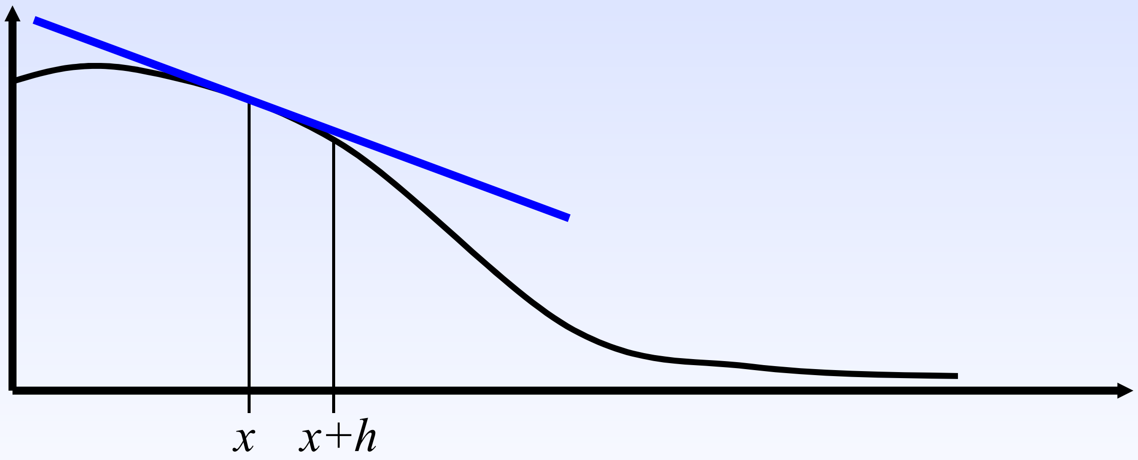
Numerical Differentiation

Chapter 23

- The mathematical definition:

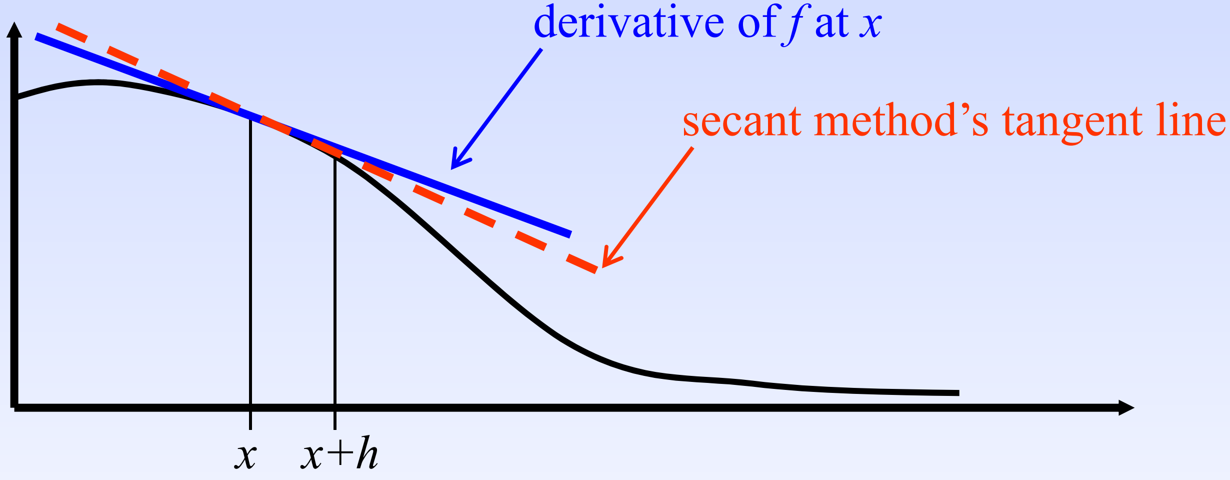
$$f'(x) = \lim_{h \to 0} \frac{f(x+h) - f(x)}{h}$$

- Can also be thought of as the tangent line.



