Math/CS 467/667 Homework 1 Solutions Part 1

14.1 Show that the midpoint rule is exact for $f(x) = mx+c$ along any interval $x \in [a, b]$. Let $f(x) = mx + c$. The exact integral along the interval $[a, b]$ is

$$\int_a^b f(x)dx = \int_a^b (mx + c)dx = \left(\frac{m}{2}x^2 + cx\right)\Big|_a^b = \frac{m}{2}(b^2 - a^2) + c(b - a).$$

On the other hand, the midpoint rule gives

$$\begin{aligned}\texttt{mprule}(a, b, f) &= f\Big(\frac{a+b}{2}\Big)(b-a) = \Big\{m\Big(\frac{a+b}{2}\Big) + c\Big\}(b-a) \\ &= \frac{m}{2}(b+a)(b-a) + c(b-a) = \frac{m}{2}(b^2 - a^2) + c(b-a).\end{aligned}$$

As these two formula agree then the rule is exact for $f(x) = mx + c$.

14.2 Derive α, β, and x_1 such that the following quadrature rule holds exactly for polynomials of degree less than or equal 2.

$$\int_0^2 f(x)dx \approx \alpha f(0) + \beta f(x_1).$$

Note that polynomials of degree two are specified by three coefficients and there are three unknowns α, β and x_1 to solve for. Solving for these unknowns such that polynomials of degree two are exact is equivalent to solving so that the the formula is exact for the functions $\{1, x, x^2\}$. Thus, we solve the system

$$\int_0^2 1\,dx = \alpha \cdot 1 + \beta \cdot 1 = 2,$$
$$\int_0^2 x\,dx = \alpha \cdot 0 + \beta \cdot x_1 = 2,$$
$$\int_0^2 x^2\,dx = \alpha \cdot 0^2 + \beta \cdot x_1^2 = 8/3.$$

Eliminating β from the second and third equations gives

$$\frac{2}{x_1} = \beta = \frac{8}{3x_1^2}.$$

Consequently, $x_1 = 4/3$. Substituting in the second equation implies $\beta = 2/x_1 = 3/2$. Now, solve the first equation for α in terms of β to obtain $\alpha = 2 - \beta = 2 - 3/2 = 1/2$. It follows that the desired quadrature formula is given by

$$\int_0^2 f(x)dx \approx \frac{1}{2} f(0) + \frac{3}{2} f(4/3).$$

14.4a Some quadrature problems can be solved by applying a suitable change of variables. Our strategies for quadrature break down when the interval of integration is not of finite length. Derive the following relationships for $f\colon \mathbf{R} \to \mathbf{R}$.

$$\int_{-\infty}^{\infty} f(x)dx = \int_{-1}^{1} f\Big(\frac{t}{1-t^2}\Big)\frac{1+t^2}{(1-t^2)^2}dt,$$
$$\int_{0}^{\infty} f(x)dx = \int_{0}^{1} \frac{f(-\log t)}{t}dt$$
$$\int_{c}^{\infty} f(x)dx = \int_{0}^{1} f\Big(c+\frac{t}{1-t}\Big)\frac{1}{(1-t)^2}dt.$$

How can these formulas be used to integrate over intervals of infinite length? What might be a drawback of evenly spacing t samples?

To obtain the first equation substitute

$$x = \frac{t}{1-t^2} \qquad \text{so that} \qquad dx = \frac{(1-t^2)-t(-2t)}{(1-t^2)^2}dt = \frac{1+t^2}{(1-t^2)^2}dt.$$

Since

$$\lim_{t\searrow -1}\frac{t}{1-t^2} = \lim_{t\searrow -1}\frac{t}{1-t}\,\frac{1}{1+t} = \frac{-1}{2}\cdot\infty = -\infty$$

and

$$\lim_{t\nearrow 1}\frac{t}{1-t^2} = \lim_{t\nearrow 1}\frac{t}{1+t}\,\frac{1}{1-t} = \frac{1}{2}\cdot\infty = \infty$$

the limits of integration transform as required and the result follows.

