BLG 202E

Numerical Differentiation

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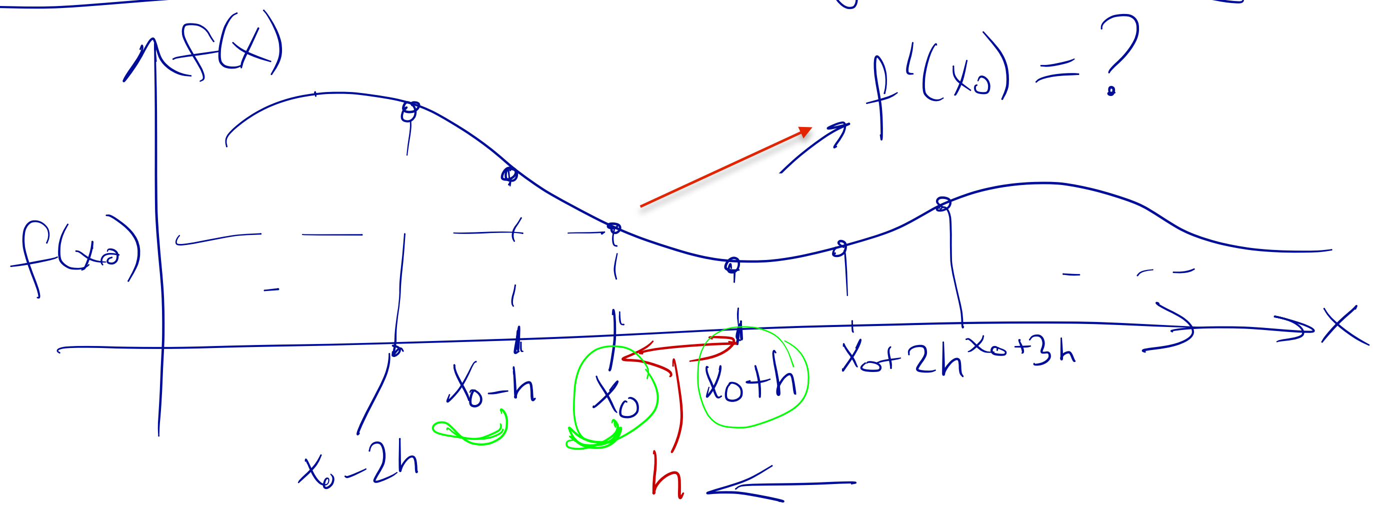
Chapter 14 Numerical Differentiation :



We'll use points nearby x_0

Outline:

1) Taylor series approach : error analysis
2) Richardson extrapolation
3) Polynomial interpolation to do derivation
4) Round-off vs discretization error
   = truncation error

① Taylor Series Approach:

(i) Two-point formulas: $f(x)$: expand about x_0: $x = x_0 - h$

$$f(x_0-h) = f(x_0) - h\,f'(x_0) + \frac{h^2}{2} f''(\xi), \quad \xi \in [x_0-h, x_0]$$

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

error we make: $e(h) = f'(x_0) - \boxed{\frac{f(x_0)-f(x_0-h)}{h}} = \frac{h}{2} f''(\xi)$ C

1st order accurate.

$e(h) \leq C \cdot h \Rightarrow \boxed{O(h)}$

$\Rightarrow$ This is 1^{st} order accurate $= O(h)$.

Truncation error (Discretization) $= \frac{h}{2} f''(\xi)$

(one-sided deriv formulas)

$$\Rightarrow f'(x_0) = \frac{f(x_0) - f(x_0 - h)}{h}$$: Backward difference

Exercise:
$\Rightarrow$ You can derive forward difference formula for $f'(x_0)$

(ii) 3-pt formula: A centered formula (at x_0):

Expand about $x = x_0$ at $x = x_0 - h$, $x = x_0 + h$

$$f(x_0+h) = f(x_0) + h f'(x_0) + \frac{h^2}{2!} f''(x_0) + \frac{h^3}{3!} f'''(\xi_1)$$

$$f(x_0-h) = f(x_0) - h f'(x_0) + \frac{h^2}{2} f''(x_0) - \frac{h^3}{3!} f'''(\xi_2)$$

$$f(x_0+h) - f(x_0-h) = 2h f'(x_0) + \frac{h^3}{3!}\underbrace{\left(f'''(\xi_1) + f'''(\xi_2)\right)}_{f'''(\xi)\text{ by mean value thm.}}$$

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

Centered derivative
2^{nd} order accurate.

