Numerical Solutions to Differential Equations

Lecture Notes #2 — Calculus and Math 541 Review

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Outline

Current Lecture — Reviewing Math 541 and Calculus

The purpose of this lecture is to "warm up" by reviewing some forgotten(?) material from the past.

Note that **complete lecture notes** for Math 541 are available on-line at http://terminus.sdsu.edu/SDSU/Math541_f2014/.

Why Review Calculus???

It's a good warm-up for our brains!

When developing numerical schemes we will use theorems from calculus to guarantee that our algorithms make sense.

If the theory is sound, when our programs fail we look for bugs in the code!

Background Material — A Crash Course in Calculus

Key concepts from Calculus

- Limits
- Continuity
- Convergence
- Differentiability
- Rolle's Theorem
- Mean Value Theorem
- Extreme Value Theorem
- Intermediate Value Theorem
- **Taylor's Theorem**

Limit / Continuity

Definition (Limit)

A function f defined on a set X of real numbers $X \subset \mathbb{R}$ has the limit L at x_0, written

$$\lim_{x \to x_0} f(x) = L,$$

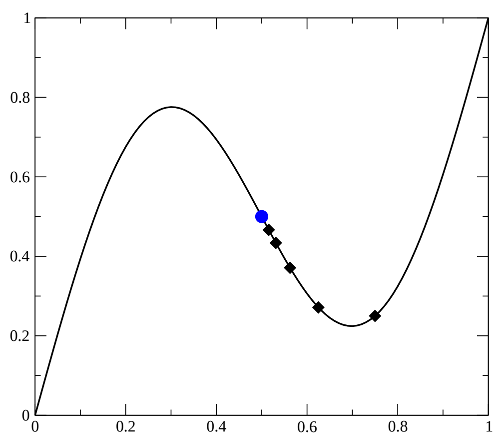
if given any real number $\epsilon > 0$ ($\forall \epsilon > 0$), there exists a real number $\delta > 0$ ($\exists \delta > 0$) such that $|f(x) - L| < \epsilon$, whenever $x \in X$ and $0 < |x - x_0| < \delta$.

Definition (Continuity (at a point))

Let f be a function defined on a set X of real numbers, and $x_0 \in X$. Then f is continuous at x_0 if

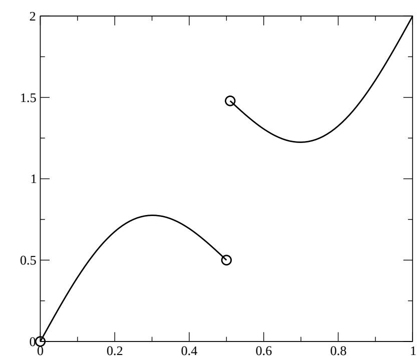
$$\lim_{x \to x_0} f(x) = f(x_0).$$

Example: Continuity at x_0



Here we see how the limit $x \to x_0$ (where $x_0 = 0.5$) exists for the function $f(x) = x + \frac{1}{2}\sin(2\pi x)$.

Examples: Jump Discontinuity

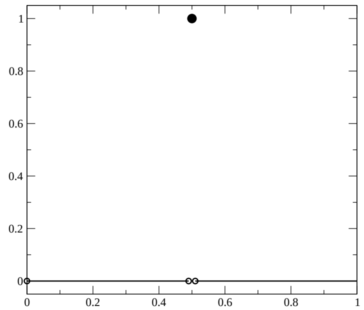


The function

$$f(x) = \begin{cases} x + \frac{1}{2}\sin(2\pi x) & x < 0.5 \\ x + \frac{1}{2}\sin(2\pi x) + 1 & x > 0.5 \end{cases}$$

has a jump discontinuity at $x_0 = 0.5$.

Examples: "Spike" Discontinuity



The function

$$f(x) = \begin{cases} 1 & x = 0.5 \\ 0 & x \neq 0.5 \end{cases}$$

has a discontinuity at $x_0 = 0.5$.

