Math 541 - Numerical Analysis

Lecture Notes – Quadrature – Part A

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Outline

SDSU

Definite Integral

Theorem (Fundamental Theorem of Calculus)

Let $f(x)$ be a continuous function on the interval $[a, b]$ and assume that $F(x)$ is any ***antiderivative*** *of $f(x)$. The* ***definite integral****, which gives the* ***area under the curve*** *of $f(x)$ between a and b, satisfies the following formula:*

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

- Finding integrals was a significant part of Calculus
- Developed many techniques for solving a variety of integrals
- Many integrals are impossible to solve with classic techniques
- We need **numerical methods** to evaluate these **definite integrals**

Definition of Riemann Integral

Definition of Riemann Integral: The standard integral from Calculus is the **Riemann Integral**

- Let $f(x)$ be a continuous function in the interval $[a, b]$
- Partition the interval $[a, b]$ into n subintervals $[x_{i-1}, x_i]$ with $\Delta x_i = x_i - x_{i-1}$ and Δx_k being the largest
- Let c_i be some point in the subinterval $[x_{i-1}, x_i]$
- The n^{th} **Riemann sum** is given by

$$S_n = \sum_{i=1}^{n} f(c_i) \Delta x_i$$

- The **Riemann integral** is defined by

$$\int_a^b f(x)dx = \lim_{\Delta x_k \to 0} \sum_{i=1}^{n} f(c_i) \Delta x_i$$

Midpoint Rule 1

The **Midpoint Rule** is based directly on the **definition of the Riemann integral**.

Suppose that we want to approximate the area under some continuous function $f(x)$ between $x = a$ and $x = b$

- Divide the interval $[a, b]$ into a number of small intervals
- Assume there are n evenly spaced intervals (which Riemann sums do not require this restriction)
- Evaluate the function, $f(x)$, at the midpoint of any subinterval
- Technically, it is important in the definition of the Riemann integral that one chooses arbitrarily any point in the interval, but that is left to other analysis courses

Midpoint Rule

The **Midpoint Rule** is given by the following:

- Let $x_0 = a$ and $x_n = b$ and define $\Delta x = \frac{b-a}{n}$ with $x_i = a + i\Delta x$ for $i = 0, ..., n$
- This **partitions the interval** $[a, b]$ into n subintervals $[x_{i-1}, x_i]$ each with length Δx
- The height of the approximating rectangle is found by evaluating the function at the **midpoint**, $c_i = \frac{x_i + x_{i-1}}{2}$
- The **area of the rectangle**, R_i, over the interval $[x_{i-1}, x_i]$ is given by its height times its width or

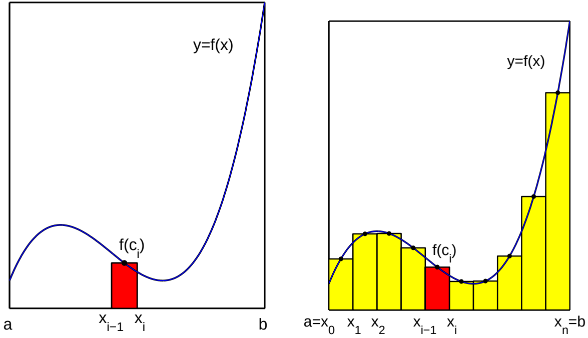
$$R_i = f(c_i)\Delta x$$

- The area under $f(x)$ is approximated by adding the areas of the rectangles

$$S_n = \sum_{i=1}^{n} f(c_i)\Delta x \approx \int_a^b f(x)dx$$

Midpoint Rule

Figures below show a single rectangle in computing area of the **Riemann Integral** and all of the rectangles using the **Midpoint Rule** for approximating the area under the curve



Midpoint Rule

Riemann Sums and Riemann Integral

- The **Midpoint Rule** described above is a specialized form of **Riemann sums**
- The more general form of Riemann sums allows the subintervals to have varying lengths, Δx_i
- The choice of where the function is evaluated need not be at the midpoint as described above
- The **Riemann integral** is defined using a limiting process, similar to the one described above

Area under a Curve 1

Area under a Curve: Consider the function

$$f(x) = x^3 - 6\,x^2 + 9\,x + 2 \qquad \text{for} \quad x \in [0,5]$$

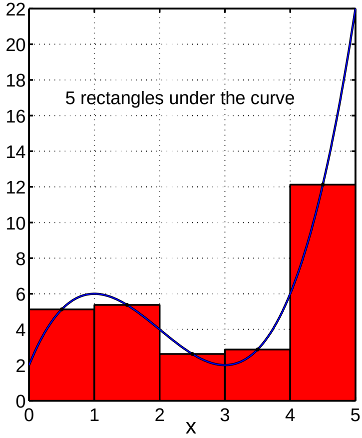
From the **Fundamental Theorem of Calculus** the area under the curve is

$$A_* = \int_0^5 f(x)dx = \frac{x^4}{4} - 2x^3 + \frac{9x^2}{2} + 2x\Big|_0^5 = 28.75$$

- Approximate area with rectangles under the curve
- Divide the interval $x \in [0,5]$ into even intervals
- Use the midpoint of the interval to get height of the rectangle
- Examine approximation as intervals get smaller

Area under a Curve 2

Area under a Curve Divide $x \in [0, 5]$ into 5 intervals



Area under a Curve 3

Area under a Curve: Height of rectangles from the function

$$f(x) = x^3 - 6\,x^2 + 9\,x + 2 \qquad \text{for} \quad x \in [0,5]$$

- Width of the rectangles are $\Delta x = 1$
- Height of rectangles evaluated at midpoints
- Approximate area satisfies

$$A_1 \approx \left(f\left(\tfrac{1}{2}\right) + f\left(\tfrac{3}{2}\right) + f\left(\tfrac{5}{2}\right) + f\left(\tfrac{7}{2}\right) + f\left(\tfrac{9}{2}\right)\right)\Delta x = \sum_{i=0}^{4} f\left(i + \tfrac{1}{2}\right)\cdot 1$$