Truncation error
$O(h^2)$ $\rightarrow$ accuracy $>$ 1-sided deriv.

Exercise: Derive one-sided 2^{nd} order formula for $f'(x_0)$:

Expand $\longrightarrow$ get rid of $f''(x_0)$ term

$f(x_0+2h) =$

$f(x_0+h) =$

$\underline{f'''(\xi)}$
expand until.

(iii) 5-pt formulas:

eg. Derive a 4^{th} order centered formula for $f'(\cdot)$

$$f(x_0 \pm h) = f(x_0) \pm h f'(x_0) + \frac{h^2}{2} f''(x_0) \pm \frac{h^3}{6} f'''(x_0) + \frac{h^4}{24} f^{(iv)}(x_0) \pm \frac{h^5}{120} f^{(v)}(x_0) + \frac{h^6}{720} f^{(vi)}(x_0) + O(h^7)$$

$$f(x_0 \pm 2h) = f(x_0) \pm 2h f'(x_0) + \frac{(2h)^2}{2} f''(x_0) \pm \frac{8h^3}{6} f'''(x_0) + \frac{16h^4}{24} f^{(iv)}(x_0) \pm \frac{32h^5}{120} f^{(v)}(x_0) + \frac{64h^6}{720} f^{(vi)}(x_0) + O(h^7)$$

Subtract the pair $f(x_0 \pm h)$ from each other
" " $f(x_0 \pm 2h)$ " " "

$$\times 8 \left\{ f(x_0+h) - f(x_0-h) = 2h f'(x_0) + \frac{2h^3}{6} f'''(x_0) + \frac{2h^5}{120} f^{(v)}(x_0) + O(h^7) \right.$$

$$\times(-1) \left\{ f(x_0+2h) - f(x_0-2h) = 4h f'(x_0) + \frac{16}{6} h^3 f'''(x_0) + \frac{64h^5}{120} f^{(v)}(x_0) + O(h^7) \right.$$

eliminate these

$$+$$

$$\boxed{f'(x_0) = \frac{1}{12h}\left(f(x_0-2h) - 8f(x_0-h) + 8f(x_0+h) - f(x_0+2h)\right)}$$

$$+ \underbrace{\frac{48}{120}\frac{h^5}{12h} f^{(v)}(\xi)}_{+O(h^4)} \longrightarrow e(h) = \frac{h^4}{30} f^{(v)}(\xi)$$

(iv) 3-pt formula: for the 2^{nd} derivative:

Add $f(x_0 \pm h)$; all odd powers will cancel.

$$f(x_0+h)+f(x_0-h) = 2f(x_0)+h^2 f''(x_0)+\frac{h^4}{24}\left(f^{(iv)}(\xi_1)+f^{(iv)}(\xi_2)\right)$$

$\Rightarrow$ Solve for $f''(x_0)$ to get second derivative formula:

$$\boxed{f''(x_0) = \frac{1}{h^2}\left(f(x_0+h)-2f(x_0)+f(x_0-h)\right)} - \underbrace{\frac{h^2}{12}f^{(iv)}(\xi)}_{O(h^2)}$$

truncation error

Ex 14.1.: $\longrightarrow$ Slides

$\boxed{O(h^q)} \Leftarrow \boxed{e(h) \leq C\cdot h^q}$

(2) Richardson Extrapolation: Want to generate higher-order formulas from lower order ones

with more than one step size

Ex 14.2: Example method of derivation

Derive a centered 4^{th} order formula for the 2^{nd} derivative

Write the centered 3-pt formula for h:

Also write it for $2h$:

to cancel $f^{(iv)}(\cdot)$ term

$$4\times \left\{ f''(x_0) = \frac{1}{h^2}\left(\underbrace{f_{-1}}_{f(x_0-h)} - 2\underbrace{f_0}_{f(x_0)} + \underbrace{f_1}_{f(x_0+h)}\right) - \frac{h^2}{12}f^{(iv)}(x_0) - \frac{h^4}{360}f^{(vi)}(x_0) + O(h^6) \right.$$

$$-1\left\{ f''(x_0) = \frac{1}{(2h)^2}\left(f_{-2}-2f_0+f_2\right) - \frac{(2h)^2}{12}f^{(iv)}(x_0) - \frac{16h^4}{360}f^{(vi)}(x_0) + O(h^6) \right.$$