The **limit exists**, but

$$\lim_{x \to 0.5} f(x) = 0 \neq 1$$

Continuity / Convergence

Definition (Continuity (in an interval))

The function f is continuous on the set X ($f \in C(X)$) if it is continuous at each point x in X.

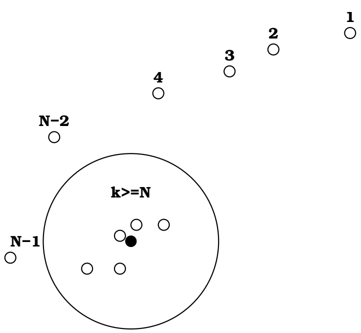
Definition (Convergence of a sequence)

Let $\underline{\mathbf{x}} = \{x_n\}_{n=1}^{\infty}$ be an infinite sequence of real (or complex numbers). The sequence $\underline{\mathbf{x}}$ converges to x (has the limit x) if $\forall \epsilon > 0$, $\exists N(\epsilon) \in \mathbb{Z}^+$: $|x_n - x| < \epsilon \; \forall n > N(\epsilon)$. The notation

$$\lim_{n \to \infty} x_n = x$$

means that the sequence $\{x_n\}_{n=1}^{\infty}$ converges to x.

Illustration: Convergence of a Complex Sequence



A sequence in $\underline{\mathbf{z}} = \{z_k\}_{k=1}^{\infty}$ converges to $z_0 \in \mathbb{C}$ (the black dot) if for any ϵ (the radius of the circle), there is a value N (which depends on ϵ) so that the "tail" of the sequence $\underline{\mathbf{z}}_t = \{z_k\}_{k=N}^{\infty}$ is inside the circle.

Differentiability

Theorem

If f is a function defined on a set X of real numbers and $x_0 \in X$, the the following statements are **equivalent***:*

(a) *f is continuous at x_0*

(b) *If $\{x_n\}_{n=1}^{\infty}$ is any sequence in X converging to x_0, then $\lim_{n \to \infty} f(x_n) = f(x_0)$.*

Definition (Differentiability (at a point))

Let f be a function defined on an open interval containing x_0 ($a < x_0 < b$). f is differentiable at x_0 if

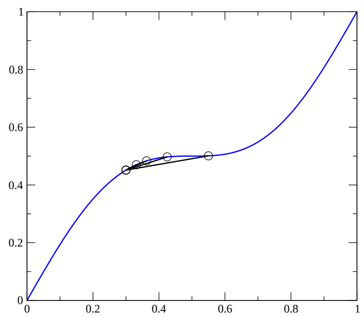
$$f'(x_0) = \lim_{x \to x_0} \frac{f(x) - f(x_0)}{x - x_0} \quad \text{exists.}$$

If the limit exists, $f'(x_0)$ is the derivative at x_0.

Definition (Differentiability (in an interval))

If $f'(x_0)$ exists $\forall x_0 \in X$, then f is differentiable on X.

Illustration: Differentiability



Here we see that the limit

$$\lim_{x \to x_0} \frac{f(x) - f(x_0)}{x - x_0}$$

exists — and approaches the slope / derivative at x_0, $f'(x_0)$.

Calculus Review
Math 541 Review
Limits, Continuity, and Convergence
Differentiability, Rolle's, and the Mean Value Theorem
Extreme Value, Intermediate Value, and Taylor's Theorem

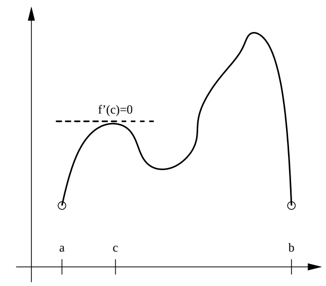
Continuity / Rolle's Theorem

Theorem (Differentiability $\Rightarrow$ Continuity)

If f is differentiable at x_0, then f is continuous at x_0.

