51 Numerical Differentiation

We develop finite difference formulas for approximating derivatives.

### 8.1.1 Finite Difference Formulas

Recall from Calculus:

\[
    f'(x) = \lim_{h \to 0} \frac{f(x+h) - f(x)}{h}
\]

Using Taylor's Theorem (with "center" : \( x \)) we have:

\[
    f(x+h) = f(x) + hf'(x) + \frac{h^2}{2} f''(\xi)
\]

for some \( \xi \in (x, x+h) \). This equation implies the following:

**Two-point forward-difference formula**

\[
    f'(x) \approx \frac{f(x+h) - f(x)}{h} - \frac{h}{2} f''(\xi)
\]

where \( \xi \in (x, x+h) \).

(*Note: For small \( h \), this gives us a small error.

**Quantity.** We call the Two-point forward-difference formula a first-order method for approximating \( f'(x) \).

In general, we say a method is *an order* \( n \) if the error is \( O(h^n) \), for an approximation.

The idea here is that for first-order approximation, the error is proportional to \( h \) as \( h \to 0 \).
Ex. Use the Two-point forward-difference formula with \( h = 0.1 \) to approximate \( f'(x) \), where \( f(x) = \frac{1}{x} \) @ \( x = 2 \).

\[
f'(x) \approx \frac{f(x+h) - f(x)}{h} = \frac{\frac{1}{2.1} - \frac{1}{2}}{0.1} = \mathbf{2.387}
\]

True value: \( f'(x) = -\frac{1}{x^2} \) @ \( x = 2 \) \( \rightarrow \) error: \( 2.387 - (-0.25) = 2.637 \)

Compare the error to the predicted error given by \( \frac{h^2}{2} f''(c) \text{ for } c \in (2, 2.1) \)

\[
f''(x) = \frac{2}{x^3} \rightarrow \text{error in b/w } (0.1)2^3 a. 0.0155 \text{ & } (0.1)(2.1)^3 a. 0.0138
\]

which is consistent with our result.

Next we consider a means to develop a second-order formula.

By Taylor's Theorem:

\[
f(x+h) = f(x) + hf'(x) + \frac{h^2}{2} f''(x) + \frac{h^3}{6} f'''(c_1)
\]

\[
f(x-h) = f(x) - hf'(x) + \frac{h^2}{2} f''(x) - \frac{h^3}{6} f'''(c_2)
\]

Solving for \( f'(x) \):

\[
f'(x) = \frac{f(x+h) - f(x-h)}{2h} - \frac{h^2}{12} \left[ f''(c_1) - f''(c_2) \right]
\]

Before arriving at a "nice" clean answer, we would like to first consolidate the error terms above. To do so, we use an extension of the IVP method called...
Theorem [Generalized Intermediate Value Theorem]

Let \( f \) be a continuous function on \([a, b]\). Let \( x_1, \ldots, x_n \) be points in \([a, b]\) with \( a < x_1 < \cdots < x_n > b \). Then there exists a number \( c \in (x_1, x_n) \) such that

\[
\sum_{i=1}^{n} a_i f(x_i) = \left( \sum_{i=1}^{n} a_i \right) f(c) = a_1 f(x_1) + \cdots + a_n f(x_n)
\]

Proof

Let \( f(x_i) \) be the minimum and \( f(x_j) \) be the maximum of \( f \) in each interval \([x_{i-1}, x_i]\). Then

\[
a_1 f(x_1) + \cdots + a_n f(x_n) \leq a_1 f(x_i) + \cdots + a_n f(x_j) \leq a_1 f(x_1) + \cdots + a_n f(x_n)
\]

which implies

\[
f(x_i) \leq \frac{a_1 f(x_1) + \cdots + a_n f(x_n)}{a_1 + \cdots + a_n} \leq f(x_j)
\]

By the IMVT, there exists a number \( c \in (x_i, x_j) \) such that

\[
f(c) = \frac{a_1 f(x_1) + \cdots + a_n f(x_n)}{a_1 + \cdots + a_n}
\]

Observe that the Generalized IMVT (above) indicates that we may consolidate the error terms from before, whereas:

Three-point centered difference formula

\[
f''(c) = \frac{f(x+h)-f(x-h)}{2h} \quad \text{and} \quad \frac{h^2}{6} f'''(c)
\]

Order Two approximation!
Ex. Use the three-point central difference formula with \( h = 0.1 \) to approximate \( f'(x) \) with \( f(x) = \frac{1}{x} \), \( x = 2 \).

\[
f'(x) \approx \frac{f(x+h) - f(x-h)}{2h} = \frac{\frac{1}{2.1} - \frac{1}{1.9}}{0.2} = -2.506
\]

The error here is \( 0.006 \), a significant improvement on the two-point forward difference used previously.

Q: How do we numerically approximate higher derivatives?
A: Simply use Taylor series, as usual, and algebraically eliminate \( f''(x) \) terms, solve for \( f'''(x) \).