To obtain the second equation substitute

$$x = -\log t \qquad \text{so that} \qquad dx = -\frac{1}{t}dt.$$

Since

$$-\log t\Big|_{t=1} = -\log 1 = 0 \qquad \text{and} \qquad \lim_{t\searrow 0}\big(-\log t\big) = \infty$$

the limits of integration transform as required and we obtain

$$\int_0^\infty f(x)dx = \int_1^0 f(-\log t)\frac{-1}{t}dt = \int_0^1 \frac{f(-\log t)}{t}dt.$$

To obtain the third equation substitute

$$x = c + \frac{t}{1-t} \qquad \text{so that} \qquad dx = \frac{(1-t)-t(-1)}{(1-t)^2}dt = \frac{1}{(1-t)^2}dt.$$

Since

$$\Big(c+\frac{t}{1-t}\Big)\Big|_{t=0} = c \qquad \text{and} \qquad \lim_{t\nearrow 1}\Big(c+\frac{t}{1-t}\Big)\Big|_{t=0} = c+\infty = \infty$$

the limits of integration transform as required and the result follows.

These formulas can be used to integrate over intervals of infinite length because they transform infinite intervals of integration on the left side to finite intervals on the right side. Note, that the resulting integrals are still improper integrals and need to be interpreted as limits. For example,

$$\int_{-1}^{1} f\Big(\frac{t}{1-t^2}\Big)\frac{1+t^2}{(1-t^2)^2}dt = \lim_{\alpha\searrow -1}\lim_{\beta\nearrow 1}\int_{\alpha}^{\beta} f\Big(\frac{t}{1-t^2}\Big)\frac{1+t^2}{(1-t^2)^2}dt.$$

What this means from a practical point of view, is that the left and right endpoints of the transformed integral can't appear in the quadrature formula used to approximate the integral. Thus, it would be okay to use an open Newton–Cotes formula but not the closed Newton–Cotes formula for the approximation. Similarly, the Gaussian quadrature formula would be fine.

A drawback of using equally spaced t samples to perform the quadrature is that the derivatives of the integrand becomes larger at the endpoints due to the singularity there. Thus, the error bounds near the endpoints become large and more closely spaced samples in t be necessary to achieve the required tolerance. This difficulty could be overcome by using a recursive-adaptive method that further subdivides intervals based on error estimates.

14.5 The methods in this chapter for differentiation were limited to functions $f\colon \mathbf{R} \to \mathbf{R}$. Suppose $g\colon \mathbf{R}^n \to \mathbf{R}^m$. How would you use these techniques to approximate the Jacobian Dg? How does the timing of your approach scale with m and n?

Upon writing $g(x) = \big(g_1(x), g_2(x), \ldots, g_m(x)\big)$ and $x = (x_1, x_2, \ldots, x_n)$ we may write the Jacobian Dg as the matrix

$$Dg = \begin{bmatrix} \partial g_1/\partial x_1 & \partial g_1/\partial x_2 & \cdots & \partial g_1/\partial x_n \\ \partial g_2/\partial x_1 & \partial g_2/\partial x_2 & \cdots & \partial g_2/\partial x_n \\ \vdots & \vdots & \ddots & \vdots \\ \partial g_m/\partial x_1 & \partial g_m/\partial x_2 & \cdots & \partial g_m/\partial x_n \end{bmatrix}.$$

To approximate Dg it is sufficient to approximate each of the partial derivatives. This can be done, for example, using the centered difference approximation

$$\frac{\partial g_i(x)}{\partial x_j} \approx \frac{g_i(x+he_j) - g_i(x-he_j)}{2h}$$

where e_j denote the standard basis of $\mathbf{R}^n$ given by

$$e_1 = \begin{bmatrix} 1 \\ 0 \\ 0 \\ \vdots \\ 0 \end{bmatrix}, \quad e_2 = \begin{bmatrix} 0 \\ 1 \\ 0 \\ \vdots \\ 0 \end{bmatrix}, \quad e_3 = \begin{bmatrix} 0 \\ 0 \\ 1 \\ \vdots \\ 0 \end{bmatrix}, \quad \ldots, \quad e_n = \begin{bmatrix} 0 \\ 0 \\ 0 \\ \vdots \\ 1 \end{bmatrix}.$$

Note that any other method for approximating derivatives from the chapter could be adapted in a similar way to approximate partial derivatives.

The timing of this approach is as follows. Since each Jacobian matrix has $m \times n$ entries, then it takes $\mathcal{O}(mn)$ amount of computational effort to compute the entire matrix. The same estimate is obtained no matter what method is used to approximate the individual partial derivatives, provided the time needed to approximate each entry is is bounded by a constant independent of m and n.

14.10 Give examples of closed and open Newton-Cotes quadrature rules with negative coefficients for integrating $f(x)$ on $[0,1]$. What unnatural properties can be exhibited by these approximations?