Theorem (Rolle's Theorem Wiki-Link)

Suppose $f \in C[a,b]$ and that f is differentiable on (a,b). If $f(a) = f(b)$, then $\exists c \in (a,b)$: $f'(c) = 0$.



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Limits, Continuity, and Convergence
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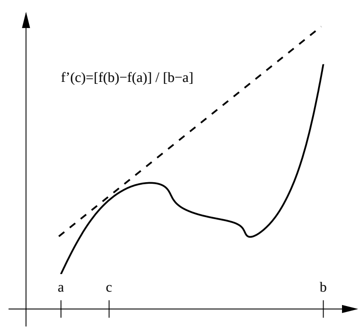
Mean Value Theorem

Theorem (Mean Value Theorem Wiki-Link)

If $f \in C[a,b]$ and f is differentiable on (a,b), then $\exists c \in (a,b)$:

$$f'(c) = \frac{f(b) - f(a)}{b - a}.$$



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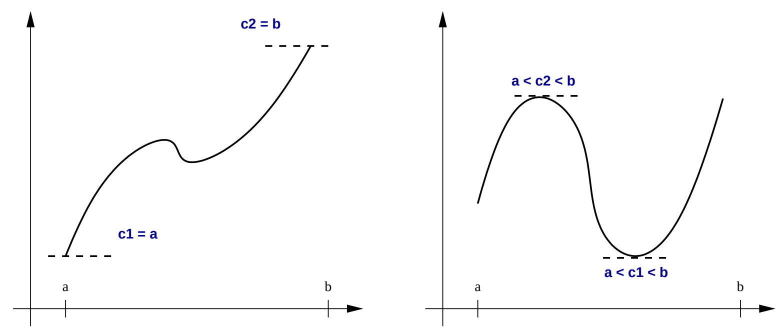
Extreme Value Theorem

Theorem (Extreme Value Theorem Wiki-Link)

If $f \in C[a,b]$ then $\exists c_1, c_2 \in [a,b]$: $f(c_1) \le f(x) \le f(c_2)$ $\forall x \in [a,b]$. If f is differentiable on (a,b) then the numbers c_1, c_2 occur either at the endpoints of $[a,b]$ or where $f'(x) = 0$.



Intermediate Value Theorem

Theorem (Intermediate Value Theorem Wiki-Link **)**

if $f \in C[a,b]$ and K is any number between $f(a)$ and $f(b)$, then there exists a number c in (a,b) for which $f(c) = K$.

Taylor's Theorem

Theorem (Taylor's Theorem Wiki-Link **)**

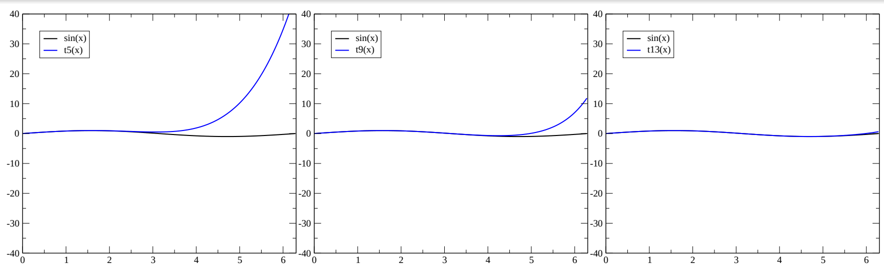
Suppose $f \in C^n[a,b]$, $f^{(n+1)}\exists$ on $[a,b]$, and $x_0 \in [a,b]$. Then $\forall x \in (a,b)$, $\exists \xi(x) \in (x_0, x)$ with $f(x) = P_n(x) + R_n(x)$ where

$$P_n(x) = \sum_{k=0}^{n} \frac{f^{(k)}(x_0)}{k!}(x-x_0)^k, \quad R_n(x) = \frac{f^{(n+1)}(\xi(x))}{(n+1)!}(x-x_0)^{(n+1)}.$$

$P_n(x)$ is called the **Taylor polynomial of degree** *n, and $R_n(x)$ is the* **remainder term** *(truncation error).*

This theorem is **extremely important** for numerical analysis; Taylor expansion is a fundamental step in the derivation of many of the algorithms we see in this class (and in Math 542 & 693ab).