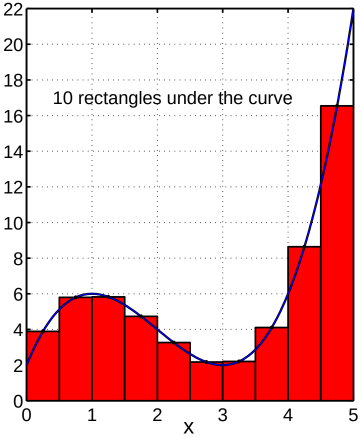
- This gives

$$A_1 \approx \sum_{i=0}^{4}\left(\left(i+\tfrac{1}{2}\right)^3 - 6\left(i+\tfrac{1}{2}\right)^2 + 9\left(i+\tfrac{1}{2}\right) + 2\right) = 28.125$$

- This is 2.17% less than the actual area

Area under a Curve

Area under a Curve Divide $x \in [0, 5]$ into 10 intervals



Area under a Curve

Area under a Curve: Height of rectangles from the function

$$f(x) = x^3 - 6\,x^2 + 9\,x + 2 \qquad \text{for} \quad x \in [0, 5]$$

- Width of the rectangles are $\Delta x = \frac{1}{2}$
- Height of rectangles evaluated at midpoints
- Approximate area satisfies

$$A_2 \approx \sum_{i=0}^{9} f\left(\tfrac{i}{2} + \tfrac{1}{4}\right)\Delta x$$

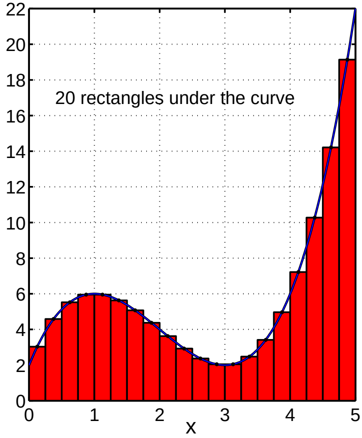
- This gives

$$A_2 \approx \frac{1}{2}\sum_{i=0}^{9}\left(\left(\tfrac{i}{2} + \tfrac{1}{4}\right)^3 - 6\left(\tfrac{i}{2} + \tfrac{1}{4}\right)^2 + 9\left(\tfrac{i}{2} + \tfrac{1}{4}\right) + 2\right) = 28.59375$$

- This is 0.543% less than the actual area

Area under a Curve

Area under a Curve Divide $x \in [0, 5]$ into 20 intervals



Area under a Curve

Area under a Curve: Height of rectangles from the function

$$f(x) = x^3 - 6\,x^2 + 9\,x + 2 \qquad \text{for} \quad x \in [0,5]$$

- Width of the rectangles are $\Delta x = \frac{1}{4}$
- Height of rectangles evaluated at midpoints
- Approximate area satisfies

$$A_3 \approx \sum_{i=0}^{19} f\left(\frac{i}{4} + \frac{1}{8}\right)\Delta x$$

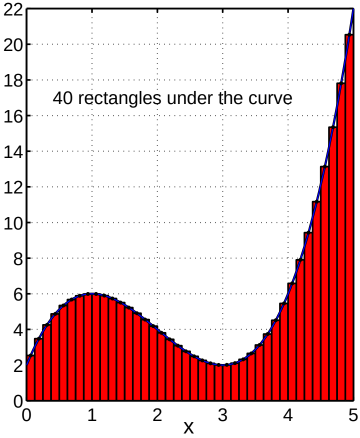
- This gives

$$A_3 \approx \frac{1}{4}\sum_{i=0}^{19}\left(\left(\frac{i}{4}+\frac{1}{8}\right)^3 - 6\left(\frac{i}{4}+\frac{1}{8}\right)^2 + 9\left(\frac{i}{4}+\frac{1}{8}\right) + 2\right) = 28.7109$$

- This is 0.135% less than the actual area

Area under a Curve

Area under a Curve Divide $x \in [0, 5]$ into 40 intervals



Area under a Curve

Area under a Curve: Height of rectangles from the function

$$f(x) = x^3 - 6\,x^2 + 9\,x + 2 \qquad \text{for} \quad x \in [0,5]$$

- Width of the rectangles are $\Delta x = \frac{1}{8}$
- Height of rectangles evaluated at midpoints
- Approximate area satisfies

$$A_4 \approx \sum_{i=0}^{39} f\left(\tfrac{i}{8} + \tfrac{1}{16}\right)\Delta x$$

- This gives

$$A_4 \approx \frac{1}{8}\sum_{i=0}^{39}\left(\left(\tfrac{i}{8} + \tfrac{1}{16}\right)^3 - 6\left(\tfrac{i}{8} + \tfrac{1}{16}\right)^2 + 9\left(\tfrac{i}{8} + \tfrac{1}{16}\right) + 2\right) = 28.7402$$

- This is 0.034% less than the actual area

Area under a Curve

Area under a Curve: The actual area is,

$$A_* = \int_0^5 f(x)dx = 28.75$$

The approximate areas were

$\Delta x_1 = 1$	$\Delta x_2 = \frac{1}{2}$	$\Delta x_3 = \frac{1}{4}$	$\Delta x_4 = \frac{1}{8}$
$A_1 = 28.125$	$A_2 = 28.59375$	$A_3 = 28.7109$	$A_4 = 28.7402$

