1. a) Consider the formula
\[ f(x, h) = \frac{f(x+h) - f(x-h)}{2h} \]
to approximate the derivative of a function \( f \). Assume we are able to evaluate \( f \) with about 5 decimal precision. Assume, further, that \( f'''(1) \approx 1 \). What is the best value of \( h \) to approximate the derivative?

**Solution.** We have
\[ f'(x) = f(x, h) + c_1 h^2 + c_2 h^4 \ldots \]
We are able to evaluate \( f(x) \) with 5 decimal precision, i.e., with an error of \( 5 \cdot 10^{-6} \). Thus, the (absolute value of the maximum) error in evaluating \( \frac{f(x+h) - f(x-h)}{2h} \) is \( 5 \cdot 10^{-6} / h \). So the total error (roundoff error plus truncation error) in evaluating \( f'(x) \) is
\[ \frac{5 \cdot 10^{-6}}{h} + \frac{f'''(x)}{6} h^2 \approx \frac{5 \cdot 10^{-6}}{h} + h^2 / 6, \]
as \( f'''(x) \approx 1 \). The derivative of the right-hand side with respect to \( h \) is
\[ - \frac{5 \cdot 10^{-6}}{h^2} + \frac{h}{3}. \]
Equating this with 0 gives the place of minimum error when \( h^3 = 15 \cdot 10^{-6} \), i.e., \( h \approx 0.0246 \).

b) Given a certain function \( f \), we are using the formula
\[ f(x, h) = \frac{f(x+h) - f(x-h)}{2h} \]
to approximate its derivative. We have
\[ \tilde{f}(1, 0.1) = 5.135, 466, 136 \quad \text{and} \quad \tilde{f}(1, 0.2) = 5.657, 177, 752 \]
Using Richardson extrapolation, find a better approximation for \( f'(1) \).

**Solution.** We have
\[ f'(x) = \tilde{f}(x, h) + c_1 h^2 + c_2 h^4 \ldots \]
\[ f'(x) = \tilde{f}(x, 2h) + c_1 (2h)^2 + c_2 (2h)^4 \ldots \]
with some \( c_1, c_2, \ldots \). Multiplying the first equation by 4 and subtracting the second one, we obtain
\[ 3f'(x) = 4\tilde{f}(x, 2h) - \tilde{f}(x, h) + 12 c_2 h^4 + \ldots . \]
That is, with \( h = 0.1 \) we have
\[ f'(x) \approx \frac{4\tilde{f}(x, h) - \tilde{f}(x, 2h)}{3} \approx \frac{4 \cdot 5.135, 466, 136 - 5.657, 177, 752}{3} = 4.961, 56 \]
The function in the example is \( f(x) = x \tan x \) and \( f'(1) = 4.982, 93 \).

2. We want to evaluate
\[ \int_{-1}^{1} e^{1/x} \, dx \]

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1 All computer processing for this manuscript was done under Fedora Linux. *AMSTeX* was used for typesetting.
using the composite trapezoidal rule with three decimal precision, i.e., with an error less than $5 \cdot 10^{-4}$. What value of $n$ should one use when dividing the interval $[1, 2]$ into $n$ parts?

**Solution.** The error term in the composite Simpson formula when integrating $f$ on the interval $[a, b]$ and dividing the interval into $2n$ parts is

$$\frac{(b-a)^3}{12n^2} f''(\xi)$$

with some $\xi \in (a, b)$. We want to use this with $a = 1$, $b = 2$, and $f(x) = e^{1/x}$. We have

$$f''(x) = (2x^{-3} + x^{-4})e^{1/x}.$$  

This function is decreasing on the interval $[1, 2]$ (because both factors are decreasing). Hence it assumes its maximum at the left end point, that is, at $x = 1$. We have $f''(1) = 3e \approx 8.154, 846$. Since $f''(x) > 0$ on $[1, 2]$, we therefore have $|f''(x)| < 3e$ for $x \in (1, 2)$. So, noting that $a = 1$ and $b = 2$, the absolute value of the error is

$$\frac{(b-a)^3}{12n^2}|f''(\xi)| = \frac{1}{12n^2} |f''(\xi)| < \frac{3e}{12n^2} = \frac{e}{4n^2}.$$  

In order to ensure that this error is less than $5 \cdot 10^{-4}$, we need to have $e/(4n^2) < 5 \cdot 10^{-4}$, i.e.,

$$n > \sqrt{500e} \approx \sqrt{1359.141} \approx 36.87.$$  

So one needs to make sure that $n \geq 37$. Thus one needs to divide the interval $[1, 2]$ into (at least) 37 parts in order to get the result with 4 decimal precision while using the trapezoidal rule.