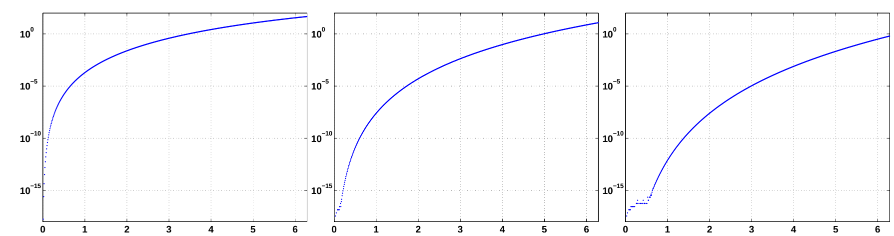
Illustration: Taylor's Theorem $f(x) = \sin(x)$



$P_5(x)$ $P_9(x)$ $P_{13}(x)$

$$P_{13}(x) = \underbrace{\underbrace{x - \frac{1}{3!}x^3 + \frac{1}{5!}x^5}_{P_5(x)} - \frac{1}{7!}x^7 + \frac{1}{9!}x^9}_{P_9(x)} - \frac{1}{11!}x^{11} + \frac{1}{13!}x^{13}$$

Illustration: Taylor's Theorem Errors $f(x) = \sin(x)$



$E_5(x)$ $E_9(x)$ $E_{13}(x)$

$$P_{13}(x) = \underbrace{\underbrace{x - \frac{1}{3!}x^3 + \frac{1}{5!}x^5}_{P_5(x)} - \frac{1}{7!}x^7 + \frac{1}{9!}x^9}_{P_9(x)} - \frac{1}{11!}x^{11} + \frac{1}{13!}x^{13}$$

Taylor Expansions — Matlab

- A **Taylor polynomial of degree** n requires all derivatives up to order n, and order $n+1$ for the **remainder**.
- Derivatives may be [more] complicated expression [than the original function].
- **Matlab** can compute derivatives for you:

Matlab: Symbolic Computations Try this!!!

```
>> syms x
>> diff(sin(2*x))
>> diff(sin(2*x),3)
>> taylor(exp(x),5)
>> taylor(exp(x),5,1)
```


Background Material

Key concepts from Math 541

- Polynomial Interpolation and Approximation
  $\to$ Approximation of Derivatives
- Numerical Integration
  $\to$ Approximation of

$$\int_{t_i}^{t_{i+1}} f(t, y, y', \ldots, y^{(n)})\, dt$$

Math 541 Review

Key topics:

Lagrange Coefficients — Lagrange Polynomials

Newton's Divided Differences — An expression for the polynomial

Using polynomials to approximate $f'(x)$

Richardson's Extrapolation

Numerical Integration — Return of the Lagrange Polynomials

Interpolation: Lagrange Polynomials

Instead of working hard at *one point* (Taylor polynomials), we are going to construct a polynomial passing through the points $(x_0, f(x_0))$, $(x_1, f(x_1))$, $(x_2, f(x_2))$, $\ldots$, $(x_n, f(x_n))$.
We define

Definition (the Lagrange coefficients, $L_{n,k}(x)$)

