Numerical Differentiation: Part 2

Math 131: Numerical Analysis

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April 4, 2024

Outline

- Higher-order finite difference formulas
- Stability of numerical differentiation
- Richardson Extrapolation

Section 1

Higher-order Finite Difference formulas

Motivation

- First order numerical differentiaion formulas good, but sometimes we desire more accuracy
- Higher order required in certain computing applications
- Already seen one example of higher order in the last lecture - *centered differences*
- Another strategy is to use the Lagrange interpolating polynomials.

($n + 1$)-point Formulas

Idea

- Replace the function $f(x)$ by a Lagrange interpolating polynomial.
- Use the derivative of the Lagrange polynomial in place of the derivative of $f(x)$.

Remark: Appropriate error estimates can also be produced.

General $(n+1)-$point formula

The $(n+1)$-point formula (Equation 4.2, p. 176, textbook) is given by:

$$f'(x_j) = \sum_{k=0}^{n} f(x_k) L_k'(x_j) + \frac{f^{(n+1)}(\xi(x_j))}{(n+1)!} \prod_{k=0, k\neq j}^{n} (x_j - x_k)$$

where $[x_0, x_1, \ldots, x_n]$ are $n+1$ distinct points on some interval.

Observations

1. In general, more points leads to higher accuracy.
2. This comes at the expense of more function evaluations and greater roundoff error.
3. Formulas most useful when we choose equally spaced points

3-point formulas

The ***3-point midpoint(centered)***approximation for the first derivative

$$f'(x) = \frac{f(x+h) - f(x-h)}{2h} - \frac{h^2}{6} f^{(3)}(\xi) \tag{1}$$

The ***3-point endpoint*** approximation for the first derivative

$$f'(x) = \frac{-3f(x) + 4f(x+h) - f(x+2h)}{2h} + \frac{h^2}{3} f^{(3)}(\xi) \tag{2}$$

Comparison

Note the difference in the number of function evaluations and the constant in the error term.

5-point formulas

The ***5-point midpoint (centered)*** approximation for the first derivative

$$f'(x) = \frac{f(x-2h) - 8f(x-h) + 8f(x+h) - f(x+2h)}{12h} + \frac{h^4}{30} f^{(5)}(\xi) \tag{3}$$

The ***5-point endpoint*** approximation for the first derivative

$$\begin{aligned} f'(x) = \frac{1}{12h}\Big[&\frac{-25f(x) + 48f(x+h) - 36f(x+2h)}{2h} \\ &+ 16f(x+3h) - 3f(x+4h)\Big] + \frac{h^4}{5} f^{(5)}(\xi) \end{aligned} \tag{4}$$

Practical Tips

- More points yield more accurate approximations.
- More points also means more funcation evaluations.
- Roundoff error will also increase with higher-order.
- In general midpoint formulas have smaller errors for same number of points.
- In practice, most commonly used formulas are the 3 and 5 point formulas.

Section 2

Stability

Stability

- Sometimes an algorithm will fail to yield a good result due to stability.
- Computing derivatives by using finite differences is a prime example of such a possibility. This is due to the properties of computer arithmetic.
- In practice there is a delicate balance between truncation error and roundoff error. As a result one needs to be careful when choosing the ***step size***, h.

We briefly looked at an example earlier where we looked at the accuracy of the forward difference approximation as a function of h.

Forward Difference Example (Recap of earlier lecture)

Example

Approximate $f'(x)$ for $f(x) = \cos(x)$ and $h = 10^{-3} - 10^{-15}, x = \pi/6$.