3. We would like to evaluate the integral

$$\int_0^4 \sqrt{1 + x^3} \, dx$$

with a precision of $\epsilon = 5 \cdot 10^{-4}$ using the adaptive Simpson Rule. Writing $f(x) = \sqrt{1 + x^3}$, on the interval $[2, 3]$ we find that

$$S_{[2,3]} = \frac{1}{6} \left( f(2) + 4f \left( \frac{2}{2} \right) + f(3) \right) \approx 4.100, 168, 175.$$  

and

$$S_{[2,2\frac{1}{4}]} + S_{[2\frac{1}{4}, 3]} = \frac{1}{12} \left( f(2) + 4f \left( \frac{2}{4} \right) + 2f \left( \frac{2}{2} \right) + 4f \left( \frac{3}{4} \right) + f(3) \right) = 4.100, 102, 756.$$  

Do we have to subdivide the interval $[2, 3]$ further or the result is already precise enough. *Justify your answer.*

**Solution.** The error allowed on the interval $[2, 3]$ is $\epsilon/4 = 1.25 \cdot 10^{-4}$. The error can be estimated as

$$\frac{1}{15} \left( S_{[2,2\frac{1}{4}]} + S_{[2\frac{1}{4}, 3]} - S_{[2,3]} \right) \approx \frac{4.100, 102, 756 - 4.100, 168, 175}{15} = -0.363, 27 \cdot 10^{-6}.$$  

This is considerably smaller in absolute value than the permissible error, so the interval does not need to be further subdivided; one can accept $S_{[2,2\frac{1}{4}]} + S_{[2\frac{1}{4}, 3]} = 4.100, 102, 756$ as the integral on this interval.

4.a) In estimating the error of the trapezoidal rule and Simpson’s rule, the following lemma was used.

**Lemma.** Let $g(x) \geq 0$ for all $x \in [a, b]$. Assume $f$ is differentiable on $(a, b)$, and for each $x \in [a, b]$ we have $\xi_x \in (a, b)$. Then there is an $\eta \in (a, b)$ such that

$$\int_a^b f'(\xi_x)g(x) \, dx = f'(\eta) \int_a^b g(x) \, dx.$$  

provided that the integrals on both sides of this equation exist.

Briefly outline the proof of this lemma.

Solution. We may assume that \( \int_a^b g(x) \, dx \neq 0 \). Indeed, if \( \int_a^b g = 0 \) then both integrals in the above equation are zero, so the equation holds with any \( \eta \in (a, b) \).\(^2\) Assume \( m < f'(x) < M \) for all \( x \in (a, b) \), where we allow \( m = -\infty \) and \( M = +\infty \), if \( f' \) is not bounded. Then

\[
m \int_a^b g(x) \, dx < \int_a^b f'(\xi_x) g(x) \, dx < M \int_a^b g(x) \, dx,
\]
or else

\[
\int_a^b f'(\xi_x) g(x) \, dx = H \int_a^b g(x) \, dx,
\]

with some \( H \) with \( m < H < M \). In fact, one only needs to take

\[
H = \frac{\int_a^b f'(\xi_x) g(x) \, dx}{\int_a^b g(x) \, dx}.
\]

Since the derivative satisfies the Intermediate Value Property,\(^3\) it is easy to conclude that we have \( H = f'(\eta) \) for some \( \eta \in (a, b) \). Hence above Lemma follows.

b) Describe how to deal with the singularity in the integral

\[
\int_0^1 x^{-1/2} e^{-x^2} \, dx
\]

if one wants to evaluate this integral using Simpson’s rule.

Solution. One can subtract the singularity by taking an initial segment of the Taylor series at \( x = 0 \) of \( e^{-x^2} \). We have

\[
e^x = \sum_{n=0}^{\infty} \frac{x^n}{n!};
\]

this Taylor series is convergent on the whole real line. Therefore, we have

\[
e^{-x^2} = 1 - x^2 + \frac{x^4}{2} + O(x^6),
\]

where the symbol \( O(\cdot) \) is meant as \( x \to 0 \). Hence

\[
x^{-1/2} \left( e^{-x^2} - 1 + x^2 - \frac{x^4}{2} \right) = O(x^{6-1/2}) = O(x^{11/2}).
\]

\(^2\)To show that

\[
\int_a^b f'(\xi_x) g(x) \, dx = 0
\]

assuming

\[
\int_a^b g(x) \, dx = 0
\]

is a little messy when one works with the Riemann integral, but quite easy if one works with the Lebesgue integral, the latter being a generalization of the Riemann integral, in common use in modern mathematics. We cannot go into details here.

\(^3\)Let \( \phi \) be a real-valued function whose domain includes the interval \( I \). We say that \( \phi \) satisfies the Intermediate Value Property on \( I \) if for any two points \( x_1 < x_2 \) in \( I \) and for any real number \( c \) with \( \phi(x_1) < c < \phi(x_2) \) or with \( \phi(x_1) > c > \phi(x_2) \) there is a \( \xi \in (x_1, x_2) \) such that \( \phi(\xi) = c \). This property is to be distinguished from the Intermediate Value Theorem. This theorem says that a function continuous on an interval satisfies the Intermediate Value Property on this interval. The result we are using about derivatives says that if \( f \) is differentiable on the interval \( I \) then \( f' \) satisfies the Intermediate Value Property on \( I \) – note that \( f' \) need not be continuous for this.

