Numerical Differentiation

MATH 375

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Background and Objectives

Recall: the definition of the derivative:

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

provided the limit exists.

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Objectives:

- Develop formulas which approximate the derivative.
- Quantify the errors in these formulas.

Taylor Polynomial Approximation

Suppose $f \in \mathcal{C}^2[a, b]$ and $x_0 \in (a, b)$, then

$$f(x) = f(x_0) + f'(x_0)(x - x_0) + \frac{f''(z(x))}{2}(x - x_0)^2$$

where $z(x)$ lies between x and x_0.

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where $z(x)$ lies between x and x_0.

Let $x = x_0 + h$, then

$$\begin{aligned} f(x_0 + h) &= f(x_0) + f'(x_0)h + \frac{f''(z(x))}{2}h^2 \\ \frac{f(x_0 + h) - f(x_0)}{h} &= f'(x_0) + \frac{f''(z(x))}{2}h \\ f'(x_0) &= \frac{f(x_0 + h) - f(x_0)}{h} - \frac{f''(z(x))}{2}h. \end{aligned}$$

Error Analysis

If h is small then

$$f'(x_0) \approx \frac{f(x_0+h) - f(x_0)}{h}.$$

If $\max_{a \le z \le b} |f''(z)| = M$ then the error in this approximation is bounded by

$$E \le \frac{M}{2}|h|.$$

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If $\max\limits_{a \le z \le b} |f''(z)| = M$ then the error in this approximation is bounded by

$$E \le \frac{M}{2}|h|.$$

- If $h > 0$ this is a **forward difference.**
- If $h < 0$ this is a **backward difference.**

More Accurate Formulas

Remark: the previous approximation to $f'(x_0)$ used the evaluation of f at only two points. If we use more than two points we can improve our approximation.

We will explore several **three-point formulas**.

Lagrange Interpolating Polynomial

- Let $\{x_0, x_1, x_2\}$ be distinct points in $[a, b]$ and suppose $f \in \mathcal{C}^3[a, b]$.
- Using the Lagrange Interpolating Polynomial of degree two:

$$
\begin{aligned}
f(x) &= \sum_{k=0}^{2} f(x_k) L_{2,k}(x) + \frac{f^{(3)}(z(x))}{3!}(x - x_0)(x - x_1)(x - x_2) \\
f'(x) &= \sum_{k=0}^{2} f(x_k) L'_{2,k}(x) \\
&\quad + \frac{d}{dx}\left[\frac{f^{(3)}(z(x))}{3!}\right](x - x_0)(x - x_1)(x - x_2) \\
&\quad + \frac{f^{(3)}(z(x))}{3!}\frac{d}{dx}\left[(x - x_0)(x - x_1)(x - x_2)\right]
\end{aligned}
$$

Evaluation of the Derivative (1 of 2)

If $x = x_i$ for $i = 0, 1, 2$ then the derivative simplifies to

$$f'(x_i) = \sum_{k=0}^{2} f(x_k) L'_{2,k}(x_i) + \frac{f^{(3)}(z(x_i))}{3!} \prod_{k=0, k \neq i}^{2} (x_i - x_k).$$

Note that

$$\begin{aligned} L'_{2,0}(x) &= \frac{2x - x_1 - x_2}{(x_0 - x_1)(x_0 - x_2)} \\ L'_{2,1}(x) &= \frac{2x - x_0 - x_2}{(x_1 - x_0)(x_1 - x_2)} \\ L'_{2,2}(x) &= \frac{2x - x_0 - x_1}{(x_2 - x_0)(x_2 - x_1)}. \end{aligned}$$

Evaluation of the Derivative (2 of 2)

Thus we may write:

$$
\begin{aligned}
f'(x_i) = f(x_0)\frac{2x_i - x_1 - x_2}{(x_0 - x_1)(x_0 - x_2)} + f(x_1)\frac{2x_i - x_0 - x_2}{(x_1 - x_0)(x_1 - x_2)} \\
+ f(x_2)\frac{2x_i - x_0 - x_1}{(x_2 - x_0)(x_2 - x_1)} + \frac{f^{(3)}(z(x_i))}{6} \prod_{k=0, k \neq i}^{2} (x_i - x_k).
\end{aligned}
\tag{1}
$$

Evenly Spaced Nodes (1 of 2)