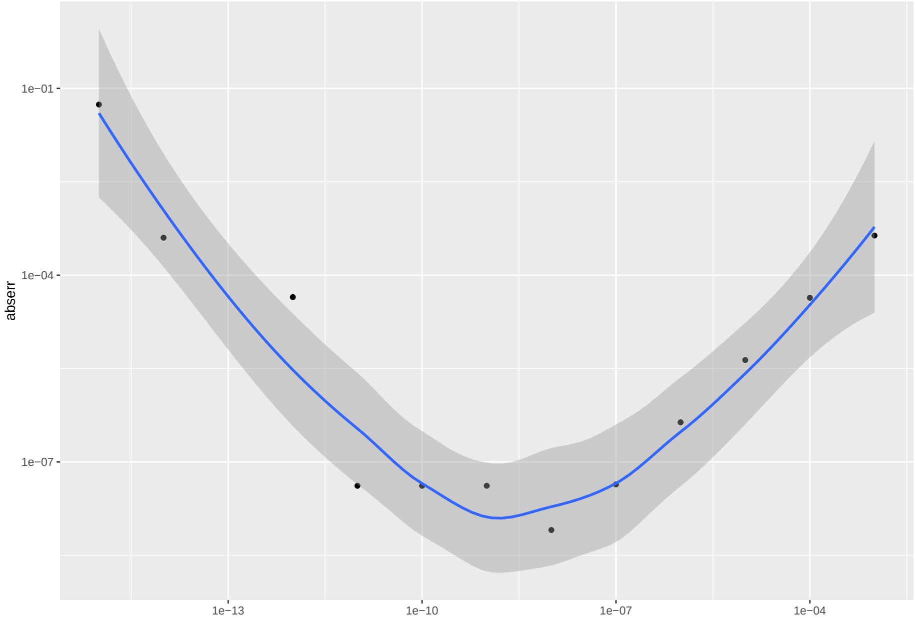
$$f'(x_0) \approx \frac{f(x_0 + h) - f(x_0)}{h}$$

Forward Difference Example Solution

Table 1: Absolute and Relative Error in finite difference (F.D) approximation as a function of stepsize h.

h	F.D	abserr	relerr
1e-03	-0.5004329	4.329293e-04	8.658587e-04
1e-04	-0.5000433	4.330044e-05	8.660088e-05
1e-05	-0.5000043	4.330117e-06	8.660235e-06
1e-06	-0.5000004	4.330569e-07	8.661137e-07
1e-07	-0.5000000	4.359063e-08	8.718126e-08
1e-08	-0.5000000	8.063495e-09	1.612699e-08
1e-09	-0.5000000	4.137019e-08	8.274037e-08
1e-10	-0.5000000	4.137019e-08	8.274037e-08
1e-11	-0.5000000	4.137019e-08	8.274037e-08
1e-12	-0.5000445	4.445029e-05	8.890058e-05
1e-14	-0.4996004	3.996389e-04	7.992778e-04
1e-15	-0.5551115	5.511151e-02	1.102230e-01

Forward Difference Example Solution



Remarks

Important

- Notice that for each decrease in the value of h by an order of magnitude, both the absolute and relative error have a corresponding decrease in their values.
- *This is exactly what the theory predicts.*
- However, it is important to note that this is true only up to a certain point. We'll discuss this more fully when we get to the sections on computer arithmetic and roundoff error.

Analysis

Let's try to analyze what is happening here.

Consider the central difference formula for $f'(x)$ at some point x_0.

$$f'(x_0) = \frac{f(x_0 + h) - f(x_0 - h)}{2h} - \frac{h^2}{6} f^{(3)}(\xi(x))$$

When evaluating a function on a computer, we know that we do not have infinite precision, hence suppose:

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

where $e(x)$ is the roundoff error as a result of computing $f(x)$ and $\hat{f}(x)$ is the computed value of the function.

(cont.)