$+$

$$3f''(x_0) = \frac{4}{h^2}\left(f_{-1}-2f_0+f_1\right) - \frac{1}{(2h)^2}\left(f_{-2}-2f_0+f_2\right) + \underbrace{\frac{12h^4}{360}f^{(vi)}}_{O(h^4)}$$

$\Rightarrow$ Re-arrange

$$f''(x_0) = \frac{1}{12h^2}\left(-f_{-2} + 16f_{-1} - 30f_0 + 16f_1 - f_2\right) + O(h^4).$$

$\left.\begin{array}{l} 4^{th} \text{ order formula for} \\ \quad 2^{nd} \text{ derivative} \end{array}\right\}$ $e(h) = \frac{h^4}{90} f^{(vi)}(\xi)$, $\xi \in [x_0-2h, x_0+2h]$

The idea in this ex. can be applied to higher order derivative approximations. (Richardson extrapolation)

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③ Deriving methods using polynomial interpolation:

— T.S. method may be difficult to apply when the points are NOT equally spaced; also when desired order of accuracy is high.

Soln: $\Rightarrow$

Idea:

$f(x) \approx p_n(x)$

$f'(x) \approx p_n'(x)$

use an interpolating polynomial $p_n(x)$, and take its derivative.

We'll use Lagrange polyn. interp:

$$p_n(x) = \sum_{j=0}^{n} \underbrace{c_j}_{f(x_j)} L_j(x)$$

$\longrightarrow$ Lagrange is the most natural.

Chapter 10: Want to obtain an expression for the error in polynomial interpolation (p. 314)

$f(x) \approx p_n(x)$ $\qquad f \in C[a,b]$

$e_n(x) = f(x) - p_n(x)$

$$f(x) = p_{n+1}(x) = p_n(x) + f[x_0, x_1, \dots, x_n, x]\, \psi_n(x)$$

(10.4).

divided differences.

$$\psi_n(x) = \prod_{i=0}^{n} (x - x_i)$$

$$e_n(x) = f(x) - p_n(x) = f[x_0, x_1, \dots, x_n, x]\, \psi_n(x)$$

Theorem (Divided Differences & Derivatives):

(page 312)

If f has $n+1$ bdd (bounded) derivatives, then

$\exists$ a point $\xi = \xi(x)$, $\xi \in [a,b]$ s.t.

$$f[x_0, x_1, \dots, x_n, x] = \frac{f^{(n+1)}(\xi)}{(n+1)!}$$

We assumed that x is another interpolation point:

$$\boxed{f(x) - p_n(x) = \frac{f^{(n+1)}(\xi)}{(n+1)!}\, \psi_n(x)}$$

expression for the error we make in polynomial interp.

$$\max_{a \le x \le b} |f(x) - p_n(x)| \le \frac{1}{(n+1)!} \max_{a \le t \le b} |f^{(n+1)}(t)| \max |\psi_n(x)|$$

Back to Chapter 14.3:

$\ast$ x_0, $x_1 = x_0 + h$ } Derive interpolant $p_1(x)$ to $f(x)$ using abscissae x_0, x_1.

$$p_1(x) = \sum_{j=0}^{1} f(x_j) L_j(x)$$

$$L_0(x) = \frac{(x - x_1)}{(x_0 - x_1)}, \quad L_1(x) = \frac{(x - x_0)}{(x_1 - x_0)}$$

$$p_1(x) = f(x_0) L_0(x) + f(x_1) L_1(x)$$

exercise derive

$$p_1(x) = f(x_0) + \frac{f(x_1) - f(x_0)}{h} (x - x_0)$$

Assume, x is another interpolation point:

$$f(x) = p_1(x) + f[x_0, x_1, x] (x - x_0)(x - x_1)$$

$$f'(x) = \frac{f(x_1) - f(x_0)}{h} + ((x - x_0) + (x - x_1)) f[x_0, x_1, x] + \frac{d}{dx} f[x_0, x_1, x] (x - x_0)(x - x_1)$$

- We get rid of the last term by evaluating the $f'(x)$ at $x = x_0$:

$$\boxed{f'(x_0) = \frac{f(x_0+h) - f(x_0)}{h}} - h \frac{f''(\xi)}{2!}, \quad \xi \in [x_0, x_1]$$

1st order forward difference formula for $f'(\cdot)$.