Now suppose that x_0, x_1, and x_2 are evenly spaced in the sense that

$$x_1 = x_0 + h \quad \text{and} \quad x_2 = x_0 + 2h,$$

then the derivative $f'(x_0)$ given by Eq. (1) can be written as

$$\begin{aligned}
f'(x_0) &= f(x_0)\frac{2x_0 - x_1 - x_2}{(x_0 - x_1)(x_0 - x_2)} + f(x_1)\frac{2x_0 - x_0 - x_2}{(x_1 - x_0)(x_1 - x_2)} \\
&\quad + f(x_2)\frac{2x_0 - x_0 - x_1}{(x_2 - x_0)(x_2 - x_1)} + \frac{f^{(3)}(x_0)}{6}(x_0 - x_1)(x_0 - x_2) \\
&= \frac{-3}{2h}f(x_0) + \frac{2}{h}f(x_0 + h) - \frac{1}{2h}f(x_0 + 2h) + \frac{f^{(3)}(x_0)}{6}2h^2 \\
f'(x_0) &= \frac{1}{2h}\left[-3f(x_0) + 4f(x_0 + h) - f(x_0 + 2h)\right] + \frac{h^2}{3}f^{(3)}(z(x_0)). \quad (2)
\end{aligned}$$

Evenly Spaced Nodes (2 of 2)

In a similar way we may derive by setting $x_i = x_2$ in Eq. (1)

$$\begin{aligned}
f'(x_2) &= f(x_0)\frac{2x_2 - x_1 - x_2}{(x_0 - x_1)(x_0 - x_2)} + f(x_1)\frac{2x_2 - x_0 - x_2}{(x_1 - x_0)(x_1 - x_2)} \\
&\quad + f(x_2)\frac{2x_2 - x_0 - x_1}{(x_2 - x_0)(x_2 - x_1)} + \frac{f^{(3)}(x_2)}{6}(x_2 - x_0)(x_2 - x_1) \\
&= \frac{1}{2h}f(x_0) - \frac{2}{h}f(x_0 + h) + \frac{3}{2h}f(x_0 + 2h) + \frac{f^{(3)}(x_2)}{6}2h^2 \\
f'(x_2) &= \frac{1}{2h}\left[f(x_0) - 4f(x_1) + 3f(x_2)\right] + \frac{h^2}{3}f^{(3)}(z(x_2)). \qquad (3)
\end{aligned}$$

Change of Variables

In Eq. (3) replace x_0 by $x_0 - 2h$ to obtain

$$f'(x_0) = \frac{1}{2h}\left[f(x_0 - 2h) - 4f(x_0 - h) + 3f(x_0)\right] + \frac{h^2}{3} f^{(3)}(z(x_0)). \quad (4)$$

Note that Eq. (4) is merely Eq. (2) (repeated below) with h replaced by $-h$. Thus they constitute only one expression for $f'(x_0)$.

$$f'(x_0) = \frac{1}{2h}\left[-3f(x_0) + 4f(x_0 + h) - f(x_0 + 2h)\right] + \frac{h^2}{3} f^{(3)}(z(x_0))$$

Centered Difference (1 of 2)

If we set $x_i = x_1$ in Eq. (1) then we have

$$\begin{aligned}
f'(x_1) &= f(x_0)\frac{2x_1 - x_1 - x_2}{(x_0 - x_1)(x_0 - x_2)} + f(x_1)\frac{2x_1 - x_0 - x_2}{(x_1 - x_0)(x_1 - x_2)} \\
&\quad + f(x_2)\frac{2x_1 - x_0 - x_1}{(x_2 - x_0)(x_2 - x_1)} + \frac{f^{(3)}(x_1)}{6}(x_1 - x_0)(x_1 - x_2) \\
&= \frac{-1}{2h}f(x_0) - (0)f(x_0 + h) + \frac{1}{2h}f(x_0 + 2h) - \frac{f^{(3)}(x_2)}{6}h^2 \\
f'(x_1) &= \frac{1}{2h}\left[f(x_2) - f(x_0)\right] - \frac{h^2}{6}f^{(3)}(z(x_1)). \qquad (5)
\end{aligned}$$

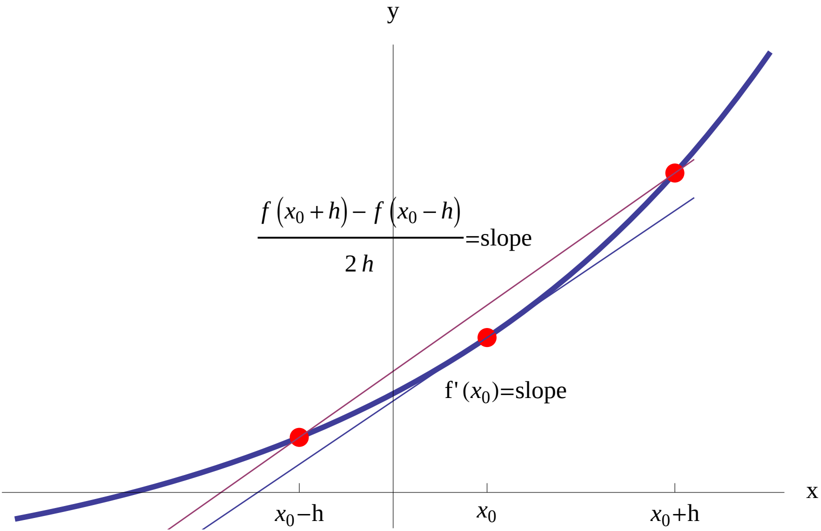
This is called the **centered difference formula** or **three-point midpoint formula**.