The error ratio for this example is

$$\frac{|A_{n+1} - A_*|}{|A_n - A_*|} \approx 0.25$$

Thus, as the stepsize decreases by $\frac{1}{2}$, the error in the approximate area decreases by a factor of $\frac{1}{4}$

We will demonstrate that the error of the **Midpoint Rule** is $\mathcal{O}((\Delta x)^2)$, depending on the stepsize

Numerical Methods for Integration

Numerical Methods for Integration

- As noted before, many integrals cannot be solved exactly, so **numerical methods** need to be used to estimate **definite integrals**

$$\int_a^b f(x)dx$$

- The **Midpoint Rule** is an approximation based on the definition of a **Riemann integral**
- The **Midpoint Rule** is **NOT** a very efficient way to estimate the area under the curve
- Once again we turn to **polynomials** to approximate our functions and improve the convergence of the **numerical routine** to the actual value of the **definite integral**

Interpolation and Polynomial Approximation

Interpolation and Polynomial Approximation

- Polynomials provide "nice" smooth functions for approximations
- **Taylor's series** give excellent estimates near a point
- For integration, we need to extend over an interval
- **Interpolating polynomials** have many applications to fit functions or data at various x values

Weierstrass Approximation Theorem

The following theorem is the basis for polynomial approximation:

Theorem (Weierstrass Approximation Theorem)

Suppose $f \in C[a,b]$. Then for every $\epsilon > 0$ there exists a polynomial $P(x): \ |f(x) - P(x)| < \epsilon$, for all $x \in [a,b]$.

Note: The bound is *uniform*, *i.e.*, valid for all x in the interval.

Note: The theorem says nothing about how to find the polynomial, or about its order.

Illustrated: Weierstrass Approximation Theorem

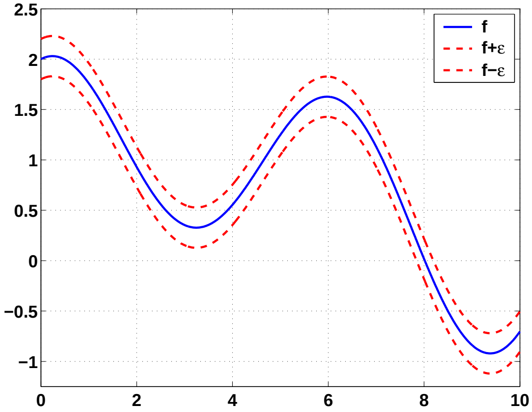


Figure: Weierstrass approximation Theorem guarantees that we (maybe with substantial work) can find a polynomial which fits into the "tube" around the function f, no matter how thin we make the tube.

Candidates: the Taylor Polynomials???

Natural Question:

Are our old friends, the Taylor Polynomials, good candidates for polynomial interpolation?

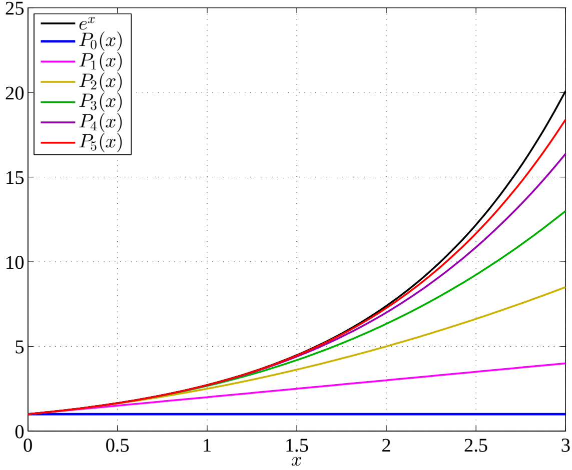
Answer:

No. The Taylor expansion works very hard to be accurate in the neighborhood of *one point*. But we want to fit data at many points (in an extended interval).

[Next slide: The approximation is great near the expansion point $x_0 = 0$, but get progressively worse at we get further away from the point, even for the higher degree approximations.]

Taylor Approximation of e^x on the Interval $[0, 3]$

We learned that e^x outgrows any polynomial



Interpolation: Lagrange Polynomials

Idea: Instead of working hard at *one point*, we will prescribe a number of points through which the polynomial must pass.

Consider a function that passes through the points $(x_0, f(x_0))$ and $(x_1, f(x_1))$. From techniques of algebra, we have the slope

$$m = \frac{f(x_1) - f(x_0)}{x_1 - x_0},$$

so the point slope form of a line gives

$$y(x) - f(x_0) = \frac{f(x_1) - f(x_0)}{x_1 - x_0}(x - x_0).$$

This is rearranged to give

$$\begin{aligned} y(x) &= \frac{f(x_1) - f(x_0)}{x_1 - x_0}(x - x_0) + f(x_0), \\ y(x) &= f(x_1)\frac{(x - x_0)}{x_1 - x_0} + f(x_0)\frac{(x - x_0)}{x_0 - x_1} + f(x_0)\frac{(x_0 - x_1)}{x_0 - x_1}, \\ y(x) &= f(x_1)\frac{(x - x_0)}{x_1 - x_0} + f(x_0)\frac{(x - x_1)}{x_0 - x_1}, \end{aligned}$$

Interpolation: Lagrange Polynomials

From the previous slide we have:

$$y(x) = f(x_1)\frac{(x-x_0)}{x_1-x_0} + f(x_0)\frac{(x-x_1)}{x_0-x_1}.$$

If we define:

$$L_0(x) = \frac{x-x_1}{x_0-x_1}, \quad L_1(x) = \frac{x-x_0}{x_1-x_0},$$

then we obtain the interpolating polynomial

$$P(x) = L_0(x)f(x_0) + L_1(x)f(x_1),$$

with $P(x_0) = f(x_0)$, and $P(x_1) = f(x_1)$.