Truncation error $O(h)$

Goals of this Chapter:
— to develop useful formulas for approximating derivatives of a function $f(x)$ at $x = x_0$.
[redacted]

Chapter 14: Numerical Differentiation

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Slides for the book
A First Course in Numerical Methods (published by SIAM, 2011)
http://www.ec-securehost.com/SIAM/CS07.html

— to understand errors in numerical differentiation.

Outline

- Deriving formulas using Taylor series
- Richardson extrapolation
- Deriving formulas using polynomial interpolation
- Roundoff and data errors
- ~~*Differentiation matric~~es

*advanced

What is numerical differentiation

- Given a function $f(x)$ that is differentiable in the vicinity of a point x_0, it is often necessary to estimate the derivative $f'(x)$ and higher derivatives using nearby values of f.
- Example 1.2 in Chapter 1 provides a simple instance of numerical differentiation. Here we consider the more complete picture. For instance, we ask
  - how to achieve more, higher order difference formulas in an easy and orderly fashion?
  - how to control or altogether avoid the strong cancellation error effect demonstrated in Example 1.3?

  These and several other questions are considered here.

Why numerical differentiation?

- Numerical differentiation is a major tool in deriving methods for differential equations (see Chapter 16).
- Approximating derivatives is ubiquitous in continuous optimization and nonlinear equations (see Chapters 3 and 9).
- The need to estimate derivatives from discrete data often arises in applications.

Outline

- Deriving formulas using Taylor series
- Richardson extrapolation
- Deriving formulas using polynomial interpolation
- Roundoff and data errors
- *~~Differentiation matrices~~

Difference formulas using Taylor series

- This is the most convenient, ad hoc approach.
- Start from Taylor's expansion, generally written for a small $h > 0$ as

$$\begin{aligned} f(x_0 \pm h) &= f(x_0) \pm hf'(x_0) + \frac{h^2}{2} f''(x_0) \pm \frac{h^3}{6} f'''(x_0) + \\ &+ \frac{h^4}{24} f^{(iv)}(x_0) \pm \frac{h^5}{120} f^{(v)}(x_0) + \frac{h^6}{720} f^{(vi)}(x_0) + \mathcal{O}(h^7). \end{aligned}$$

- Truncate this as needed and derive an expression for $f'(x_0)$.
- Simplest example is the forward difference of Example 1.2. Likewise, backward difference is obtained by writing $f(x_0 - h) = f(x_0) - hf'(x_0) + \frac{h^2}{2} f''(\xi)$, hence $f'(x_0)$ is approximated by $\frac{f(x_0) - f(x_0 - h)}{h}$ with truncation error $\frac{h}{2} f''(\xi)$ for some $x_0 - h \le \xi \le x_0$.
- The forward and backward formulas are one-sided, two-point formulas with truncation error $\mathcal{O}(h)$, i.e., they are 1st order methods.

Higher order formulas

- We can easily derive 2nd order, three-point formulas.
  - Centered: subtract expressions for $f(x_0+h)$ and $f(x_0-h)$:
  $$f(x_0+h)-f(x_0-h)=2hf'(x_0)+\frac{2h^3}{6}f'''(x_0)+\frac{2h^5}{120}f^{(v)}(x_0)+\mathcal{O}(h^7).$$
  Thus, $f'(x_0)$ is approximated by $\frac{f(x_0+h)-f(x_0-h)}{2h}$ with truncation error $-\frac{h^2}{6}f'''(\xi)$.
  - One-sided: Please verify that the approximation $\frac{1}{2h}\left(-3f(x_0)+4f(x_0+h)-f(x_0+2h)\right)$ has truncation error $\frac{h^2}{3}f'''(\xi)$ where $\xi\in[x_0,x_0+2h]$.
- Using five points we can derive 4th order formulas, e.g., the formula
$$f'(x_0)\approx\frac{1}{12h}\left(f(x_0-2h)-8f(x_0-h)+8f(x_0+h)-f(x_0+2h)\right),$$
has the truncation error $e(h)=\frac{h^4}{30}f^{(v)}(\xi)$.
- A similar approach may be used to eliminate for the 2nd derivative. For instance, the famous centred, three-point, 2nd order formula is
$$f''(x_0)=\frac{1}{h^2}\left(f(x_0-h)-2f(x_0)+f(x_0+h)\right)-\frac{h^2}{12}f^{(iv)}(\xi).$$