Centered Difference (2 of 2)

If we replace x_0 by $x_0 - h$,

$$f'(x_0) = \frac{1}{2h}\left[f(x_0 + h) - f(x_0 - h)\right] - \frac{h^2}{6} f^{(3)}(z(x_0)). \tag{6}$$

Graphical Interpretation



Summary of Formulae

We have two approximations to $f'(x_0)$:

$$f'(x_0) \approx \frac{1}{2h}\left[-3f(x_0) + 4f(x_0+h) - f(x_0+2h)\right] \tag{7}$$

$$f'(x_0) \approx \frac{1}{2h}\left[-f(x_0-h) + f(x_0+h)\right] \tag{8}$$

Remarks

- The approximation in Eq. (7) makes use of x_0 and two forward points $x_0 + h$ and $x_0 + 2h$.
- The approximation in Eq. (8) makes use of a point to the left of x_0 and a point to the right of x_0.
- The error in the approximation in Eq. (8) is half the size of the error in Eq. (7).
- The approximation in Eq. (7) can only be used if $x_0 + h$ and $x_0 + 2h$ both lie in $[a, b]$.
- The approximation in Eq. (8) can only be used if $x_0 - h$ and $x_0 + h$ both lie in $[a, b]$.

Example (1 of 2)

Suppose $f(x) = x \sin x$. Using Eq. (7) to approximate $f'(1)$ with $h = 0.1$ yields

$$f'(1) = \frac{1}{0.2}\left[-3f(1) + 4f(1.1) - f(1.2)\right] \approx 1.39226$$

Using Eq. (8) to approximate $f'(1)$ with $h = 0.1$ yields

$$f'(1) = \frac{1}{0.2}\left[f(1.1) - f(0.9)\right] \approx 1.37677$$

For purposes of comparison, the correct value to six significant digits is $f'(1) \approx 1.38177$.

Example (2 of 2)

- A bound for the error in the 3-point forward approximation is

$$M = \frac{(0.1)^2}{3} \max_{1 \leq z \leq 1.2} \left| f^{(3)}(z) \right| = \frac{0.01}{3}(3.23095) = 0.0107698.$$

Absolute error: 0.0104893

Example (2 of 2)

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  Absolute error: 0.0104893
- A bound for the error in the centered difference approximation is

  $$M = \frac{(0.1)^2}{6} \max_{0.9 \leq z \leq 1.1} \left| f^{(3)}(z) \right| = \frac{0.01}{6}(3.17258) = 0.00528763.$$

  Absolute error: 0.0051039

Five-Point Formulas

Five-point Midpoint Formula

$$\begin{aligned} f'(x_0) &= \frac{1}{12h}\left[f(x_0-2h)-8f(x_0-h)+8f(x_0+h)-f(x_0+2h)\right] \\ &\quad + \frac{h^4}{30}f^{(5)}(z) \end{aligned}$$

where z is between x_0-2h and x_0+2h.

Five-point Endpoint Formula

$$\begin{aligned} f'(x_0) = \frac{1}{12h}&\left[-25f(x_0)+48f(x_0+h)-36f(x_0+2h)\right. \\ &\left. + 16f(x_0+3h)-3f(x_0+4h)\right] \\ &+ \frac{h^4}{5}f^{(5)}(z) \end{aligned}$$

where z is between x_0 and x_0+4h.

Higher Order Derivatives

Suppose $f \in \mathcal{C}^4[a, b]$ and $x_0 \in (a, b)$ then using Taylor's Theorem

$$f(x) = f(x_0) + f'(x_0)(x - x_0) + \frac{f''(x_0)}{2}(x - x_0)^2 + \frac{f'''(x_0)}{6}(x - x_0)^3 + \frac{f^{(4)}(z)}{24}(x - x_0)^4$$

where z is between x_0 and x.

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where z is between x_0 and x.

Evaluate this function at $x = x_0 \pm h$.