Recall:
\[
f(x+h) = f(x) + hf'(x) + \frac{h^2}{2} f''(x) + \frac{h^3}{6} f'''(x) + \frac{h^4}{24} f^{(4)}(c_1)
\]
\[
f(x-h) = f(x) - hf'(x) + \frac{h^2}{2} f''(x) - \frac{h^3}{6} f'''(x) + \frac{h^4}{24} f^{(4)}(c_2)
\]

\[
f(x+h) + f(x-h) = 2f(x) = h^2 f''(x) + \frac{h^3}{3!} \left[ f'''(c_1) + f'''(c_2) \right]
\]

One again we need the Generalized T dovT...

Three-Point Central-Difference Formula for Second Derivative

\[
f''(x) = \frac{f(x-h) - 2f(x) + f(x+h)}{h^2} - \frac{h^2}{12} f^{(4)}(c)
\]

where \( c \in (x-h, x+h) \).
A caveat for numerical differentiation

Each of the previous methods in §5.1 relies, fundamentally, on subtracting/adding nearly equal quantities. Unfortunately, when using floating point arithmetic (i.e., performing computations on a computer with a finite 

\[ E_{\text{mach}} \]

such computation can lead to significant deterioration in the quality of approximations due to loss of significance. We illustrate this phenomenon with an example.

**Example:** Approximate \( f'(x) \) when \( f(x) = e^x \) as \( x \to 0 \).

**Two-point formula:**

\[ f'(x) \approx \frac{e^{x+h} - e^x}{h} \]

**Three-point:**

\[ f'(x) \approx \frac{e^{x+h} - e^{x-h}}{2h} \]

(set \( h = 0.1 \))

<table>
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<th>( n )</th>
<th>error for 2-point</th>
<th>error for 3-point</th>
</tr>
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<td>-0.0517...</td>
<td>-0.001664</td>
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</tbody>
</table>

Why does this happen? Consider 3-point error:

\[ f'(x) - f'(p) = f'(x) - \frac{f(x+h) - f(x) + f(x-h)}{2h} = \cdots \]

\[ = f''(x) + \frac{h^2 E_2 - E_1}{2h} \]

**Error:** when \( h \) becomes too small 

error can actually increase!
**Extrapolation**

Assume that we have an \( n \)-order formula \( F(n) \) for approximately

The quantity \( Q \). This tells us that:

\[
Q = F(n) + Kh^n + \text{error}
\]

where \( K \) is roughly constant over

The range of \( h \). \( (x) \)

As before, we would like to algebraically manipulate this formula of order \( n \) so as to produce a higher order approximation. The key insight here is: that we use \( \frac{h}{2} \) instead of \( h \), as this should reduce the error from a constant times \( h^n \) to a constant times \( (\frac{1}{2})^n \); i.e. we reduce the error by a factor of \( 2^n \).

That is to say, we expect:

\[
Q - F(\frac{h}{2}) \approx \frac{1}{2^n} \left[ Q - F(n) \right]
\]

Solve for \( Q \)...

**Extrapolation for order- \( n \) formula** (Richardson Extrapolation)

\[
Q \approx \frac{2^n F(n/2) - F(n)}{2^n - 1}
\]

\[
Q = \frac{F_n(h) + Kh^n + O(h^{n+1})}{n\text{-order formula}}
\]
Now we cut \( h \) in half.

\[
Q = F_n \left( \frac{h}{2} \right) + k \left( \frac{h^m}{2^n} \right) + o \left( h^{n+1} \right)
\]

4. The extrapolated version which we call \( F_{\text{extr}}(h) \) satisfies

\[
F_{\text{extr}}(h) = \frac{2^n F_n \left( \frac{h}{2} \right) - F_n(h)}{2^n - 1}
\]

\[
= \frac{2^n \left( Q - Kh^n/2^n - o(h^{n+1}) \right) - \left( Q - Kh^n - o(h^{n+1}) \right)}{2^n - 1}
\]

\[
= Q - \frac{Kh^n + o(h^{n+1})}{2^n - 1} = Q + o(h^{n+1})
\]

This shows that \( F_{\text{extr}}(h) \) is at least an order \( n+1 \) formula for approximating the quantity \( Q \).

Exercise: Apply the extrapolation formula for second order central difference

\[
F_2(h) = \frac{2 F_n \left( \frac{h}{2} \right) - F_n(h)}{2^2 - 1}
\]

\[
= \left[ \frac{f(x + h/2) - 2 f(x) + f(x - h/2)}{h^2/4} \right]^{1/3}
\]

\[
= \left[ \frac{-f(x-h) - 8 f(x-h/2) + 8 f(x+h/2) - f(x+h)}{64} \right]^{1/3}
\]

\[
\rightarrow \text{A five-point central difference formula!}
\]

(This is an order \( n+1 \) formula.