For the closed formula the Maple worksheet

```
restart;
kernelopts(printbytes=false):
n:=8;
h:=1/n;
approx:=sum(w[k]*f(k*h),k=0..n);
eq:=int(f(x),x=0..1)=approx;
eqf:=unapply(eq,f);
eqs:={seq(eqf(x->x^k),k=0..n)};
vbls:={seq(w[k],k=0..n)};
solve(eqs,vbls);
```

yields the output

```
    |\^/|     Maple 9.5 (IBM INTEL LINUX)
._|\|   |/|_. Copyright (c) Maplesoft, a division of Waterloo Maple Inc. 2004
 \  MAPLE  /  All rights reserved. Maple is a trademark of
 <____ ____>  Waterloo Maple Inc.
      |       Type ? for help.
> restart;
> kernelopts(printbytes=false):
> n:=8;
                                     n := 8

> h:=1/n;
                                    h := 1/8

> approx:=sum(w[k]*f(k*h),k=0..n);
approx := w[0] f(0) + w[1] f(1/8) + w[2] f(1/4) + w[3] f(3/8) + w[4] f(1/2)

     + w[5] f(5/8) + w[6] f(3/4) + w[7] f(7/8) + w[8] f(1)

> eq:=int(f(x),x=0..1)=approx;
         1
        /
       |
eq :=  |   f(x) dx = w[0] f(0) + w[1] f(1/8) + w[2] f(1/4) + w[3] f(3/8)
       |
      /
        0
```

```
     + w[4] f(1/2) + w[5] f(5/8) + w[6] f(3/4) + w[7] f(7/8) + w[8] f(1)

> eqf:=unapply(eq,f);
               1
              /
             |
eqf := f ->  |   f(x) dx = w[0] f(0) + w[1] f(1/8) + w[2] f(1/4) + w[3] f(3/8)
             |
            /
              0

     + w[4] f(1/2) + w[5] f(5/8) + w[6] f(3/4) + w[7] f(7/8) + w[8] f(1)

> eqs:={seq(eqf(x->x^k),k=0..n)};
eqs := {1 = w[0] + w[1] + w[2] + w[3] + w[4] + w[5] + w[6] + w[7] + w[8], 1/2

     = 1/8 w[1] + 1/4 w[2] + 3/8 w[3] + 1/2 w[4] + 5/8 w[5] + 3/4 w[6]

     + 7/8 w[7] + w[8], 1/3 = 1/64 w[1] + 1/16 w[2] + 9/64 w[3] + 1/4 w[4]

       25                    49
     + -- w[5] + 9/16 w[6] + -- w[7] + w[8], 1/4 = 1/512 w[1] + 1/64 w[2]
       64                    64

       27                    125        27        343
     + --- w[3] + 1/8 w[4] + --- w[5] + -- w[6] + --- w[7] + w[8], 1/5 =
       512                   512        64        512

                                81                      625         81
    1/4096 w[1] + 1/256 w[2] + ---- w[3] + 1/16 w[4] + ---- w[5] + --- w[6]
                               4096                    4096        256

       2401                                                   243
     + ---- w[7] + w[8], 1/6 = 1/32768 w[1] + 1/1024 w[2] + ----- w[3]
       4096                                                 32768

                   3125         243         16807
     + 1/32 w[4] + ----- w[5] + ---- w[6] + ----- w[7] + w[8], 1/7 =
                   32768        1024        32768

                                   729                        15625
    1/262144 w[1] + 1/4096 w[2] + ------ w[3] + 1/64 w[4] + ------ w[5]
                                  262144                     262144
```

```
        729          117649
     + ---- w[6] + ------ w[7] + w[8], 1/8 = 1/2097152 w[1] + 1/16384 w[2]
        4096         262144

         2187                        78125         2187         823543
     + ------- w[3] + 1/128 w[4] + ------- w[5] + ----- w[6] + ------- w[7]
        2097152                     2097152       16384        2097152

                                                                6561
     + w[8], 1/9 = 1/16777216 w[1] + 1/65536 w[2] + -------- w[3] + 1/256 w[4]
                                                              16777216

         390625         6561         5764801
     + -------- w[5] + ----- w[6] + -------- w[7] + w[8]}
        16777216        65536        16777216

> vbls:={seq(w[k],k=0..n)};
         vbls := {w[0], w[1], w[2], w[3], w[4], w[5], w[6], w[7], w[8]}

> solve(eqs,vbls);
         989          2944          -464          5248          -454
{w[8] = -----, w[7] = -----, w[6] = -----, w[5] = -----, w[4] = ----,
        28350         14175         14175         14175         2835

           5248          -464           989          2944
    w[3] = -----, w[2] = -----, w[0] = -----, w[1] = -----}
           14175         14175         28350         14175

> quit
bytes used=2126536, alloc=1769148, time=0.05
```