Evaluation

$$f(x_0 - h) = f(x_0) - f'(x_0)h + \frac{f''(x_0)}{2}h^2 - \frac{f'''(x_0)}{6}h^3 + \frac{f^{(4)}(z)}{24}h^4$$

$$f(x_0 + h) = f(x_0) + f'(x_0)h + \frac{f''(x_0)}{2}h^2 + \frac{f'''(x_0)}{6}h^3 + \frac{f^{(4)}(w)}{24}h^4$$

with $x_0 - h \leq z \leq x_0 \leq w \leq x_0 + h$.

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with $x_0 - h \leq z \leq x_0 \leq w \leq x_0 + h$.

Now add the two expressions.

$$f(x_0 - h) + f(x_0 + h) = 2f(x_0) + f''(x_0)h^2 + \frac{h^4}{24}\left[f^{(4)}(z) + f^{(4)}(w)\right]$$

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\begin{aligned}
f(x_0-h) &= f(x_0) - f'(x_0)h + \frac{f''(x_0)}{2}h^2 - \frac{f'''(x_0)}{6}h^3 + \frac{f^{(4)}(z)}{24}h^4 \\
f(x_0+h) &= f(x_0) + f'(x_0)h + \frac{f''(x_0)}{2}h^2 + \frac{f'''(x_0)}{6}h^3 + \frac{f^{(4)}(w)}{24}h^4
\end{aligned}
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with $x_0 - h \leq z \leq x_0 \leq w \leq x_0 + h$.

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f(x_0-h) + f(x_0+h) = 2f(x_0) + f''(x_0)h^2 + \frac{h^4}{24}\left[f^{(4)}(z) + f^{(4)}(w)\right]
$$

Now solve this equation for $f''(x_0)$.

Approximating $f''(x)$

$$f''(x_0) = \frac{1}{h^2}\left[f(x_0 - h) - 2f(x_0) + f(x_0 + h)\right] - \frac{h^2}{24}\left[f^{(4)}(z) + f^{(4)}(w)\right]$$

Thus if h is small then

$$f''(x_0) \approx \frac{1}{h^2}\left[f(x_0 - h) - 2f(x_0) + f(x_0 + h)\right]. \tag{9}$$

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The error term involves two evaluations of $f^{(4)}(x)$, but can be simplified.

Error Term

Since $x_0 - h \leq z \leq w \leq x_0 + h$ then

$$\begin{aligned}
\frac{h^2}{24}\left|f^{(4)}(z) + f^{(4)}(w)\right| &\leq \frac{h^2}{24}\left(\left|f^{(4)}(z)\right| + \left|f^{(4)}(w)\right|\right) \\
&\leq \frac{h^2}{12}\max_{|x_0 - y| \leq h}\left|f^{(4)}(y)\right|
\end{aligned}$$

which we will use as a bound for the error in the approximation to $f''(x)$.

Example

Suppose $f(x) = x \sin x$. Using Eq. (9) to approximate $f''(1)$ with $h = 0.1$ yields

$$f''(1) = \frac{1}{(0.1)^2}\left[f(0.9) - 2f(1) + f(1.1)\right] \approx 0.238035.$$

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A bound for the error is

$$E = \frac{(0.1)^2}{12} \max_{|1-y| \le 0.1} \left| f^{(4)}(y) \right| = 0.00148454.$$

Absolute error: 0.00109912

Behavior of the Absolute Error

Let $f(x) = x \sin x$ and use the centered-difference formula to approximate $f'(1)$ for various values of h.

h	**Absolute Error**
1.0×10^{-5}	5.53118×10^{-11}
5.0×10^{-6}	1.99396×10^{-13}
2.5×10^{-6}	2.20051×10^{-11}
1.0×10^{-6}	1.99618×10^{-13}
5.0×10^{-7}	1.11222×10^{-10}
2.5×10^{-7}	2.22244×10^{-10}
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There appears to be an h below which the absolute error is roughly constant.

Truncation *versus* Round-off Error

Consider the centered-difference formula:

$$f'(x_0) = \frac{1}{2h}\left[f(x_0+h) - f(x_0-h)\right] - \underbrace{\frac{h^2}{6} f^{(3)}(z)}_{\text{truncation error}} .$$

The **truncation error** is due to using only a finite number of terms of the Taylor series for $f(x)$.

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The **truncation error** is due to using only a finite number of terms of the Taylor series for $f(x)$.

Our arithmetic is also subject to **round-off error** which we will denote $e(x)$.

Total Error (1 of 2)

Suppose $f(x) = \hat{f}(x) + e(x)$ where

- $f(x)$ is the true value of the function
- $\hat{f}(x)$ is the calculated value of the function, and
- $e(x)$ is the round-off error.

