Numerical Differentiation

Omer F Koru and Ethan Feilich

University of Pennsylvania

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Basic Concepts

Why numerical differentiation?

- We have a function we'd like to differentiate, but we only have function values at discrete points
- We'd like to study changes in data, where it may not be obvious that an underlying function exists
- Exact formulas for a function may be available, but computationally expensive
- Discrete approximating solutions to differential equations are defined on a grid, and we need to evaluate derivatives at the grid points

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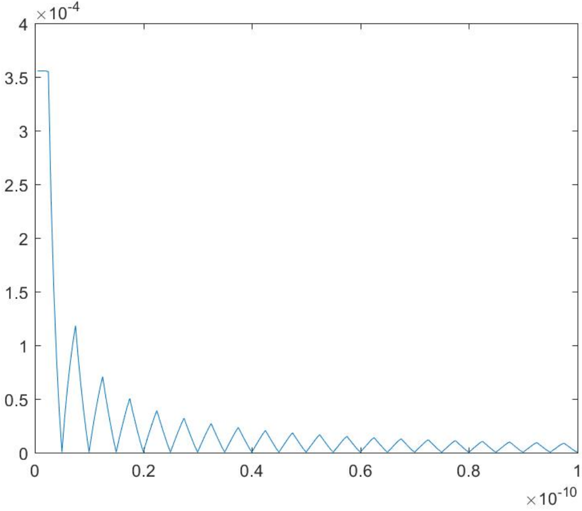
Centered differencing carries a smaller truncation error which converges “faster”.

Error for Different h



$f(x) = x^2$, derivative at 2 with forward differencing
h from 10^{-12} to 10^{-10}

Optimal Choice of h

To minimize the sum of round-off and truncation error, choose $h = h^*$ by

$$h = \sqrt{\frac{\epsilon_f f}{f''}} \approx \sqrt{\epsilon_f} x_c$$

where ϵ_f is the fractional accuracy with which f is computed. Without information about f and f'' we typically assume $x_c = x$.

Interpolation

Assuming we have $f(x_0), \ldots, f(x_n)$, the Lagrange form of the interpolation polynomial is:

$$Q_n(x) = \sum_{j=0}^{n} f(x_j) l_j(x)$$

The numerical differentiation formula, derived from the interpolation error formula is:

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

where $\xi_{x_k} \in (min(x, x_0, ..., x_k), max(x, x_0, ..., x_k))$.

Undetermined Coefficients

The method of undetermined coefficients is described by the algorithm:

- Express the derivative as a linear combination of function values at certain points
- Derive the Taylor expansions of the function at the approximation points
- Equate the coefficients of the function and its derivatives on both sides

Undetermined Coefficients

Suppose we have three points, then the linear combination and Taylor approximation around x_1 are:

$$f'(x_1) \approx af(x_1) + bf(x_2) + cf(x_3)$$

$$f(x_i) = f(x_1) + f'(x_1)(x_i - x_1) + \frac{f''(x_1)(x_i - x_1)^2}{2} + \frac{(x_i - x_1)^3 f'''(\xi_i)}{6}$$

for $i = 2, 3$ and $\xi_i \in (x_1, x_i)$. Solving for a,b, and c gives the 3x3 system:

$$\begin{aligned} a + b + c &= 0 \\ b(x_2 - x_1) + c(x_3 - x_1) &= 1 \\ b(x_2 - x_1)^2 + c(x_3 - x_1)^2 &= 0 \end{aligned}$$

Richardson's Extrapolation

Let $L = f'(x)$. The truncation error from the center differencing approximation has the form:

$$
\begin{aligned}
L &= \frac{f(x+h) - f(x-h)}{2h} - \left[\frac{h^2}{3!} f^{(3)}(x) + \frac{h^4}{5!} f^{(5)}(x)\right] + \dots \\
&= D(h) + e_2 h^2 + e_4 h^4 + \dots
\end{aligned}
$$

where the coefficients e_k don't depend on h.

Richardson's Extrapolation

The approximation can be improved by incorporating more points.

$$L = D(2h) + e_2(2h)^4 + e_4(2h)^4 + \dots$$
$$4L = 4D(2h) + 4e_2(2h)^4 + 4e_4(2h)^4 + \dots$$

Subtracting the two approximations gives:

$$L = \frac{4D(h) - D(2h)}{3} - 4e_4 h^4 + \dots$$

Which eliminates the $e_2 h^2$ term from the error. The resulting fourth order approximation is:

$$f'(x) = \frac{-f(x+2h) + 8f(x+h) - 8f(x-h) + f(x-2h)}{12h} + O(h^4)$$

Symbolic Differentiation

```
%symbolic variables
syms a
% symbolic function
g= log(a+5)*a^2*exp(sqrt(a));
% symbolic diff
dg = diff(g);
display(dg);
% evaluation of diff at x=2
a=2;
%substitute a=2 to dg
eval(subs(dg))
```

$$g(a) = log(a+5) \times a^2 \times e^{\sqrt{a}}$$

```
dg =
2*a*log(a + 5)*exp(a^(1/2))+(a^2*exp(a^(1/2)))/(a + 5)+
(a^(3/2)*log(a+5)*exp(a^(1/2)))/2
```