which shows that the 9-point closed Newton–Cotes formula has negative weights

$$w_4 = w_6 = -\frac{464}{14175}.$$

For the open formula the Maple worksheet

```
restart;
kernelopts(printbytes=false):
n:=6;
h:=1/(n+1);
approx:=sum(w[k]*f((k+1/2)*h),k=0..n);
eq:=int(f(x),x=0..1)=approx;
eqf:=unapply(eq,f);
eqs:={seq(eqf(x->x^k),k=0..n)};
```

```
vbls:={seq(w[k],k=0..n)};
solve(eqs,vbls);
```

yields the output

```
    |\^/|     Maple 9.5 (IBM INTEL LINUX)
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 <____ ____>  Waterloo Maple Inc.
      |       Type ? for help.
> restart;
> kernelopts(printbytes=false):
> n:=6;
                                     n := 6

> h:=1/(n+1);
                                    h := 1/7

> approx:=sum(w[k]*f((k+1/2)*h),k=0..n);
approx := w[0] f(1/14) + w[1] f(3/14) + w[2] f(5/14) + w[3] f(1/2)

                             11            13
     + w[4] f(9/14) + w[5] f(--) + w[6] f(--)
                             14            14

> eq:=int(f(x),x=0..1)=approx;
         1
        /
       |
eq :=  |   f(x) dx = w[0] f(1/14) + w[1] f(3/14) + w[2] f(5/14) + w[3] f(1/2)
       |
      /
        0

                             11            13
     + w[4] f(9/14) + w[5] f(--) + w[6] f(--)
                             14            14

> eqf:=unapply(eq,f);
               1
              /
             |
eqf := f ->  |   f(x) dx = w[0] f(1/14) + w[1] f(3/14) + w[2] f(5/14)
             |
            /
```

```
              0

                                           11           13
     + w[3] f(1/2) + w[4] f(9/14) + w[5] f(--) + w[6] f(--)
                                           14           14

> eqs:={seq(eqf(x->x^k),k=0..n)};
eqs := {1 = w[0] + w[1] + w[2] + w[3] + w[4] + w[5] + w[6], 1/2 = 1/14 w[0]

                                                      11         13
     + 3/14 w[1] + 5/14 w[2] + 1/2 w[3] + 9/14 w[4] + -- w[5] + -- w[6], 1/3 =
                                                      14         14

                          25                     81         121
    1/196 w[0] + 9/196 w[1] + --- w[2] + 1/4 w[3] + --- w[4] + --- w[5]
                          196                    196        196

       169                              27          125
     + --- w[6], 1/4 = 1/2744 w[0] + ---- w[1] + ---- w[2] + 1/8 w[3]
       196                             2744        2744

       729         1331        2197                                 81
     + ---- w[4] + ---- w[5] + ---- w[6], 1/5 = 1/38416 w[0] + ----- w[1]
       2744        2744        2744                               38416

        625                      6561         14641        28561
     + ----- w[2] + 1/16 w[3] + ----- w[4] + ----- w[5] + ----- w[6], 1/6 =
       38416                     38416        38416        38416

                     243           3125                        59049
    1/537824 w[0] + ------ w[1] + ------ w[2] + 1/32 w[3] + ------ w[4]
                    537824        537824                       537824

       161051        371293                                  729
     + ------ w[5] + ------ w[6], 1/7 = 1/7529536 w[0] + ------- w[1]
       537824        537824                                7529536

        15625                      531441         1771561        4826809
     + ------- w[2] + 1/64 w[3] + ------- w[4] + ------- w[5] + ------- w[6]}
       7529536                     7529536        7529536        7529536

> vbls:={seq(w[k],k=0..n)};
               vbls := {w[0], w[1], w[2], w[3], w[4], w[5], w[6]}
```

```
> solve(eqs,vbls);
       4949          49          6223          -6257          6223
{w[6] = -----, w[5] = ----, w[4] = -----, w[3] = -----, w[2] = -----,
       27648         7680        15360          34560          15360

           49          4949
    w[1] = ----, w[0] = -----}
          7680         27648

> quit
bytes used=1968360, alloc=1638100, time=0.05
```