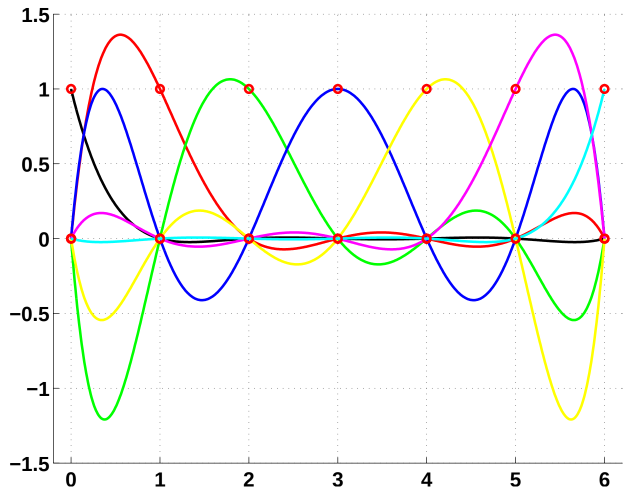
$$L_{n,k}(x) = \prod_{i=0,\, i\neq k}^{n} \frac{x - x_i}{x_k - x_i},$$

$L_{n,k}(x)$ have the properties $L_{n,i}(x_j) = \delta_{i,j}$, and we use them as building blocks for the **Lagrange interpolating polynomial**:

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

The Lagrange Coefficients, $L_{n,k}(x)$.

E.g. $L_{6,k}(x_i) = \delta_{i,k}$, $\{x_i\}_{i=0}^{6} = i$:



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Interpolation, Differentiation, Extrapolation
Integration, Degree of Accuracy
Newton-Cotes Formulas, Composite Integration

Newton's Divided Differences.

Zeroth Divided Difference:

$$f[x_i] = f(x_i).$$

First Divided Difference:

$$f[x_i, x_{i+1}] = \frac{f[x_{i+1}] - f[x_i]}{x_{i+1} - x_i}.$$

Second Divided Difference:

$$f[x_i, x_{i+1}, x_{i+2}] = \frac{f[x_{i+1}, x_{i+2}] - f[x_i, x_{i+1}]}{x_{i+2} - x_i}.$$

***k*th Divided Difference**:

$$f[x_i, x_{i+1}, \ldots, x_{i+K}] = \frac{f[x_{i+1}, x_{i+2}, \ldots, x_{i+k}] - f[x_i, x_{i+1}, \ldots, x_{i+k-1}]}{x_{i+k} - x_i}.$$

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Newton's Divided Differences: Compute the Polynomial.

We can write the interpolating polynomial with the help of the divided differences:

$$P_n(x) = f[x_0] + \sum_{k=1}^{n} \left[f[x_0, \ldots, x_k] \prod_{m=0}^{k-1} (x - x_m) \right].$$

where $f[x_0, \ldots, x_k]$ are the diagonal entries from the divided difference table:

x_0	$f[x_0]$			
x_1	$f[x_1]$	$f[x_0, x_1]$		
x_2	$f[x_2]$	$f[x_1, x_2]$	$f[x_0, x_1, x_2]$	
$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\ddots$

$$\frac{f[x_1, x_2] - f[x_0, x_1]}{x_2 - x_0}.$$

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Numerical Differentiation — Using Polynomials

Suppose $\{x_0, x_1, \ldots, x_n\}$ are distinct points in an interval $\mathcal{I}$, and $f \in C^{n+1}(\mathcal{I})$, we can write

$$f(x) = \sum_{k=0}^{n} f(x_k) L_k(x) + \frac{\prod_{k=0}^{n}(x - x_k)}{(n+1)!} f^{(n+1)}(\xi).$$

Formal differentiation gives:

$$\begin{aligned} f'(x) &= \sum_{k=0}^{n} f(x_k) L_k'(x) + \frac{d}{dx}\left[\frac{\prod_{k=0}^{n}(x - x_k)}{(n+1)!}\right] f^{(n+1)}(\xi) \\ &\quad + \frac{\prod_{k=0}^{n}(x - x_k)}{(n+1)!} \frac{d}{dx}\left[f^{(n+1)}(\xi)\right]. \end{aligned}$$

Since we will be evaluating $f'(x_j)$ the last term gives no contribution.