– **$P(x)$ is the unique linear polynomial passing through $(x_0, f(x_0))$ and $(x_1, f(x_1))$.**

An n-degree polynomial passing through $n+1$ points

We are going to construct a polynomial passing through the points $(x_0, f(x_0))$, $(x_1, f(x_1))$, $(x_2, f(x_2))$, $\dots$, $(x_n, f(x_n))$.

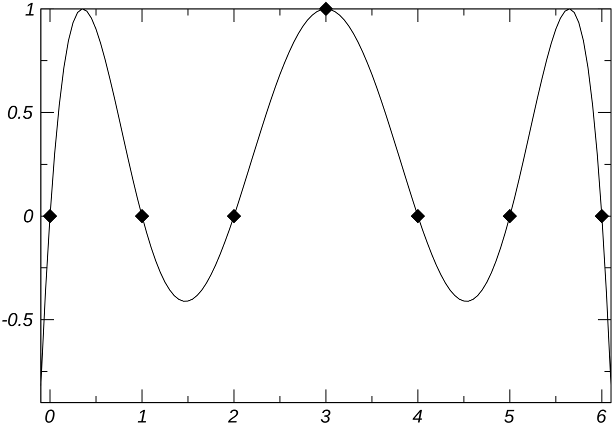
We define $L_{n,k}(x)$, the **Lagrange coefficients:**

$$\mathbf{L_{n,k}(x) = \prod_{i=0,\, i\neq k}^{n} \frac{x - x_i}{x_k - x_i}} = \frac{x - x_0}{x_k - x_0} \cdots \frac{x - x_{k-1}}{x_k - x_{k-1}} \cdot \frac{x - x_{k+1}}{x_k - x_{k+1}} \cdots \frac{x - x_n}{x_k - x_n},$$

which have the properties

$$L_{n,k}(x_k) = 1; \quad L_{n,k}(x_i) = 0, \quad \text{for all } i \neq k.$$

Example of $L_{n,k}(x)$



This is $L_{6,3}(x)$, for the points $x_i = i$, $i = 0, \ldots, 6$.

The n^{th} Lagrange Interpolating Polynomial

We use $L_{n,k}(x)$, $k = 0, \ldots, n$ as building blocks for the Lagrange interpolating polynomial:

$$P(x) = \sum_{k=0}^{n} f(x_k) L_{n,k}(x),$$

which has the property

$$P(x_i) = f(x_i), \quad \text{for all } i = 0, \ldots, n.$$

This is the unique n^{th} degree polynomial passing through the points $(x_i, f(x_i))$, $i = 0, \ldots, n$.

Error bound for the Lagrange interpolating polynomial

Suppose x_i, $i = 0, \dots, n$ *are distinct numbers in the interval* $[a, b]$, *and* $f \in C^{n+1}[a, b]$. *Then for all* $x \in [a, b]$ *there exists* $\xi(x) \in (a, b)$ *so that:*

$$f(x) = P_{\text{Lagrange}}(x) + \frac{f^{(n+1)}(\xi(x))}{(n+1)!} \prod_{i=0}^{n} (x - x_i),$$

where $P_{\text{Lagrange}}(x)$ *is the* n^{th} *Lagrange interpolating polynomial.*

Compare with the error formula for Taylor polynomials

$$f(x) = P_{\text{Taylor}}(x) + \frac{f^{(n+1)}(\xi(x))}{(n+1)!} (x - x_0)^{n+1},$$

Problem: Applying the error term may be difficult...

The Lagrange and Taylor Error Terms

Just to get a feeling for the non-constant part of the error terms in the Lagrange and Taylor approximations, we plot those parts on the interval $[0, 4]$ with interpolation points $x_i = i$, $i = 0, 1, \ldots, 4$:

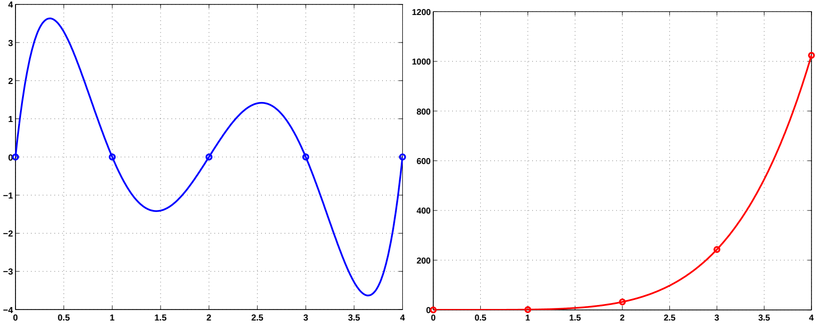


Figure: [LEFT] The non-constant error terms for the Lagrange interpolation oscillates in the interval $[-4, 4]$ (and takes the value *zero* at the node point x_k), and [RIGHT] the non-constant error term for the Taylor extrapolation grows in the interval $[0, 1024]$.