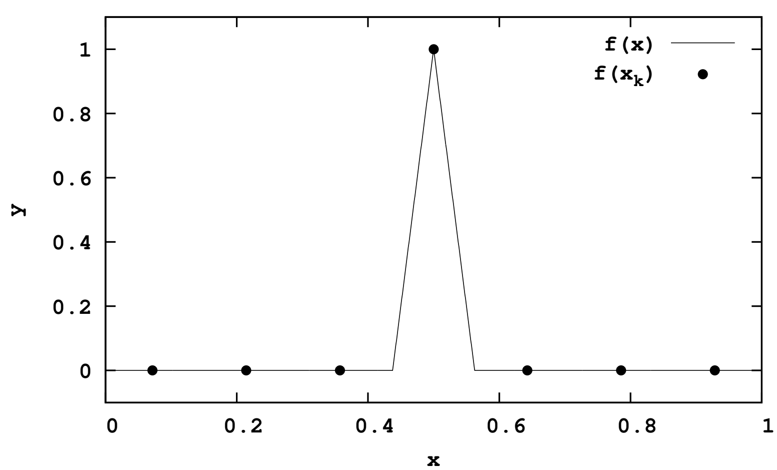
which shows that the 7-point open Newton–Cotes formula has the negative weight

$$w_3 = -\frac{6257}{34560}.$$

An unnatural property that quadrature approximations with negative weights can exhibit is the possibility of approximating the integral of a non-negative function by a negative number. For example, consider the non-negative function

$$f(x) = \begin{cases} 1 - |16x - 8| & \text{for } |x - 1/2| < 1/16 \\ 0 & \text{otherwise} \end{cases}$$

with graph



For this function the exact integral is

$$\int_0^1 f(x)dx = 1/16$$

whereas the 7-point open Newton–Cotes approximation yields the negative number

$$\sum_{k=0}^{6} w_k f(x_k) = w_3 = -\frac{6257}{34560}.$$

14.11 Provide a sequence of differentiable functions

$$f_k\colon [0,1] \to \mathbf{R} \qquad \text{and a function} \qquad f\colon [0,1] \to \mathbf{R}$$

such that as $k \to \infty$ the following limits hold:

$$\max_{x\in[0,1]} \big|f_k(x) - f(x)\big| \to 0 \qquad \text{and} \qquad \max_{x\in[0,1]} \big|f_k'(x) - f'(x)\big| \to \infty.$$

What does this example imply about numerical differentiation when function values are noisy? Is a similar counterexample possible for integration when f and the f_ks are integrable?

Consider the functions

$$f_k(x) = k^{-1}\sin(k^2 x) \qquad \text{and} \qquad f(x) = 0.$$

Then $|\sin(x)| \le 1$ implies

$$\big|f_k(x) - f(x)\big| = \big|k^{-1}\sin(k^2x) - 0\big| \le 1/k \to 0 \qquad \text{as} \qquad k \to \infty.$$

Differentiating yields

$$f_k'(x) = k\cos(k^2x) \qquad \text{and} \qquad f'(x) = 0.$$

Consequently

$$\big|f_k'(0) - f'(0)\big| = \big|k\cos(0) - 0\big| = k \to \infty \qquad \text{as} \qquad k \to \infty.$$

It follows that f_k and f satisfy the desired limits.

In the case that the function values are noisy with noise level ϵ, one might take $k > 1/\epsilon$ and imagine that f_k represents a noisy approximation of f such that

$$\big|f_k(x) - f(x)\big| < \epsilon \qquad \text{for every} \qquad x \in [0,1].$$

If f_k is used to obtain a numerical approximation of the derivative, then what we really have is an approximation of the derivative f_k'. However, since f_k' and f' are quite different, a good approximation of f_k' would be a bad approximation of f'.

There are no similar counterexamples possible for integration, because

$$\max_{x\in[0,1]} \big|f_k(x) - f(x)\big| < \epsilon$$

implies

$$\Big|\int_0^1 f_k(x)dx - \int_0^1 f(x)dx\Big| \le \int_0^1 \big|f_k(x) - f(x)\big|dx \le \int_0^1 \epsilon\, dx = \epsilon.$$

Therefore, as $\epsilon \to 0$ the difference in the integrals of f_k and f also tends to zero.