Lecture 7: Difference Approximations

1. Taylor Series

A function \( f(x) \) can be expanded about a point \( x_0 \) within some radius of convergence \( C \) as

\[
 f(x) = f(x_0) + \sum_{j=1}^{\infty} \frac{f^{(j)}(x_0)}{j!} (x - x_0)^j.
\]

- Taylor series

Proof

Write

\[
\int_{x_0}^{x} f'(\xi) \, d\xi = f(x) - f(x_0)
\]

or

\[
 f(x) = f(x_0) + \int_{x_0}^{x} f'(\xi) \, d\xi
\]

Use integration by parts ( \( Su' \, d\xi = uv - Su \, v \, d\xi \)),

with \( u = f'(\xi) \) and \( v = \xi - x \) to write

\[
f(x) = f(x_0) + [ (\xi-x) f'(\xi) ]_{x_0}^{x} - \int_{x_0}^{x} (\xi-x) f''(\xi) \, d\xi
\]

or

\[
f(x) = f(x_0) + (x-x_0) f'(x_0) + \int_{x_0}^{x} (x-\xi) f''(\xi) \, d\xi.
\]
Use integration by parts again with 
\[ u = f''(x) \] and 
\[ v = -\frac{1}{2}(x-x_0)^2 \] to get

\[ f(x) = f(x_0) + (x-x_0)f'(x_0) + \frac{(x-x_0)^2}{2}f''(x_0) \]

\[ + \int_{x_0}^{x} \frac{(x-\xi)^2}{2} f''(\xi) \, d\xi \]

Keep repeating integration by parts to obtain Taylor series.

**Radius of Convergence**

Consider power series with center \( x_0 \)

\[ y = \sum_{n=1}^{\infty} a_n (x-x_0)^n \]

(A special case of this is the Taylor series).

Series will converge for \( |x-x_0| < R \), where

\( R = \text{radius of convergence} \), and diverge for \( |x-x_0| > R \).
If the series is to converge, we require that for sufficiently large $C$, the terms get smaller in magnitude, such that

$$|a_n|/|x-x_0|^n > |a_{n+1}|/|x-x_0|^{n+1}$$

as $n \to \infty$. Divide by $|a_{n+1}|/|x-x_0|^{n+1}$ to get convergence criterion.

$$|x-x_0| < \frac{|a_n|}{|a_{n+1}|} = \left|\frac{a_n}{a_{n+1}}\right|$$

as $n \to \infty$. $C =$ maximum value of $|x-x_0|$ such that this convergence criterion holds, or

$$C = \lim_{n \to \infty} \left|\frac{a_n}{a_{n+1}}\right|.$$
Examples: Find radius of convergence of the following series.

1. \( e^x = \sum_{n=0}^{\infty} \frac{x^n}{n!} \)

   Soln:
   \[ \left| \frac{x^n}{n!} \right| > \left| \frac{x^{n+1}}{(n+1)!} \right| \quad \text{as} \quad n \to \infty \]

   \[ |x| < \frac{(n+1)!}{n!} \quad \text{as} \quad n \to \infty \]

   \[ \therefore C = \infty \] Series is everywhere convergent

2. \( \frac{1}{1-x} = \sum_{n=1}^{\infty} x^n \)

   Soln.
   \[ \left| x^n \right| > \left| x^{n+1} \right| \quad \text{as} \quad n \to \infty \]

   \[ |x| < 1 \quad \text{as} \quad n \to \infty \]

   \[ \therefore C = 1 \]
3. \[ \cos x = \sum_{n=0}^{\infty} \frac{(-1)^n}{n!} x^{2n} \]

**Soln:**

\[ \left| \frac{(-1)^n}{n!} x^{2n} \right| < \left| \frac{(-1)^{n+1}}{(n+1)!} x^{2n+2} \right| \quad \text{as} \quad n \to \infty \]

\[ |x|^2 < \left| \frac{(-1)^n}{(-1)^{n+1}} \frac{(n+1)!}{n!} \right| \quad \text{as} \quad n \to \infty \]

\[ C = \lim_{n \to \infty} \left| \frac{(-1)^n}{(-1)^{n+1}} (n+1) \right|^{1/2} = 0 \]

series everywhere convergent

4. \[ \sum_{n=0}^{\infty} n x^{3n} \]

**Soln:**

\[ |nx^{3n}| < |(n+1) x^{3n+3}| \quad \text{as} \quad n \to \infty \]

\[ |x|^3 < \left| \frac{n}{n+1} \right| \quad \text{as} \quad n \to \infty \]

\[ C = \lim_{n \to \infty} \left| \frac{n}{n+1} \right|^{1/3} = 1 \]

\[ \text{If } C = 0, \text{ series is divergent.} \]
Error Estimate for Truncated Taylor Series

Truncate Taylor series after \( n \) terms to write

\[
f(x) = f(x_0) + \sum_{j=1}^{n} \frac{f^{(j)}(x_0)}{j!} (x-x_0)^j + R_n,
\]

where from the derivation of the Taylor series using integration by parts, we find that

\[
R_n = \int_{x_0}^{x} \frac{(x-\xi)^n}{n!} f^{(n+1)}(\xi) \, d\xi.
\]