The $(n+1)$ point formula for approximating $f'(x_j)$

$$\boxed{\mathbf{f'(x_j) = \sum_{k=0}^{n} f(x_k) L_k'(x_j) + \frac{f^{(n+1)}(\xi)}{(n+1)!} \left[\prod_{\substack{k=0 \\ k \neq j}}^{n} (x_j - x_k) \right]}}$$

The formula is most useful when the node points are equally spaced, *i.e.*

$$x_k = x_0 + kh.$$

Example: 3-point Formulas, I/III

Building blocks:

$$L_{2,0}(x) = \frac{(x-x_1)(x-x_2)}{(x_0-x_1)(x_0-x_2)}, \quad L_{2,0}'(x) = \frac{2x-x_1-x_2}{(x_0-x_1)(x_0-x_2)}$$

$$L_{2,1}(x) = \frac{(x-x_0)(x-x_2)}{(x_1-x_0)(x_1-x_2)}, \quad L_{2,1}'(x) = \frac{2x-x_0-x_2}{(x_1-x_0)(x_1-x_2)}$$

$$L_{2,2}(x) = \frac{(x-x_0)(x-x_1)}{(x_2-x_0)(x_2-x_1)}, \quad L_{2,2}'(x) = \frac{2x-x_0-x_1}{(x_2-x_0)(x_2-x_1)}.$$

Formulas:

$$\begin{aligned} f'(x_j) &= f(x_0)\left[\frac{2x_j-x_1-x_2}{(x_0-x_1)(x_0-x_2)}\right] + f(x_1)\left[\frac{2x_j-x_0-x_2}{(x_1-x_0)(x_1-x_2)}\right] \\ &+ f(x_2)\left[\frac{2x_j-x_0-x_1}{(x_2-x_0)(x_2-x_1)}\right] + \frac{f^{(3)}(\xi_j)}{6} \prod_{\substack{k=0 \\ k \neq j}}^{2} (x_j - x_k). \end{aligned}$$

Example: 3-point Formulas, II/III

$$\begin{cases} f'(x_0) = \frac{1}{2h}\left[-3f(x_0) + 4f(x_1) - f(x_2)\right] + \frac{h^2}{3} f^{(3)}(\xi_0) \\ f'(x_1) = \frac{1}{2h}\left[-f(x_0) + f(x_2)\right] - \frac{h^2}{6} f^{(3)}(\xi_1) \\ f'(x_2) = \frac{1}{2h}\left[f(x_0) - 4f(x_1) + 3f(x_2)\right] + \frac{h^2}{3} f^{(3)}(\xi_2) \end{cases}$$

Use $x_k = x_0 + kh$:

$$\begin{cases} f'(x_0) = \frac{1}{2h}\left[-3f(x_0) + 4f(x_0+h) - f(x_0+2h)\right] + \frac{h^2}{3} f^{(3)}(\xi_0) \\ f'(x_0+h) = \frac{1}{2h}\left[-f(x_0) + f(x_0+2h)\right] - \frac{h^2}{6} f^{(3)}(\xi_1) \\ f'(x_0+2h) = \frac{1}{2h}\left[f(x_0) - 4f(x_0+h) + 3f(x_0+2h)\right] + \frac{h^2}{3} f^{(3)}(\xi_2) \end{cases}$$

Example: 3-point Formulas, III/III

$$\begin{cases} f'(x_0) = \frac{1}{2h}\left[-3f(x_0) + 4f(x_0+h) - f(x_0+2h)\right] + \frac{h^2}{3} f^{(3)}(\xi_0) \\ \mathbf{f'(x_0) = \frac{1}{2h}\left[-f(x_0-h) + f(x_0+h)\right] - \frac{h^2}{6} f^{(3)}(\xi_1)} \\ f'(x_0) = \frac{1}{2h}\left[f(x_0-2h) - 4f(x_0-h) + 3f(x_0)\right] + \frac{h^2}{3} f^{(3)}(\xi_2) \end{cases}$$

After the substitution $x_0 + h \to x_0$ in the second equation, and $x_0 + 2h \to x_0$ in the third equation.