Ex 14.1:

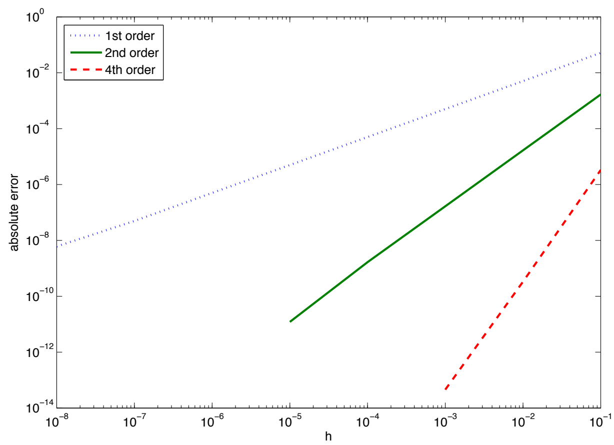
Example

Approximate $f'(0)$ for $f(x) = e^x$ using methods of order 1, 2 and 4. Record and plot errors for $h = 10^{-k}$, $k = 1, \ldots, 5$.

$f(x_0+h) - f(x_0)$

h	$\frac{e^h - 1}{h} - 1$	$\frac{e^h - e^{-h}}{2h} - 1$	$\frac{-e^{2h}+8e^h-8e^{-h}+e^{-2h}}{12h} - 1$
0.1	5.17e-2	1.67e-3	3.33e-6
0.01	5.02e-3	1.67e-5	3.33e-10
0.001	5.0e-4	1.67e-7	−4.54e-14
0.0001	5.0e-5	1.67e-9	−2.60e-13
0.00001	5.0e-6	1.21e-11	−3.63e-12

Truncation error for a method of order q decreases ~ by 10^{-q}



Straight lines terminate where the round-off errors take over.

Difference formulas

Notation: $f_j = f(x_0 + jh),\ j = 0, \pm 1, \pm 2, \ldots$.

Derivative	points	type	order	formula
$hf'(x_0)$	2	forward	1	$f_1 - f_0$
	2	backward	1	$f_0 - f_{-1}$
$2hf'(x_0)$	3	centred	2	$f_1 - f_{-1}$
	3	forward	2	$-3f_0 + 4f_1 - f_2$
$12hf'(x_0)$	5	centred	4	$f_{-2} - 8f_{-1} + 8f_1 - f_2$
$h^2 f''(x_0)$	3	centred	2	$f_{-1} - 2f_0 + f_1$
$12h^2 f''(x_0)$	5	centred	4	$-f_{-2} + 16f_{-1} - 30f_0 + 16f_1 - f_2$

Taylor series approach assessment

- Simple and natural to use.
- Directly obtain both formula and its truncation error estimate.
- However, this approach is ad hoc and does not automatically generalize:
  - Sometimes we need to approximate with a non-uniform step size, e.g., approximate $f'(x_0)$ using $f(x_0),\ f(x_0+h),\ f(x_0-h/3)$. This would require an individual treatment.
  - Tedious work (and increased chances for human error) may be required for deriving high order formulas.

Richardson extrapolation

- This is a straightforward, favourite technique based on a simple yet general principle for deriving higher order formulas from lower order ones.
- More limited than the general Taylor series approach, but methodical and easily applied.
- Can be applied repeatedly for generating methods of higher and higher order.
- Used in classical methods for numerical integration and differential equations (Chapters 15, 16).
- **Basic idea**: use lower order formula with more than one step size, and combine to eliminate the leading term of the truncation error.

Example of method derivation

Goal: Derive a centred, 4th order formula for the 2nd derivative.

- Write the centred 3-point formula for f_0 once for h and once for $2h$,

$$\begin{aligned} f''(x_0) &= \frac{1}{h^2}(f_{-1} - 2f_0 + f_1) - \frac{h^2}{12} f^{(iv)}(x_0) + \mathcal{O}(h^4) \\ &= \frac{1}{(2h)^2}(f_{-2} - 2f_0 + f_2) - \frac{(2h)^2}{12} f^{(iv)}(x_0) + \mathcal{O}(h^4). \end{aligned}$$

- The leading term of the truncation error in the second line is 4 times larger than in the first. So multiply the first line by 4 and subtract the 2nd line:

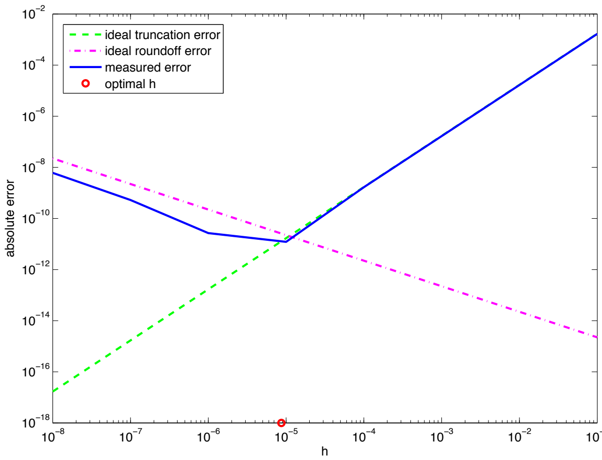
$$3f''(x_0) = \frac{4}{h^2}(f_{-1} - 2f_0 + f_1) - \frac{1}{(2h)^2}(f_{-2} - 2f_0 + f_2) + \mathcal{O}(h^4).$$

- Rearrange:

$$f''(x_0) = \frac{1}{12h^2}(-f_{-2} + 16f_{-1} - 30f_0 + 16f_1 - f_2) + \mathcal{O}(h^4).$$

Roundoff and data errors

- Recall Example 1.3: for very small h and smooth f we may encounter severe cancellation error amplified by h^{-1} when approximating the derivative f'. Then, roundoff error takes over, and it grows as h decreases.
- Clearly, this problem happens with all numerical differentiation methods we have seen thus far (e.g. see our table of difference formulas).
- In fact, for higher order methods roundoff error dominates sooner (i.e. for larger h) because truncation error decreases faster.



Example

Consider the 2nd order method $f'(x_0) \simeq D_h = \frac{f(x_0+h)-f(x_0-h)}{2h}$.

- Denote $\mathrm{fl}(f(x)) \equiv \bar{f}(x) = f(x) + e_r(x), \quad |e_r(x)| \le \epsilon$, where ϵ depends on the **rounding unit**. Assuming exact arithmetic for simplicity, $\overline{D}_h = \frac{\bar{f}(x_0+h)-\bar{f}(x_0-h)}{2h}$.
- Obtain

$$
\begin{aligned}
|\overline{D}_h - D_h| &= \left| \frac{\bar{f}(x_0+h)-\bar{f}(x_0-h)}{2h} - \frac{f(x_0+h)-f(x_0-h)}{2h} \right| \\
&= \left| \frac{e_r(x_0+h)-e_r(x_0-h)}{2h} \right| \\
&\le \left| \frac{e_r(x_0+h)}{2h} \right| + \left| \frac{e_r(x_0-h)}{2h} \right| \le \frac{\epsilon}{h}.
\end{aligned}
$$

- So, if $|f'''(\xi)| \le M$ then

$$
\begin{aligned}
\left|f'(x_0) - \overline{D}_h\right| &= \left|(f'(x_0) - D_h) + \left(D_h - \overline{D}_h\right)\right| \\
&\le |f'(x_0) - D_h| + \left|D_h - \overline{D}_h\right| \le \frac{h^2 M}{6} + \frac{\epsilon}{h}.
\end{aligned}
$$

- "Theoretically optimal" h is where this bound is minimized: $h_* = (3\epsilon/M)^{1/3}$.

How bad can this problem be, and what can we do?

- The answer highly depends on the application!
- For discretization of differential equations, can usually keep $h \gg \epsilon$ using IEEE standard "double precision" word (but not "single precision"); see Chapter 2.
- For calculating gradient and Hessian in a more controlled optimization context (also, constrained multibody simulations), it is usually fine to use h "not too small". An alternative is automatic differentiation methods, not covered here, which do not suffer from roundoff error problems.
- For applications involving numerical differentiation of measured data which may contain noise, it is easy to get stuck! A possible remedy is to smooth the data (i.e., approximate the data by a smooth function), and only then differentiate.

Example: differentiating noisy data

We create a function $f(x)$ to be differentiated by first sampling $\sin(x)$ on $[0, 2\pi]$ with $h = .01$, and then adding 1% Gaussian noise to these 200π values. The result is in the left panel below.

Next, numerical differentiation approximately gives $\cos(x)$ plus the noise magnified by $1/h = 100$. The (unacceptable) result is depicted in the right panel below.