(x-b)(x-c)(x-d)\,dx$$

i.e.

$$\text{error} = \left|\int_a^b f(x)\,dx - Q_{NC(3)}\right| \le \frac{M_4}{24}\int_a^b |(x-a)(x-b)(x-c)(x-d)|\,dx$$

d arbitrary, $d \in [a,b]$

Now set $d = c$. Then by above result,

$$\int_a^b |(x-a)(x-b)(x-c)(x-\underset{c}{\overset{\shortparallel}{d}})|\,dx = h^5 \int_{-1}^{1} |(s+1)(s-1)s^2|\,ds$$

$$= h^5 \int_{-1}^{1} (1-s^2)s^2\,ds$$

$$= h^5 \int_{-1}^{1} s^2 - s^4\,ds$$

$$= h^5 \left(\frac{s^3}{3} - \frac{s^5}{5}\right)\Big|_{-1}^{1}$$

$$= 2h^5\left(\frac{1}{3} - \frac{1}{5}\right)$$

$$= \frac{4}{15} h^5 \qquad \left(h = \frac{b-a}{2}\right)$$

$$= \frac{4}{15}\left(\frac{b-a}{2}\right)^5 = \frac{(b-a)^5}{120}$$

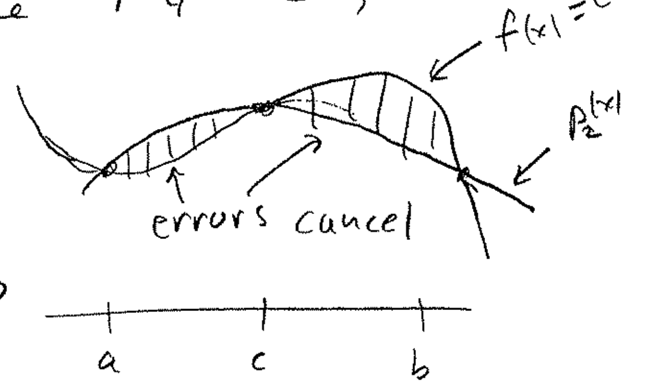
So

$$\text{error} = \left|\int_a^b f(x)\,dx - Q_{NC(3)}\right| \le \frac{M_4}{24}\frac{(b-a)^5}{120} = \frac{M_4}{2880}(b-a)^5 = O(h^5)$$

(qed

Note! If $f(x)$ is a poly. of degree ≤ 3, then we can take $M_4 = 0$, i.e. $f^{(4)}(x) \equiv 0$, so i.e. the error $= 0$.

$\therefore$ Simpson's rule integrates polynomials of degree ≤ 3 exactly! picture



In general, we have

$$\text{error} = \left| \int_a^b f(x)\,dx - Q_{NC(m)} \right| \leq |C_m|\, M_{d+1} \left(\frac{b-a}{m-1}\right)^{d+2} = O(h^{d+2})$$

$$\left(h = \frac{b-a}{m-1} \right)$$

where $d = \begin{cases} m-1 & \text{if } m \text{ even} \\ m & \text{if } m \text{ odd} \end{cases}$

and $|f^{(d+1)}(x)| \leq M_{d+1}$ for all $x \in [a,b]$

and $C_m \downarrow 0, \quad m \to \infty$

(small constant)

i.e. $\text{error} = \begin{cases} O(h^{m+1}) & m \text{ even} \quad \text{(e.g. } m=2 \text{ above)} \\ O(h^{m+2}) & m \text{ odd} \quad \text{(e.g. } m=3 \text{ above)} \end{cases}$

<u>Note</u>: m even $\Rightarrow$ $Q_{NC(m)}$ integrates poly. $f(x)$ of degree $\leq m-1$ <u>exactly</u>.

m odd $\Rightarrow$ $Q_{NC(m)}$ integrates poly. $f(x)$ of degree $\leq m$ <u>exactly</u>.

Remark

We want h <u>small</u>, but m not <u>too</u> large, since signs of w_k's alternate + cancellation will occur.

10/7/99

```
% Script File: ShowQNC
%
% Examines the closed Newton-Cotes rules.

  while input('Another exammple? (1=yes, 0=no). ')
     fname = input('Enter within quotes the name of the integrand function:');
     a = input('Enter left endpoint: ');
     b = input('Enter right endpoint: ');
     s = ['QNC(' fname sprintf(',%6.3f,%6.3f,m )',a,b)];
    clc
     disp(['  m      ' s])
     disp(' ')
     for m=2:11
        numI = QNC(fname,a,b,m);
        disp(sprintf(' %2.0f      %20.16f',m,numI))
     end
  end
```

```
  function numI = QNC(fname,a,b,m)
%
% Pre:
%   fname    string that names an available function of the
%            form f(x) that is defined on [a,b]. f should
%            return a column vector if x is a column vector.
%     a,b    real scalars
%       m    integer that satisfies 2 <= m <=11
% Post:
%    numI    the m-point Newton-Cotes approximation of the
%            integral of f(x) from a to b.
%
   w = wNC(m);
   x = linspace(a,b,m)';
   f = feval(fname,x);
   numI = (b-a)*(w'*f);
```

```
  function w=WNC(m);
%
% Pre:
%   m    integer that satisfies 2 <= m <= 11
%
% Post:
%   w    column m-vector consisting of the weights for the
%        the m-point Newton-Cotes rule.
%
  if m==2
     w=[1 1]'/2;
  elseif m==3
     w=[1 4 1]'/6;
  elseif m==4
     w=[1 3 3 1]'/8;
  elseif m==5
     w=[7 32 12 32 7]'/90;
  elseif m==6
     w=[19 75 50 50 75 19]'/288;
  elseif m==7
     w=[41 216 27 272 27 216 41]'/840;
  elseif m==8
     w=[751 3577 1323 2989 2989 1323 3577 751]'/17280;
  elseif m==9
     w=[989 5888 -928 10496 -4540 10496 -928 5888 989]'/28350;
  elseif m==10
     w=[2857 15741 1080 19344 5778 5778 19344 1080 15741 2857]'/89600;
  else
     w=[16067 106300 -48525 272400 -260550 427368 -260550 272400 -48525 106300
16067]'/598752;
  end;
```

10/7/99

```
function y = fextd(x)
% examples of functions for numerical integration
   y = x.^3;
```

```
» cd ..
» cd toolbox\scicompfiles\chapter.4
» showqnc
Another exammple? (1=yes, 0=no). 1
Enter within quotes the name of the integrand function:'fextd'
Enter left endpoint: 0
Enter right endpoint: 1



  m      QNC(fextd, 0.000, 1.000,m )

  2        0.500000000000000
  3        0.250000000000000
  4        0.250000000000001
  5        0.250000000000000
  6        0.250000000000001
  7        0.250000000000001
  8        0.250000000000001
  9        0.250000000000000
 10        0.250000000000001
 11        0.250000000000000
Another exammple? (1=yes, 0=no).
```