MatLab and Lagrange Polynomials

Example: Find the **Lagrange polynomial** through the points:

$$(0,-5),\quad (1,-6),\quad (2,-1),\quad \text{and}\quad (3,16).$$

The **Lagrange polynomial** satisfies

$$\begin{aligned} P(x) &= \frac{(x-1)(x-2)(x-3)}{(0-1)(0-2)(0-3)}(-5) + \frac{x(x-2)(x-3)}{(1-0)(1-2)(1-3)}(-6) \\ &\quad + \frac{x(x-1)(x-3)}{(2-0)(2-1)(2-3)}(-1) + \frac{x(x-1)(x-2)}{(3-0)(3-1)(3-2)}(16) \\ &= x^3 - 2x - 5 \end{aligned}$$

This example was reverse engineered to have clean numbers

MatLab Lagrange Program

Below is a code for accepting vector data x and y and generating the **Lagrange polynomial**

It outputs points on this polynomial at $(u(k), v(k))$

```
function v = polyinterp(x,y,u)
% Creates Lagrange polynomial
n = length(x);
v = zeros(size(u));
for k = 1:n
    w = ones(size(u));
    for j = [1:k-1 k+1:n]
        w = (u-x(j))./(x(k)-x(j)).*w;
    end
    v = v + w*y(k);
end
```

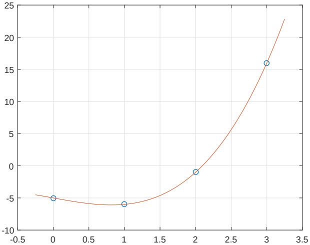
MatLab and Lagrange Polynomials

Example (with MatLab): Our example satisfies

```
x = 0:3; y = [-5 -6 -1 16];
```

We enter closely spaced points, u, the function `polyinterp`, and plot the results

```
u = -0.25:0.01:3.25;
v = polyinterp(x,y,u);
plot((x,y,'o',u,v,'-');grid;
```



MatLab and Lagrange Polynomials

Example (with MatLab): Continuing our example we can use the **symbolic package** in MatLab to obtain the polynomial expression:

```
symx = sym('x')
```

The polynomial is given by:

```
P = polyinterp(x,y,symx)
P = (x*(x - 1)*(x - 3))/2 + 5*(x/2 - 1)*(x/3 - ...
1)*(x - 1)+ (16*x*(x/2 - 1/2)*(x - 2))/3 - ...
6*x*(x/2 - 3/2)*(x - 2)
```

This is simplified with

```
P = simplify(P)
P = x^3 - 2*x - 5
```

Vandermonde Matrix and Interpreting Polynomial

Alternate Scheme: Suppose we want an interpreting polynomial of the form:

$$P(x) = c_1x^{n-1} + c_2x^{n-2} + \cdots + c_{n-1}x + c_n$$

Given data points $x = [x_1, ..., x_n]$ and $y = [y_1, ..., y_n]$ we can obtain the coefficients $c_1, ..., c_n$ by solving the system:

$$\begin{pmatrix} x_1^{n-1} & x_1^{n-2} & \cdots & x_1 & 1 \\ x_2^{n-1} & x_2^{n-2} & \cdots & x_2 & 1 \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ x_n^{n-1} & x_n^{n-2} & \cdots & x_n & 1 \end{pmatrix} \begin{pmatrix} c_1 \\ c_2 \\ \vdots \\ c_n \end{pmatrix} = \begin{pmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{pmatrix}$$

This system $Vc = y$ contains the important ***Vandermonde matrix***, V

Vandermonde Matrix and MatLab

Given the data $x = [x_1, ..., x_n]$, the elements of the ***Vandermonde matrix***, V, satisfy

$$v_{k,j} = x_k^{n-j}$$

MatLab has the function `vander`, which generates the ***Vandermonde matrix***, V

For our example above, `x = 0:3; y = [-5 -6 -1 16];`
`V = vander(x)` produces

$$V = \begin{pmatrix} 0 & 0 & 0 & 1 \\ 1 & 1 & 1 & 1 \\ 8 & 4 & 2 & 1 \\ 27 & 9 & 3 & 1 \end{pmatrix}$$

Then `c = V\y'` produces $c = [1, 0, -2, -5]^t$ or

$$P(x) = x^3 - 2x - 5$$

Numerical Quadrature – Basics

Numerical Quadrature: Basics

- Integration is valuable in many ***applications*** – often the anti-derivative is unavailable
- Introduction showed the definition of the ***Riemann integral***
  - **Midpoint rule** directly uses the definition with even intervals and function evaluations at the midpoint of the subintervals
  - The ***convergence*** of this method appeared to be $\mathcal{O}((\Delta x)^2)$
- Can we do better with interpolating functions on the subintervals $[x_j, x_{j+1}]$?

Numerical Quadrature – Basics

There are **two** primary means of improving **Numerical integration**

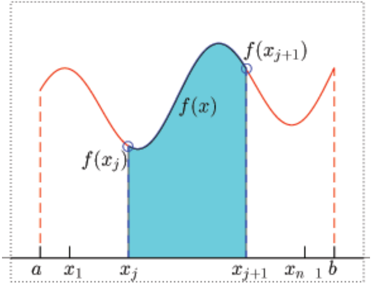
1. If $a = x_0 < x_1 < \cdots < x_{n-1} < x_n = b$, then ***properties of the integral*** give

$$\int_a^b f(x)dx = \int_{x_0}^{x_1} f(x)dx + \cdots + \int_{x_{n-1}}^{x_n} f(x)dx.$$

   We create **composite integrals** and choose appropriate x_i's, which subdivide our function $f(x)$ into n subintervals with each subinterval providing a smaller domain and better approximation of f on that subinterval.

2. Take a particular subinterval, then partition that subinterval further to obtain a reasonable approximation of $f(x)$ on the subinterval by an ***interpreting polynomial***, which is precisely integrable and has a known error bound.

