5 Numerical Integration & Differentiation

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Outline of Chapter 5

1. **The Trapezoidal and Simpson Rules**
2. **Error Formulas**
3. **Gaussian Numerical Integration**
4. **Numerical Differentiation**

- Why do we need numerical methods for evaluating the definite integrals? Recall the F.T. Calculus part II:

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

where $F' = f$. Most integrals cannot be applied by the F.T., because finding their antiderivatves is generally impossible over the elementary calculus. The examples of such integrals are

$$\int_0^{\pi/2} \frac{\sin x}{x}\,dx, \quad \int_0^1 e^{-x^2}\,dx.$$

Those integrals will be approximated by the **T. R., S. R., G. N. I,** ... .

- In this section, two numerical integrations (**quadratures**) will be discussed: one is the **trapezoidal rule** and the other is the **Simpson rule**.
- The **trapezoidal rule** is based on using **a piecewise linear** interpolation and **Simpson rule** is on using **a piecewise quadratic** interpolation.
- Consider the following definite integral:

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

$I(f)$ will be the actual value for the integral. It will be approximated by the two rules.

- **Trapezoid Rule**

Consider the approximation of $I(f)$ by $T_1(f)$:

$$T_1(f) = (b-a)\frac{f(a)+f(b)}{2}.$$

Note that subindex 1 means that one trapezoid is considered in one interval. We can see that $T_1(f)$ is the area of the trapezoid.

Example1

The function $f(x) = 1/(2x+1)$ on $[0, 1]$. Then
1. find $I(f)$ and $T_1(f)$.
2. find the absolute error $|I(f) - T_1(f)|$.

- **How do we obtain greater accuracy?** The answer is to split the interval $[a, b]$ into small subintervals and consider a linear interpolation on each subinterval. This is called the **composite trapezoidal rule.** So we can consider $T_n(f)$ with n subintervals.

Example2

1. Evaluate $T_2(f)$ for the function $f(x)$ in Example 1. Note that we use the same length of subintervals.
2. Find the absolute error $|I(f) - T_2(f)|$. Do you have better accuracy than $T_1(f)$?

- Let $h = (b-a)/n$. Then the endpoints of the subintervals are $x_i = a + i\,h$ for $i = 0, 1, 2, \cdots, n$. We can derive the general formula for the composite trapezoidal rule:

$$
\begin{aligned}
T_n(f) = h & \left[\left(\frac{1}{2} f(a) + \frac{1}{2} f(x_1) \right) + \left(\frac{1}{2} f(x_1) + \frac{1}{2} f(x_2) \right) + \right. \\
& \left. \cdots \left(\frac{1}{2} f(x_{n-2}) + \frac{1}{2} f(x_{n-1}) \right) + \left(\frac{1}{2} f(x_{n-1}) + \frac{1}{2} f(b) \right) \right] \\
&= h \left[\frac{1}{2} f(a) + f(x_1) + f(x_2) + \cdots + f(x_{n-1}) + \frac{1}{2} f(b) \right] \\
&= \frac{h}{2} \left(f(x_0) + f(x_n) + 2 \sum_{i=1}^{n-1} f(x_i) \right).
\end{aligned}
$$

Simpson Rule

To develop the Simpson Rule, we consider two examples:

1. For the quadratic interpolation $p\ ((-h,0),(0,1),(h,0))$,
$$\int_{-h}^{h} p(x)dx = \frac{4}{3}h.$$
2. For the quadratic interpolation $p\ ((-h,1),(0,0),(h,0))$ or $((-h,0),(0,0),(h,1))$,
$$\int_{-h}^{h} p(x)dx = \frac{1}{3}h.$$

Let $P_2(x)$ be the quadratic polynomial that interpolates the actual function $f(x)$ at $x = a$, $c = (a+b)/2$, b. Then we can obtain

$$I(f) \approx S_2(f) = \int_a^b P_2(x)\,dx = \frac{h}{3}\left[f(a) + 4f\left(\frac{a+b}{2}\right) + f(b)\right].$$

Example3

1. Find $S_2(f)$ for the function $f(x) = 1/(2x+1)$ on $[0,1]$.
2. Find the absolute error $|I(f) - S_2(f)|$

- **Composite Simpson Rule**

Let $h = (b-a)/n$ with **even** integers n. Then the evaluation points for the actual function $f(x)$ are given by

$$x_i = a + i\,h \quad \text{for } i = 0, 1, 2, \cdots, n.$$

We can derive the general formula for the composite Simpson rule:

$$\begin{aligned} S_n(f) &= \frac{h}{3}\left[(f(x_0) + 4f(x_1) + f(x_2)) + (f(x_2) + 4f(x_3) + f(x_4)) \cdots \right. \\ &\quad \left. + (f(x_{n-2}) + 4f(x_{n-1}) + f(x_n))\right] \\ &= \frac{h}{3}\left[f(x_0) + 4f(x_1) + 2f(x_2) + 4f(x_3) + 2f(x_4) \cdots \right. \\ &\quad \left. + 2f(x_{n-2}) + 4f(x_{n-1}) + f(x_n)\right]. \end{aligned}$$

Example4

1. Find $S_4(f)$ for the function $f(x) = 1/(2x+1)$ on $[0, 1]$.
2. Find the absolute error $|I(f) - S_4(f)|$

- **Scilab codes for Composite Trapezoidal Rule**

```
// a and b are endpoints
// n is the number of subintervals
// func is a integrand
function approx = trapez(a,b,n,func)
  h = (b-a)/n; sum_trap = 0; // initialize for trapezoidal rule
    for i = 1:n
      sum_trap = sum_trap + func(a+(i-1)*h) + func(a+i*h);
    end
  approx = sum_trap*h/2;
endfunction
////////////////////////////////////////////////////
// This is a test function
function value = f(x)
  value = sin(x);
endfunction
```

1. **Scilab codes for Composite Simpson Rule**

```
// a and b are endpoints
// n is the number of subintervals. Note that n must be even.
// func is a integrand
function approx = simpson(a,b,n,func)
  h = (b-a)/n; sum_int = 0; // initialize for Simpson rule
  for i = 1:n/2
    sum_int = sum_int + func(a+2*(i-1)*h) + ...
          4*func(a+(2*(i-1)+1)*h) + func(a+(2*(i-1)+2)*h);
  end
  approx = sum_int*h/3;
endfunction
/////////////////////////////////////////////////////
// This is a test function
function value = f(x)
  value = 1/x;
endfunction
```

- Using your Scilab code,
  (1) find $T_n(f)$ and $S_n(f)$ for $n = 10, 20, 100$.
  (2) find their errors for $n = 10, 20, 100$.
  (3) discuss your numerical results.

1. The actual value of $I(f)$ is given by

$$\int_0^{\pi} e^x \cos(4x)dx = \frac{e^{\pi} - 1}{17}.$$

2. The actual value of $I(f)$ is given by

$$\int_0^{\pi/4} e^{\cos x} dx \doteq 1.939735.$$