Note#1: The third equation can be obtained from the first one by setting $h \to -h$.

Note#2: The error is smallest in the second equation.

Note#3: The second equation is a two-sided approximation, the first and third one-sided approximations.

Richardson's Extrapolation

What it is: A general method for generating high-accuracy results using low-order formulas.

Applicable when: The approximation technique has an error term of predictable form, *e.g.*

$$M - N_j(h) = \sum_{k=j}^{\infty} E_k h^k,$$

where M is the unknown value we are trying to approximate, and $N_j(h)$ the approximation (which has an error $\mathcal{O}(h^j)$.)

Procedure: Use two approximations of the same order, but with *different* h; *e.g.* $N_j(h)$ and $N_j(h/2)$. Combine the two approximations in such a way that the error terms of order h^j cancel.

Building High Accuracy Approximations

Consider two first order approximations to M:

$$M - N_1(h) = \sum_{k=1}^{\infty} E_k h^k,$$

and

$$M - N_1(h/2) = \sum_{k=1}^{\infty} E_k \frac{h^k}{2^k}.$$

If we let $\mathbf{N_2(h) = 2N_1(h/2) - N_1(h)}$, then

$$M - N_2(h) = \underbrace{2E_1\frac{h}{2} - E_1 h}_{0} + \sum_{k=2}^{n} E_k^{(2)} h^k,$$

where

$$E_k^{(2)} = E_k\left(\frac{1}{2^{k-1}} - 1\right).$$

Hence, $N_2(h)$ is now a **second order approximation** to M.

Building High Accuracy Approximations

We can play the game again, and combine $N_2(h)$ with $N_2(h/2)$ to get a third-order accurate approximation, etc.

$$N_3(h) = \frac{4N_2(h/2) - N_2(h)}{3} = N_2(h/2) + \frac{N_2(h/2) - N_2(h)}{3}$$

$$N_4(h) = N_3(h/2) + \frac{N_3(h/2) - N_3(h)}{7}$$

$$N_5(h) = N_4(h/2) + \frac{N_4(h/2) - N_4(h)}{2^4 - 1}$$

In general, combining two jth order approximations to get a $(j+1)$st order approximation:

$$\boxed{\mathbf{N_{j+1}(h) = N_j(h/2) + \frac{N_j(h/2) - N_j(h)}{2^j - 1}}}$$

Building Integration Schemes with Lagrange Polynomials

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

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

to obtain

$$\int_a^b f(x)\,dx = \int_a^b P_n(x)\,dx + \int_a^b E_n(x)\,dx.$$

Identifying the Coefficients

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

Hence we write

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

with error given by

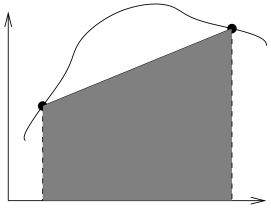
$$E(f) = \int_a^b E_n(x)\,dx = \int_a^b \frac{f^{(n+1)}(\xi(x))}{(n+1)!} \prod_{i=0}^n (x-x_i)\,dx.$$

Example #1: Trapezoidal Rule

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

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

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



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

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

Taylor expand $f(x)$ about x_1:

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

Integrating the error term gives

$$\int_a^b \frac{f^{(4)}(\xi(x))}{24}(x-x_1)^4\,dx = \frac{f^{(4)}(\xi_1)}{60} h^5.$$

Using the approximation $f''(x_1) = \frac{1}{h^2}[f(x_0) - 2f(x_1) + f(x_2)] - \frac{h^2}{12} f^{(4)}(\xi)$

$$\int_{x_0}^{x_2} f(x)\,dx = 2hf(x_1) + \frac{h^3}{3}\left[\frac{1}{h^2}[f(x_0)-2f(x_1)+f(x_2)] - \frac{h^2}{12} f^{(4)}(\xi_2)\right] + \frac{f^{(4)}(\xi_1)}{60} h^5$$

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

Degree of Accuracy (Precision) of an Integration Scheme

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 $\forall k = 0, 1, \ldots, n$.