Numerical Quadrature – Basics



Our aim is to obtain the greatest accuracy approximating the integral with the minimum amount of computation

- We can vary the spacing x_j, not necessarily uniform
- We can alter how $f(x)$ is approximated – Using polynomials, which are exactly integrable

Numerical Quadrature – Single Interval

We begin our analysis with the second point above (avoiding the **composite integral** for now)

We focus on a single interval and consider ***interpolating polynomials*** approximating $f(x)$ on the single interval

The basic idea is to replace integration by a clever summation:

$$\int_a^b f(x)\,dx \quad \to \quad \sum_{i=0}^{n} a_i f_i,$$

where $a \le x_0 < x_1 < \cdots < x_n \le b$, $f_i = f(x_i)$.

The coefficients a_i and the nodes x_i are to be selected.

Various means of selecting a_i and x_i alter the efficiency and accuracy of our ***algorithm***

Building Integration Schemes with Lagrange Polynomials

Given the nodes $\{x_0, x_1, \ldots, x_n\}$ we can use the **Lagrange interpolating polynomial**

$$P_n(x) = \sum_{i=0}^{n} f_i L_{n,i}(x), \quad \text{with error} \quad E_n(x) = \frac{f^{(n+1)}(\xi(x))}{(n+1)!} \prod_{i=0}^{n} (x - x_i)$$

to obtain

$$\int_a^b f(x)\,dx = \underbrace{\int_a^b P_n(x)\,dx}_{\text{The Approximation}} + \underbrace{\int_a^b E_n(x)\,dx}_{\text{The Error Estimate}}$$

Identifying the Coefficients

The **Lagrange interpolating polynomials** are readily integrated to give the weighting coefficients a_i

$$\int_a^b P_n(x)\,dx = \int_a^b \sum_{i=0}^{n} f_i L_{n,i}(x)\,dx = \sum_{i=0}^{n} f_i \underbrace{\int_a^b L_{n,i}(x)\,dx}_{a_i} = \sum_{i=0}^{n} f_i a_i.$$

Hence we write

$$\int_a^b f(x)\,dx \approx \sum_{i=0}^{n} a_i f_i$$

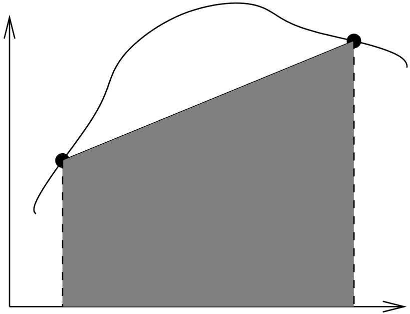
with error given by

$$E(f) = \int_a^b E_n(x)\,dx = \int_a^b \frac{f^{(n+1)}(\xi(x))}{(n+1)!} \prod_{i=0}^{n} (x - x_i)\,dx.$$

Example 1: Trapezoidal Rule

Let $a = x_0 < x_1 = b$, and use the linear interpolating polynomial

$$P_1(x) = f_0\left[\frac{x - x_1}{x_0 - x_1}\right] + f_1\left[\frac{x - x_0}{x_1 - x_0}\right].$$



Example 1: Trapezoidal Rule

Then

$$\int_a^b f(x)\,dx = \int_{x_0}^{x_1}\left[f_0\left[\frac{x-x_1}{x_0-x_1}\right]+f_1\left[\frac{x-x_0}{x_1-x_0}\right]\right]dx + \frac{1}{2}\int_{x_0}^{x_1} f''(\xi(x))(x-x_0)(x-x_1)\,dx.$$

The error term (use the Weighted Mean Value Theorem):

$$\int_{x_0}^{x_1} f''(\xi(x))(x-x_0)(x-x_1)\,dx = f''(\xi)\int_{x_0}^{x_1}(x-x_0)(x-x_1)\,dx$$

$$= f''(\xi)\left[\frac{x^3}{3}-\frac{x_1+x_0}{2}x^2+x_0x_1x\right]_{x_0}^{x_1} = -\frac{h^3}{6}f''(\xi).$$

where $h = x_1 - x_0 = b - a$.

Example 1: Trapezoidal Rule

Hence,

$$\int_a^b f(x)\,dx = \left[f_0 \left[\frac{(x-x_1)^2}{2(x_0-x_1)} \right] + f_1 \left[\frac{(x-x_0)^2}{2(x_1-x_0)} \right] \right]_{x_0}^{x_1} - \frac{h^3}{12} f''(\xi)$$

$$= \frac{(x_1-x_0)}{2}\left[f_0+f_1\right] - \frac{h^3}{12} f''(\xi)$$

$$\boxed{\int_a^b f(x)\,dx = h\left[\frac{f(x_0)+f(x_1)}{2}\right] - \frac{h^3}{12} f''(\xi), \quad h = b-a.}$$

Example 2a: Simpson's Rule (sub-optimal error bound)

Let $x_0 = a$, $x_1 = \frac{a+b}{2}$, $x_2 = b$, let $h = \frac{b-a}{2}$ and use the ***quadratic interpolating polynomial***

$$\int_a^b f(x)dx = \int_{x_0}^{x_2} \left[f(x_0)\frac{(x-x_1)(x-x_2)}{(x_0-x_1)(x_0-x_2)} + f(x_1)\frac{(x-x_0)(x-x_2)}{(x_1-x_0)(x_1-x_2)} \right.$$

$$\left. + f(x_2)\frac{(x-x_0)(x-x_1)}{(x_2-x_0)(x_2-x_1)} \right] dx$$

$$+ \int_{x_0}^{x_2} \frac{(x-x_0)(x-x_1)(x-x_2)}{6} f^{(3)}(\xi(x))\, dx \;\ldots$$

$$\int_a^b f(x)\,dx = h\left[\frac{f(x_0)+4f(x_1)+f(x_2)}{3}\right] + \mathcal{O}(h^4 f^{(3)}(\xi)).$$

Example 2b: Simpson's Rule (optimal error bound)