3
The fourth derivative of this near \( x = 0 \) is \( O(x^{3/2}) \); that is, the fourth derivative tends to zero when \( x \searrow 0 \). So the fourth derivative is bounded on \((0, 1)\), the interval of integration; therefore, Simpson’s rule can be used to calculate the integral. To sum up, we have

\[
\int_0^1 x^{-1/2} e^{-x^2} \, dx = \int_0^1 x^{-1/2} \left( e^{-x^2} - 1 + x^2 - \frac{x^4}{2} \right) \, dx + \int_0^1 \left( x^{-1/2} - x^{3/2} + \frac{x^7/2}{2} \right) \, dx.
\]

The first integral on the right-hand side can be calculated by Simpson’s rule (at \( x = 0 \) take the integrand to be 0), and the second integral can be evaluated directly, by calculating the integral explicitly.

5. a) Write a second order Taylor approximation for the solution \( y(x) \) at \( x = 3 + h \) of the differential equation \( y' = x + y^3 \) with initial condition \( y(3) = 1 \) (i.e., the error term in expressing \( y(3 + h) \) should be \( O(h^3) \)).

**Solution.** We have \( y(3) = 1, \ y'(3) = x + y^3 = 4 \); the right-hand side was obtained by substituting \( x = 3 \) and \( y = 1 \). Differentiating, then using the equation \( y' = x + y^2 \), and again substituting \( x = 3 \) and \( y = 1 \), we obtain

\[
y''(x) = (x + y^3)' = 1 + 3y^2 y' = 1 + 3y^2(x + y^3) = 1 + 3xy^2 + 3y^5 = 13.
\]

Hence

\[
y(3 + h) = y(3) + y'(3)h + y''(3) \frac{h^2}{2} + O(h^3) = 1 + 4h + \frac{13}{2} h^2 + O(h^3)
\]

for \( h \) near 0.

b) Consider the differential operators

\[
D_1 = h \frac{\partial}{\partial x} + k \frac{\partial}{\partial y} \quad \text{and} \quad D_2 = \frac{\partial}{\partial x} + f \frac{\partial}{\partial y},
\]

where \( h \) and \( k \) are fixed numbers, and \( f \) is a function of the variables \( x \) and \( y \) all whose partial derivatives (of any order) are continuous. These operators are to be applied to functions \( g \) of the variables \( x \) and \( y \) all whose partial derivatives (of any order) are continuous. Explain why one can use the Binomial Theorem to calculate \( D_1^n \), where \( n \) is a positive integer, while one cannot apply the Binomial Theorem to calculate \( D_2^n \). Do not do detailed calculation, just clearly describe the main reason.

**Solution.** The proof of Binomial Theorem saying that

\[
(A + B)^n = \sum_{k=0}^{n} \binom{n}{k} A^{n-k} B^k
\]

for the elements \( A \) and \( B \) of a ring\(^4\) makes use of the assumption that \( A \) and \( B \) commute (i.e., that \( AB = BA \)). The differential operators \( h \frac{\partial}{\partial x} \) and \( k \frac{\partial}{\partial y} \) forming \( D_1 \) commute,\(^5\) so the Binomial Theorem is applicable with \( D_1 \), while the differential operators \( \frac{\partial}{\partial x} \) and \( f \frac{\partial}{\partial y} \) do not commute, so the Binomial Theorem is not applicable with \( D_2 \).

**Note:** A more general situation involving differential operators when the Binomial Theorem is applicable is the following: let \( f \) and \( g \) be functions of one variable that are differentiable any number of times. Then the differential operators \( f(x) \frac{\partial}{\partial x} \) and \( g(y) \frac{\partial}{\partial y} \) commute when applied to functions all whose partial derivatives (of any order) are continuous. Hence, the Binomial Theorem can be used to evaluate

\[
D_3 = \left( f(x) \frac{\partial}{\partial x} + g(y) \frac{\partial}{\partial y} \right)^n
\]

\(^4\)The differential operators described generate a ring.

\(^5\)The assumption that these operators are applied to functions whose higher order derivatives are continuous is needed to make sure that in evaluating mixed partial derivatives the order of evaluation makes no difference.
for a positive integer $n$.

We need to assume that the higher order derivatives of $f$ and $g$ exist since higher order derivatives $f$ and $g$ will occur when expressing powers of $D_3$ with the Binomial Theorem. The continuity of these derivatives are also needed so the differential operators $\frac{\partial}{\partial x}$ and $\frac{\partial}{\partial y}$ can be interchanged when applied to expressions that involve various derivatives of $f(x)$ and $g(y)$.

More subtle considerations omitted here show in order to apply the Binomial Theorem to calculate $D_3^n$, the existence of $f^{(n-1)}$ and $g^{(n-1)}$ are needed, but the continuity of these derivatives are not needed. Since differentiability implies continuity, $f^{(k)}$ and $g^{(k)}$ will be continuous for any $k$ with $0 \leq k < n$ in this case.