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

Two types of Newton-Cotes Formulas:

`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.

`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

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

Closed Newton-Cotes Formulas — Error

Theorem (Newton-Cotes Formulas, Error Term)

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

$n = 2$: 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

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

Composite Simpson's Rule, I/II

For an even integer n: Subdivide the interval $[a,b]$ into n sub-intervals, and apply Simpson's rule on each consecutive pair of sub-intervals. With $h=(b-a)/n$ and $x_j = a+jh$, $j=0,1,\ldots,n$, we have

$$\int_a^b f(x)dx = \sum_{j=1}^{n/2} \int_{x_{2j-2}}^{x_{2j}} f(x)dx$$
$$= \sum_{j=1}^{n/2} \left\{ \frac{h}{3}\Big[f(x_{2j-2}) + 4f(x_{2j-1}) + f(x_{2j}) \Big] - \frac{h^5}{90} f^{(4)}(\xi_j) \right\},$$

for some $\xi_j \in [x_{2j-2}, x_{2j}]$, if $f \in C^4[a,b]$.

Since all the interior "even" x_{2j} points appear twice in the sum, we can simplify the expression a bit...

Composite Simpson's Rule, II/II

$$\int_a^b f(x)dx = \frac{h}{3}\left[f(x_0) - f(x_n) + \sum_{j=1}^{n/2}\Big[4f(x_{2j-1}) + 2f(x_{2j})\Big]\right] - \frac{h^5}{90}\sum_{j=1}^{n/2} f^{(4)}(\xi_j).$$

Theorem (Composite Simpson's Rule)

Let $f \in C^4[a,b]$, n be even, $h=(b-a)/n$, and $x_j = a+jh$, $j=0,1,\ldots,n$. There exists $\mu \in (a,b)$ for which the **Composite Simpson's Rule** *for n sub-intervals can be written with its error term as*

$$\int_a^b f(x)dx = \frac{h}{3}\left[f(a) - f(b) + \sum_{j=1}^{n/2}\big[2f(x_{2j}) + 4f(x_{2j+1})\big]\right] - \frac{(b-a)}{180} h^4 f^{(4)}(\mu).$$

Romberg Integration

Romberg Integration is the combination of the **Composite Trapezoidal Rule** (CTR)

$$\int_a^b f(x)dx = \frac{h}{2}\left[f(a) + f(b) + 2\sum_{j=1}^{n-1} f(x_j)\right] - \frac{(b-a)}{12} h^2 f''(\mu)$$

and **Richardson Extrapolation**.

It yields a method for generating high-accuracy integral approximations using several "measurements" using the relatively crude (inaccurate) Trapezoidal Rule.

Romberg Integration — Implemented

```
% Romberg Integration for sin(x) over [0,pi]
a = 0; b = pi; % The Endpoints
R = zeros(7,7);
R(1,1) = (b-a)/2*(sin(a)+sin(b));
for k=2:7
  h = (b-a)/2^(k-1);
  R(k,1)=1/2*(R(k-1,1)+2*h*sum(sin(a+(2*(1:(2^(k-2)))-1)*h)));
end
for j=2:7
  for k=j:7
   R(k,j) = R(k,j-1)+(R(k,j-1)-R(k-1,j-1))/(4^(j-1)-1);
  end
end

disp(R)
```

Next Time, and Beyond

Simulating ODEs using Euler's method, and improvements...