The optimal error bound for Simpson's rule can be obtained by Taylor expanding $f(x)$ about the mid-point x_1:

$$f(x) = f(x_1) + f'(x_1)(x - x_1) + \frac{f''(x_1)}{2}(x - x_1)^2 + \frac{f'''(x_1)}{6}(x - x_1)^3 + \frac{f^{(4)}(\xi(x))}{24}(x - x_1)^4,$$

then formally integrating this expression, to get:

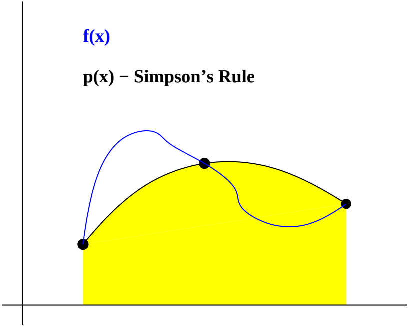
$$\int_a^b \left[f(x_1) + f'(x_1)(x - x_1) + \frac{f''(x_1)}{2}(x - x_1)^2 + \frac{f'''(x_1)}{6}(x - x_1)^3 + \frac{f^{(4)}(\xi(x))}{24}(x - x_1)^4 \right] dx.$$

After use of the weighted mean value theorem, and the approximation $f''(x_1) = \frac{1}{h^2}[f(x_0) - 2f(x_1) + f(x_2)] - \frac{h^2}{12} f^{(4)}(\xi)$, and a whole lot of algebra (**Yanofsky - UCLA Notes**) we end up with

$$\int_{x_0}^{x_2} f(x)\, dx = h \left[\frac{f(x_0) + 4f(x_1) + f(x_2)}{3} \right] - \frac{h^5}{90} f^{(4)}(\xi).$$

Example 2: Simpson's Rule

$$\int_a^b f(x)\,dx = h\left[\frac{f(x_0)+4f(x_1)+f(x_2)}{3}\right] + \mathcal{O}(h^5 f^{(4)}(\xi)).$$



Integration Examples

$f(x)$	$[a,b]$	$\int_a^b f(x)dx$	Trapezoidal	Error	Simpson	Error
x	$[0,1]$	$1/2$	0.5	0	0.5	0
x^2	$[0,1]$	$1/3$	0.5	0.16667	0.33333	0
x^3	$[0,1]$	$1/4$	0.5	0.25000	0.25000	0
x^4	$[0,1]$	$1/5$	0.5	0.30000	0.20833	0.0083333
e^x	$[0,1]$	$e-1$	1.8591	0.14086	1.7189	0.0005793

The Trapezoidal rule gives exact solutions for linear functions. — The error terms contains a second derivative.

Simpson's rule gives exact solutions for polynomials of degree less than 4. — The error term contains a fourth derivative.

Degree of Accuracy (Precision)

Definition (Degree of Accuracy)

The **Degree of Accuracy**, or **precision**, of a quadrature formula is the largest positive integer n such that the formula is exact for x^k for all $k = 0, 1, \ldots, n$.

With this definition:

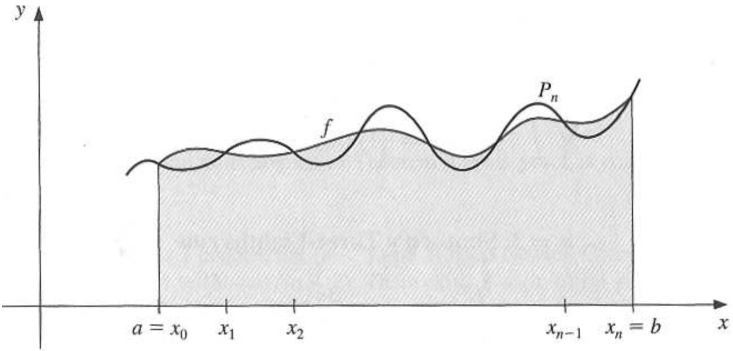
Scheme	Degree of Accuracy
Trapezoidal	1
Simpson's	3

Trapezoidal and Simpson's are examples of a class of methods known as ***Newton-Cotes formulas***.

Newton-Cotes Formulas — Two Types

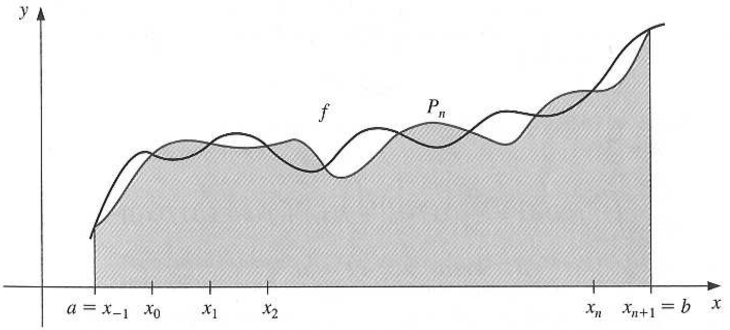
Closed

Closed The $(n+1)$ point closed NCF uses nodes $x_i = x_0 + ih$, $i = 0, 1, \ldots, n$, where $x_0 = a$, $x_n = b$ and $h = (b-a)/n$. It is called closed since the endpoints are included as nodes.



Newton-Cotes Formulas — Two Types — Open

Open The $(n+1)$ point open NCF uses nodes $x_i = x_0 + ih$, $i = 0, 1, \ldots, n$ where $h = (b-a)/(n+2)$ and $x_0 = a+h$, $x_n = b-h$. (We label $x_{-1} = a$, $x_{n+1} = b$.)