The error in the finite difference approximation can then be written as:

$$f'(x_0) - \Big(\frac{\hat{f}(x_0+h) - \hat{f}(x_0-h)}{2h}\Big)$$
$$= \frac{e(x_0+h) - e(x_0-h)}{2h} - \frac{h^2}{6} f^{(3)}(\xi(x))$$

Now assume that:

$$e(x_0 \pm h) < \tau, \quad \tau > 0,$$
$$|f^{(3)}(\xi)| < M \quad \xi \in [x_0 - h, x_0 + h].$$

The error in the finite difference approximation can be bounded by

$$\text{error} \leq \frac{\tau}{h} + \frac{h^2}{6} M$$

Proof

$$
\begin{aligned}
\Big| f'(x_0) - \Big(\frac{\hat{f}(x_0+h) - \hat{f}(x_0-h)}{2h} \Big) \Big| \\
&= \Big| \frac{e(x_0+h) - e(x_0-h)}{2h} - \frac{h^2}{6} f^{(3)}(\xi(x)) \Big| \\
&\leq \Big| \frac{e(x_0+h) - e(x_0-h)}{2h} \Big| + \Big| \frac{h^2}{6} f^{(3)}(\xi(x)) \Big| \\
&\leq \frac{1}{2h} \Big(\Big| e(x_0+h) \Big| + \Big| e(x_0-h) \Big| \Big) + \Big| \frac{h^2}{6} M \Big| \\
&\leq \frac{1}{2h}(2\tau) + \frac{h^2}{6} M \\
&\leq \frac{\tau}{h} + \frac{h^2}{6} M
\end{aligned}
$$

The proof is a simple exercise in using triangle inequality and the bounds we assumed on the roundoff error and the third derivative.

Observations

As $h \to 0$ ***the second term goes to 0, but the first term blows up.***

We need to find the "sweet spot" to minimize the error in the approximation.

Can show that the optimal h^* is given by:

$$h^* = \sqrt[3]{\frac{3\tau}{M}}$$

Unfortunately, one rarely knows either ϵ or M.

Rule of thumb

However a good rule of thumb is to choose h so that you only perturb half the digits of x. That suggests

$$h^* = \sqrt{\epsilon}$$

where ϵ is machine precision. On most modern computers $\epsilon = 10^{-16}$, so this translates into

$$h \approx 10^{-8}$$

Caution

Finite Difference approximations are an excellent example of unstable algorithms.

Section 3

Richardson Extrapolation

Richardson Extrapolation

- The methods we've studied so far for computing numerical derivatives are good and generally lead to good approximations.
- But what if we need to have greater accuracy?
- This section covers one approach to generating higher-order (more accurate) approximations to derivatives using an idea dating back to 1927

Idea

- In spirit, it is not unlike what we did when we derived the central difference approximation
- By noticing that if we took the two $O(h)$ approximations for the forward and backward difference and combined them in such a way as to cancel out one of the error terms we could get a higher-order approximation $O(h^2)$.

Idea

- Combine 2 approximations with similar error terms to obtain a more accurate approximation.
- Can be used in many different contexts including
  - interpolation (Aitken),
  - quadrature (Romberg, adaptive methods),
  - IVP,
  - acceleration of convergence of sequences.

Example: Second derivative

Let's consider how we arrived at the 3-point formula for the second derivative:

$$f''(x) = \frac{f(x+h) - 2f(x) + f(x-h)}{h^2} - \frac{h^2}{12} f^{(4)}(\xi).$$

In that derivation we started with the Taylor series about $x+h$ and $x-h$.

(cont.)

This time let's also consider one additional term, which would give us:

$$f''(x) = \frac{f(x+h) - 2f(x) + f(x-h)}{h^2} - \frac{h^2}{12} f^{(4)}(x) - \frac{h^4}{360} f^{(6)}(x) + O(h^5) \tag{5}$$

Now replace h by $2h$.

$$\begin{aligned} f''(x) = & \frac{f(x+2h) - 2f(x) + f(x-2h)}{4h^2} - \frac{4h^2}{12} f^{(4)}(x) \\ & - \frac{16h^4}{360} f^{(6)}(x) + O(h^5). \end{aligned} \tag{6}$$

Notice that the second formula has the same term for the fourth derivative except it is multiplied by 4.

(cont.)