2nd Mean Value Theorem: If \( g(\xi) \) and \( h(\xi) \) are continuous functions such that \( h(\xi) \) does not change sign in the interval \((x_0, x)\), then some point \( a \) exists such that \( x > a > x_0 \) and

\[
\int_{x_0}^{x} g(\xi) h(\xi) \, d\xi = g(a) \int_{x_0}^{x} h(\xi) \, d\xi.
\]
Let $g(\xi) = f^{(n+1)}(\xi)$

\[ h(\xi) = \frac{(x - \xi)^n}{n!} \]

to write

\[ R_n = \int_{x_0}^{x} g(\xi) h(\xi) \, d\xi = g(a) \int_{x_0}^{x} h(\xi) \, d\xi \]

\[ R_n = f^{(n+1)}(a) \int_{x_0}^{x} \frac{(x - \xi)^n}{n!} \, d\xi \]

\[ R_n = f^{(n+1)}(a) \frac{(x - x_0)^{n+1}}{(n+1)!} \]

Upper bound for $R_n$:

\[ |R_n| \leq \max_{a \in [x_0, x]} \left| f^{(n+1)}(a) \right| \frac{(x - x_0)^{n+1}}{(n+1)!} \]
2. Difference Approximations

A. First Derivative

a) Forward Difference (first order)

Suppose that \( f(x) \) is known at positions \( x_i, \ i = 1, \ldots, n \), where \( x_{i+1} - x_i = h \). We wish to estimate \( f'(x) \) at \( x \).

Expand \( f(x_{i+1}) \) about \( f(x_i) \) in Taylor series:

\[
f(x_{i+1}) = f(x_i) + h f'(x_i) + R_1
\]

where \( R_1 = \frac{h^2}{2} \max_{a \in (x_i, x_{i+1})} \left| f''(a) \right| = O(h^2) \).

Solve for \( f'(x_i) \) to get:

\[
f'(x_i) = \frac{f_{i+1} - f_i}{h} - \frac{R_1}{2h^2} \]

where \( f_i = f(x_i) \)

\[
R_1/h = O(h).
\]
6) **Backward Difference**

Expand $f(x_{i-1})$ about $f(x_i)$ in Taylor series, using similar procedure as for forward difference:

$$ f_{i-1} = f_i - hf'_i + R_1 + o(h^2) $$

so

$$ f'_i = \frac{f_i - f_{i-1}}{h} + o(h) $$

5) **Centered Difference**

Expand $f_{i+1}$ and $f_{i-1}$ about $f_i$, and subtract the two.

$$ f_{i+1} = f_i + hf'_i + \frac{h^2}{2} f''_i + R_2 + o(h^3) $$

$$ f_{i-1} = f_i - hf'_i + \frac{h^2}{2} f''_i - R_2 $$

Subtract above two equations

$$ f_{i+1} - f_{i-1} = 2hf'_i + 2R_2 $$

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solve for \( f_i' \):

\[
f_i' = \frac{f_{i+1} - f_{i-1}}{2h} - \frac{R_e}{\eta h} o(h^2)
\]

B. Second Derivative

a) Centered Difference

Use \( h/2 \) as differencing interval:

\[
f_i' = \frac{f_{i+\frac{1}{2}} - f_{i-\frac{1}{2}}}{h} + o(h^2)
\]

\[
f_i'' = (f_i')' = \frac{f_{i+\frac{1}{2}} - f_{i-\frac{1}{2}}}{h} + o(h^2)
\]

\[
f_i'' = \frac{1}{h} \left[ \frac{f_{i+1} - f_i}{h} - \frac{f_i - f_{i-1}}{h} \right] + o(h^2)
\]

\[
f_i'' = \frac{f_{i+1} - 2f_i + f_{i-1}}{h^2} + o(h^2)
\]
b) Forward Derivative

(Use $h$ as differencing increment)

$$f_i' = \frac{f_{i+1} - f_i}{h} + o(h)$$

$$f_i'' = \frac{f_{i+1} - f_i}{h^2} + o(h)$$

$$f_i''' = \frac{1}{h} \left[ \frac{f_{i+2} - f_{i+1}}{h} - \frac{f_{i+1} - f_i}{h} \right] + o(h)$$

$$f_i'' = \frac{f_{i+2} - 2f_{i+1} + f_i}{h^2} + o(h)$$

Similarly with backward differencing.
C. Higher-Order Difference Approximations

Find approximation for 1st derivative using only forward difference with error \( O(h^2) \).

Expand \( f_{i+1} \) about \( f_i \) in Taylor series

\[
f_{i+1} = f_i + h f'_i + \frac{h^2}{2} f''_i + R_2 \quad \text{with} \quad O(h^3)
\]

Solve for \( f'_i \):

\[
f'_i = \frac{f_{i+1} - f_i}{h} - \frac{h}{2} f''_i - \frac{R_2}{h} \quad \text{with} \quad O(h^3)
\]

For term \( A \) use substitution with forward diff. approximation for \( f''_i \):

\[
\frac{h}{2} f''_i = \frac{h}{2} \left( \frac{f_{i+2} - 2 f_{i+1} + f_i}{h^2} \right) + \frac{h}{2} O(h)
\]

\[
= \frac{f_{i+2} - 2 f_{i+1} + f_i}{2h} + O(h^2)
\]

\[\text{same order as } R_2/h\]
Substitute to write

\[ f'_i = \frac{f_{i+1} - f_i}{h} - \frac{f_{i+2} - 2f_{i+1} + f_i}{2h} + O(h^2) \]

\[ f'_i = -\frac{f_{i+2} + 4f_{i+1} - 3f_i}{2h} + O(h^2) \]

We can follow similar procedure to obtain difference approximations of arbitrary accuracy.