Closed Newton-Cotes Formulas

The approximation is

$$\int_a^b f(x)\,dx \approx \sum_{i=0}^{n} a_i f(x_i),$$

where

$$a_i = \int_{x_0}^{x_n} L_{n,i}(x)\,dx = \int_{x_0}^{x_n} \prod_{\substack{j=0 \\ j\neq i}}^{n} \frac{(x-x_j)}{(x_i-x_j)}\,dx.$$

Note: The Lagrange polynomial $L_{n,i}(x)$ models a function which takes the value 0 at all x_j $(j \neq i)$, and 1 at x_i. Hence, the coefficient a_i captures the integral of a function, which is 1 at x_i and zero at the other node points.

Closed Newton-Cotes Formulas — Error

Theorem

Suppose that $\sum_{i=0}^{n} a_i f(x_i)$ *denotes the* $(n+1)$ *point closed Newton-Cotes formula with* $x_0 = a$, $x_n = b$, *and* $h = (b-a)/n$. *Then there exists* $\xi \in (a,b)$ *for which*

$$\int_a^b f(x)dx = \sum_{i=0}^{n} a_i f(x_i) + \frac{h^{n+3} f^{(n+2)}(\xi)}{(n+2)!} \int_0^n t^2(t-1)\cdots(t-n)dt,$$

if n *is even and* $f \in C^{n+2}[a,b]$, *and*

$$\int_a^b f(x)dx = \sum_{i=0}^{n} a_i f(x_i) + \frac{h^{n+2} f^{(n+1)}(\xi)}{(n+1)!} \int_0^n t(t-1)\cdots(t-n)dt,$$

if n *is odd and* $f \in C^{n+1}[a,b]$.

Note that when n is an even integer, the degree of precision is $(n+1)$. When n is odd, the degree of precision is only n.

Closed Newton-Cotes Formulas — Examples

n = 1: Trapezoid Rule

$$\frac{h}{2}\Big[f(x_0)+f(x_1)\Big]-\frac{h^3}{12}f''(\xi)$$

n = 2: Simpson's Rule

$$\frac{h}{3}\Big[f(x_0)+4f(x_1)+f(x_2)\Big]-\frac{h^5}{90}f^{(4)}(\xi)$$

n = 3: Simpson's $\frac{3}{8}$-Rule

$$\frac{3h}{8}\Big[f(x_0)+3f(x_1)+3f(x_2)+f(x_3)\Big]-\frac{3h^5}{80}f^{(4)}(\xi)$$

n = 4: Boole's Rule

$$\frac{2h}{45}\Big[7f(x_0)+32f(x_1)+12f(x_2)+32f(x_3)+7f(x_4)\Big]-\frac{8h^7}{945}f^{(6)}(\xi)$$

Open Newton-Cotes Formulas

The approximation is

$$\int_a^b f(x)\,dx = \int_{x_{-1}}^{x_{n+1}} f(x)\,dx \approx \sum_{i=0}^{n} a_i f(x_i),$$

where

$$a_i = \int_{x_{-1}}^{x_{n+1}} L_{n,i}(x)\,dx = \int_{x_0}^{x_n} \prod_{\substack{j=0 \\ j \neq i}}^{n} \frac{(x - x_j)}{(x_i - x_j)}\,dx.$$

Open Newton-Cotes Formulas — Error

Theorem

Suppose that $\sum_{i=0}^{n} a_i f(x_i)$ *denotes the* $(n+1)$ *point open Newton-Cotes formula with* $x_{-1} = a$, $x_{n+1} = b$, *and* $h = (b-a)/(n+2)$. *Then there exists* $\xi \in (a,b)$ *for which*

$$\int_a^b f(x)dx = \sum_{i=0}^{n} a_i f(x_i) + \frac{h^{n+3} f^{(n+2)}(\xi)}{(n+2)!} \int_{-1}^{n+1} t^2(t-1)\cdots(t-n)dt,$$

if n *is even and* $f \in C^{n+2}[a,b]$, *and*

$$\int_a^b f(x)dx = \sum_{i=0}^{n} a_i f(x_i) + \frac{h^{n+2} f^{(n+1)}(\xi)}{(n+1)!} \int_{-1}^{n+1} t(t-1)\cdots(t-n)dt,$$

if n *is odd and* $f \in C^{n+1}[a,b]$.

Note that when n is an even integer, the degree of precision is $(n+1)$. When n is odd, the degree of precision is only n.

Open Newton-Cotes Formulas — Examples

n = 0: Midpoint Rule

$$2hf(x_0) + \frac{h^3}{3}f''(\xi)$$

n = 1: Trapezoid Method

$$\frac{3h}{2}\Big[f(x_0) + f(x_1)\Big] + \frac{3h^3}{4}f''(\xi)$$

n = 2: Milne's Rule

$$\frac{4h}{3}\Big[2f(x_0) - f(x_1) + 2f(x_2)\Big] + \frac{14h^5}{45}f^{(4)}(\xi)$$

n = 3: No Name

$$\frac{5h}{24}\Big[11f(x_0) + f(x_1) + f(x_2) + 11f(x_3)\Big] + \frac{95h^5}{144}f^{(4)}(\xi)$$

Divide and Conquer!

Say you want to compute:

$$\int_0^{100} f(x)\,dx.$$

Is it a Good Idea$^{\text{TM}}$ to directly apply your favorite Newton-Cotes formula to this integral?!?

No!

With the closed 5-point NCF, we have $h = 25$ and $h^5/90 \sim 10^5$ so even with a bound on $f^{(6)}(\xi)$ the error will be large.

Better: Apply the closed 5-point NCF to the integrals

$$\int_{4i}^{4(i+1)} f(x)\,dx, \quad i = 0, 1, \ldots, 24$$

then sum. **"Composite Numerical Integration"**