Numerical Solutions to Differential Equations
Lecture Notes #2 — Calculus and Math 541 Review

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Outline

1. **Calculus Review**
   - Limits, Continuity, and Convergence
   - Differentiability, Rolle’s, and the Mean Value Theorem
   - Extreme Value, Intermediate Value, and Taylor’s Theorem

2. **Math 541 Review**
   - Interpolation, Differentiation, Extrapolation
   - Integration, Degree of Accuracy
   - Newton-Cotes Formulas, Composite Integration
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!
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 $f(x) = x + \frac{1}{2} \sin(2\pi x)$. 
The function

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

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 \( x = \{x_n\}_{n=1}^{\infty} \) be an infinite sequence of real (or complex numbers). The sequence \( x \) 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 $z = \{z_k\}_{k=1}^{\infty}$ converges to $z_0 \in \mathbb{C}$ (the black dot) if for any $\epsilon$ (the radius of the circle), there is a value $N$ (which depends on $\epsilon$) so that the “tail” of the sequence $z_t = \{z_k\}_{k=N}^{\infty}$ 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 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

\[
f'(x_0) = \lim_{x \to x_0} \frac{f(x) - f(x_0)}{x - x_0}
\]

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 \( X \).
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 $x_0$, $f'(x_0)$. 
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 $\exists c \in (a, b): f'(c) = 0$. 
Theorem (Mean Value Theorem)

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

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

If \( f \in C[a, b] \) then \( \exists c_1, c_2 \in [a, b] : f(c_1) \leq f(x) \leq f(c_2) \) \( \forall x \in [a, b] \).

If \( f \) is differentiable on \((a, b)\) then the numbers \( c_1, c_2 \) occur either at the endpoints of \([a, b]\) or where \( f'(x) = 0 \).
Theorem (Intermediate Value Theorem)

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

\[ f(x) = \sin(x) \]

\[ P_5(x) = x - \frac{1}{3!}x^3 + \frac{1}{5!}x^5 - \frac{1}{7!}x^7 + \frac{1}{9!}x^9 - \frac{1}{11!}x^{11} + \frac{1}{13!}x^{13} \]

\[ P_9(x) \]

\[ P_{13}(x) \]
Illustration: Taylor’s Theorem  

Errors  

\( f(x) = \sin(x) \)

\[
P_{13}(x) = x - \frac{1}{3!}x^3 + \frac{1}{5!}x^5 - \frac{1}{7!}x^7 + \frac{1}{9!}x^9 - \frac{1}{11!}x^{11} + \frac{1}{13!}x^{13}
\]

\( E_5(x) \)  

\( E_9(x) \)  

\( E_{13}(x) \)
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

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

  Try this!!!
Background Material

Key concepts from Math 541

• Polynomial Interpolation and Approximation
  → Approximation of Derivatives

• Numerical Integration
  → Approximation of

\[ \int_{t_i}^{t_{i+1}} f(t, y, y', \ldots, y^{(n)}) \, dt \]
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. $L_{6,k}(x_i) = \delta_{i,k}$, $\{x_i\}_{i=0}^{6} = i$: 
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:

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

<table>
<thead>
<tr>
<th>$x_0$</th>
<th>$f[x_0]$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$x_1$</td>
<td>$f[x_1]$</td>
</tr>
<tr>
<td>$x_2$</td>
<td>$f[x_2]$</td>
</tr>
<tr>
<td>...</td>
<td>...</td>
</tr>
</tbody>
</table>

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

\[
f'(x) = \sum_{k=0}^{n} f(x_k) L'_k(x) + \frac{d}{dx} \left[ \frac{\prod_{k=0}^{n}(x - x_k)}{(n + 1)!} \right] f^{(n+1)}(\xi)
+ \frac{\prod_{k=0}^{n}(x - x_k)}{(n + 1)!} \frac{d}{dx} \left[ f^{(n+1)}(\xi) \right].
\]

Since we will be evaluating \( f'(x_j) \) the last term gives no contribution.
The \((n + 1)\) point formula for approximating \(f'(x_j)\)

\[
f'(x_j) = \sum_{k=0}^{n} f(x_k)L'_k(x_j) + \frac{f^{(n+1)}(\xi)}{(n + 1)!} \left[ \prod_{k=0}^{n} (x_j - x_k) \right]
\]

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:

\[ f'(x_j) = f(x_0) \left[ \frac{2x_j - x_1 - x_2}{(x_0 - x_1)(x_0 - x_2)} \right] + f(x_1) \left[ \frac{2x_j - x_0 - x_2}{(x_1 - x_0)(x_1 - x_2)} \right] \]

\[ + f(x_2) \left[ \frac{2x_j - x_0 - x_1}{(x_2 - x_0)(x_2 - x_1)} \right] + \frac{f^{(3)}(\xi_j)}{6} \prod_{k=0}^{2} (x_j - x_k). \]
Example: 3-point Formulas, II/III

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

Use \( x_k = x_0 + kh \):

\[
\begin{align*}
    f'(x_0) &= \frac{1}{2h} \left[ -3f(x_0) + 4f(x_0 + h) - f(x_0 + 2h) \right] + \frac{h^2}{3} f^{(3)}(\xi_0) \\
    f'(x_0 + h) &= \frac{1}{2h} \left[ -f(x_0) + f(x_0 + 2h) \right] - \frac{h^2}{6} f^{(3)}(\xi_1) \\
    f'(x_0 + 2h) &= \frac{1}{2h} \left[ f(x_0) - 4f(x_0 + h) + 3f(x_0 + 2h) \right] + \frac{h^2}{3} f^{(3)}(\xi_2)
\end{align*}
\]
Example: 3-point Formulas, III/III

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

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 \( O(h^j) \).)

**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.
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 $N_2(h) = 2N_1(h/2) - N_1(h)$, then

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

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 $M$. 
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 $j$th order approximations to get a $(j + 1)$st order approximation:

\[
N_{j+1}(h) = N_j(h/2) + \frac{N_j(h/2) - N_j(h)}{2^j - 1}
\]
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

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

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

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

\[
\int_a^b f(x) \, dx = h \left[ \frac{f(x_0) + f(x_1)}{2} \right] - \frac{h^3}{12} f''(\xi), \quad h = b - a.
\]
Example #2: Simpson’s Rule (with optimal error bound)

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

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:

<table>
<thead>
<tr>
<th>Scheme</th>
<th>Degree of Accuracy</th>
</tr>
</thead>
<tbody>
<tr>
<td>Trapezoidal</td>
<td>1</td>
</tr>
<tr>
<td>Simpson’s</td>
<td>3</td>
</tr>
</tbody>
</table>

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

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

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

**n = 3: Simpson’s \( \frac{3}{8} \)-Rule**

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

**n = 4: Boole’s Rule**

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

$$
\int_a^b f(x)\,dx = \frac{n}{2} \sum_{j=1}^{n/2} \int_{x_{2j-2}}^{x_{2j}} f(x)\,dx
$$

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

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

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

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

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