- This leads to the natural idea of multiplying the first equation by 4 and subtracting the second equation from it, which will cancel that part of the error term.
- If we do this, we will (after a bit of simple algebra) get to the following formula:

$$f''(x) = \frac{1}{12h^2}\Big[-f(x+2h)+16f(x+h)-30f(x) + 16f(x-h)-f(x-2h)\Big] + \frac{h^4}{90}f^{(6)}(x) + O(h^5).$$

This formula for the second derivative is now ***fourth order*** accurate.

Another approach

- Notice that using this approach wasn't specific to the second derivative formula.
- All we needed was an approximation to some quantity where we knew the error term.
- Therefore we could use this same approach anytime.

Richardson Extrapolation

Suppose we can write an approximation to some quantity as:

$$M = N(h) + K_1 h^2 + K_2 h^4 + K_3 h^6 + \dots.$$

For example let's define:

$$M = f''(x) \quad \text{and} \quad N(h) = \frac{f(x+h) - 2f(x) + f(x-h)}{h^2}$$

Using these we can re-write Equation 5 as:

$$\begin{aligned} M &= N(h) - \frac{h^2}{12} f^{(4)}(x) - \frac{h^4}{360} f^{(6)}(x) + O(h^5). \\ &= N(h) + K_1 h^2 + K_2 h^4 + \dots \end{aligned} \tag{7}$$

(cont.)

Now let's write the formula using the step size $h/2$.

$$M = N(h/2) + K_1 \frac{h^2}{4} + K_2 \frac{h^4}{16} + \ldots \tag{8}$$

Let's multiply Equation 8 by 4 and subtract Equation 7:

$$\begin{array}{rl} 4M &= 4N(h/2) + K_1 h^2 + K_2 \dfrac{h^4}{4} + \ldots \\ - \quad M &= N(h) + K_1 h^2 + K_2 h^4 + \ldots \\ \hline 3M &= \Big[4N(h/2) - N(h)\Big] + K_2 \Big(\dfrac{h^4}{4} - h^4\Big) + \ldots \end{array}$$

Solving for M, leads to:

$$M = \frac{1}{3}\big[4N(h/2) - N(h)\big] + O(h^4)$$

(cont.)

One final adjustment is usually made - we will split

$$4N(h/2) = 3N(h/2) + N(h/2)$$

to give us the form of the formula that is commonly used.

$$M = N(h/2) - \frac{1}{3}\big[N(h/2) - N(h)\big] + O(h^4).$$

General procedure

The procedure to obtain a fourth order accurate approximation using the two second order formulas is then easily accomplished through the following procedure:

1. compute $N(h)$, for some given h
2. compute $N(h/2)$
3. Combine the two using the formula $M = N(h/2) - \frac{1}{3}\left[N(h/2) - N(h)\right]$

Practical Tips

The trick is then to find the right combination to cancel out the leading error term, when evaluating the equation at two different points, e.g. h and $h/2$.

There are advantages and disadvantages to Richardson extrapolation as for all numerical methods.

Advantages & Disadvantages

Advantages:

- it is simple and general so we can apply the technique to many different problems.
- applications in interpolation, numerical integration, and even differential equations.
- It also leads to formulas for higher-order approximations for derivatives, which are useful in certain applications.

Disadvantages

- the technique requires more points at which to evaluate the function and
- it makes an assumption that the higher-order derivatives are nicely bounded, which may or may not hold true.

Section 4

Summary

Summary

Some of the key takeaways

- Taylor series can be used to generate finite difference approximations to first derivatives, second derivatives, etc.
- We can also use Lagrange polynomials to generate similar formulas. (covered in book as well as in the optional lecture in Section 5).
- Richardson extrapolation is a simple and general approach that combines lower-order formulas to generate higher-order approximations (at additional function evaluation costs).
- ***Numerical differentiation is inherently unstable*** - but it's also (essentially) the only game in town. Care must be taken in choosing good step sizes.