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- $\hat{f}(x)$ is the calculated value of the function, and
- $e(x)$ is the round-off error.

Then we have

$$\begin{aligned} f(x_0 + h) &= \hat{f}(x_0 + h) + e(x_0 + h) \\ f(x_0 - h) &= \hat{f}(x_0 - h) + e(x_0 - h) \end{aligned}$$

and thus

$$f'(x_0) = \frac{1}{2h}\left[\hat{f}(x_0 + h) + e(x_0 + h) - \hat{f}(x_0 - h) - e(x_0 - h)\right] - \frac{h^2}{6} f^{(3)}(z).$$

Total Error (2 of 2)

$$f'(x_0) = \frac{1}{2h}\left[\hat{f}(x_0+h) + e(x_0+h) - \hat{f}(x_0-h) - e(x_0-h)\right] - \frac{h^2}{6} f^{(3)}(z).$$

Assume the round-off error is bounded by $\epsilon > 0$ and isolate the error terms on the right-hand side and take the absolute value.

Total Error (2 of 2)

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Assume the round-off error is bounded by $\epsilon > 0$ and isolate the error terms on the right-hand side and take the absolute value.

$$\begin{aligned}
\left| f'(x_0) - \frac{1}{2h}\left(\hat{f}(x_0+h) - \hat{f}(x_0-h)\right) \right| &= \left| \frac{e(x_0+h) - e(x_0-h)}{2h} - \frac{h^2}{6} f^{(3)}(z) \right| \\
&\leq \frac{\epsilon}{2h} + \frac{\epsilon}{2h} + \frac{Mh^2}{6} \\
&= \frac{\epsilon}{h} + \frac{Mh^2}{6}
\end{aligned}$$

Minimizing Total Error (1 of 2)

$$\left| f'(x_0) - \frac{1}{2h}\left(\hat{f}(x_0+h) - \hat{f}(x_0-h)\right) \right| \leq \frac{\epsilon}{h} + \frac{Mh^2}{6}$$

Remark: making *h* small reduces truncation error but increases round-off error.

Question: what is the optimal value of *h* that minimizes the total error?

Minimizing Total Error (2 of 2)

Let $g(h) = \frac{\epsilon}{h} + \frac{Mh^2}{6}$ and find its absolute minimum.

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Let $g(h) = \frac{\epsilon}{h} + \frac{Mh^2}{6}$ and find its absolute minimum.

$$\begin{aligned} g'(h) &= -\frac{\epsilon}{h^2} + \frac{Mh}{3} \\ 0 &= -\frac{\epsilon}{h^2} + \frac{Mh}{3} \\ h^* &= \sqrt[3]{\frac{3\epsilon}{M}} \end{aligned}$$

Minimizing Total Error (2 of 2)

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0 &= -\frac{\epsilon}{h^2} + \frac{Mh}{3} \\
h^* &= \sqrt[3]{\frac{3\epsilon}{M}}
\end{aligned}
$$

If we assume $\epsilon = 10^{-16}$ and $M \approx 3.23095$ then $h^* \approx 4.5 \times 10^{-6}$ which is consistent with our earlier results.

Summary

$$f'(x_0) = \frac{f(x_0+h) - f(x_0)}{h} - \frac{f''(z)}{2}h$$

$$f'(x_0) = \frac{1}{2h}\left[-3f(x_0) + 4f(x_0+h) - f(x_0+2h)\right] + \frac{h^2}{3}f^{(3)}(z)$$

$$f'(x_0) = \frac{1}{2h}\left[f(x_0+h) - f(x_0-h)\right] - \frac{h^2}{6}f^{(3)}(z)$$

$$\begin{aligned} f'(x_0) = {} & \frac{1}{12h}\left[-25f(x_0) + 48f(x_0+h) - 36f(x_0+2h) + 16f(x_0+3h) - 3f(x_0+4h)\right] \\ & + \frac{h^4}{5}f^{(5)}(z) \end{aligned}$$

$$f'(x_0) = \frac{1}{12h}\left[f(x_0-2h) - 8f(x_0-h) + 8f(x_0+h) - f(x_0+2h)\right] + \frac{h^4}{30}f^{(5)}(z)$$

$$f''(x_0) = \frac{1}{h^2}\left[f(x_0-h) - 2f(x_0) + f(x_0+h)\right] - \frac{h^2}{24}\left[f^{(4)}(z) + f^{(4)}(w)\right]$$

Homework

- Read Section 4.1
- Exercises: 1a, 3a, 5a, 7a, 20, 21, 24, 25