Numerical Differentiation

- We can not calculate the limit as *h* goes to zero, so we need to approximate it.
- Applying directly for a non-zero *h* leads to the slope of the secant curve.



- When the value of the function is known only at discrete points, the differentiation is to be automated in an algorithm.

Differentiation Formula

- Revisit Taylor Series expansion:

$$f(x_{i+1}) = f(x_i) + f'(x_i)h + \frac{f''(x_i)}{2!}h^2 + \frac{f^{(3)}(x_i)}{3!}h^3 + \cdots + \frac{f^n(x_i)}{n!}h^n + R_n$$

with $R_n = \frac{f^{(n+1)}(\xi)}{(n+1)!}h^{n+1}$ and step size $h = x_{i+1} - x_i$

Then, the first order approximation (n=1) is:

$$f(x_{i+1}) = f(x_i) + f'(x_i)h + R_1$$

$$\Rightarrow f'(x_i)h = f(x_{i+1}) - f(x_i) - R_1$$

$$\Rightarrow f'(x_i) = \frac{f(x_{i+1}) - f(x_i)}{h} - \frac{R_1}{h}$$

Forward difference approximation of the first derivative

$$\Rightarrow f'(x_i) = \frac{f(x_{i+1}) - f(x_i)}{h} - \frac{R_1}{h}$$

The derivative of f at x_i

An approximation to it

error

This equation is called a *finite divided difference*. It can be represented generally as:

$$f'(x_i) = \frac{f(x_{i+1}) - f(x_i)}{x_{i+1} - x_i} - O(x_{i+1} - x_i)$$

or simply $f'(x_i) = \dfrac{\Delta f_i}{h} - O(h)$

Forward difference approximation of the first derivative

first forward difference

$$f'(x_i) = \frac{\Delta f_i}{h} - O(h)$$

error

step size

$$\frac{\Delta f_i}{h}$$ *first finite divided difference*

It is termed a "forward" difference because it utilizes data at *i* and *i*+1 to estimate the derivative.

Backward difference approximation of the first derivative

$$f(x_{i+1}) = f(x_i) + f'(x_i)h + \frac{f''(x_i)}{2}h^2 + \cdots$$

here $x_{i+1} = x_i + h$; so,

$$f(x_i + h) = f(x_i) + f'(x_i)h + \frac{f''(x_i)}{2}h^2 + \cdots$$

Replacing $+h$ with $-h$ yields:

$$f(x_i - h) = f(x_i) + f'(x_i)(-h) + \frac{f''(x_i)}{2}(-h)^2 + \cdots$$

$$f(\underbrace{x_i - h}_{x_{i-1}}) = f(x_i) - f'(x_i)h + \frac{f''(x_i)}{2}h^2 + \cdots$$

x_{i-1} : previous term

Backward difference approximation of the first derivative

The Taylor series can be expanded backward to calculate a previous value on the basis of a present value in the following way.

$$f(x_{i-1}) = f(x_i) - f'(x_i)h + \frac{f''(x_i)}{2}h^2 + \cdots$$

first backward difference

$$f'(x_i) = \underbrace{\frac{f(x_i) - f(x_{i-1})}{x_i - x_{i-1}}}_{\text{first backward difference}} + O(x_i - x_{i-1})$$

$$f'(x_i) = \frac{\Delta f_i}{h} + O(h)$$

Centered difference approximation of the first derivative

A third way to approximate the first derivative is to subtract backward Taylor series expansion from the forward Taylor series expansion

$$f(x_{i+1}) = f(x_i) + f'(x_i)h + \frac{f''(x_i)}{2}h^2 + \cdots$$

$$f(x_{i-1}) = f(x_i) - f'(x_i)h + \frac{f''(x_i)}{2}h^2 + \cdots$$

$-$

$$\Rightarrow f(x_{i+1}) = f(x_{i-1}) + 2f'(x_i)h + \frac{2f^{(3)}(x_i)}{3!}h^3 + \cdots$$

Centered difference approximation of the first derivative

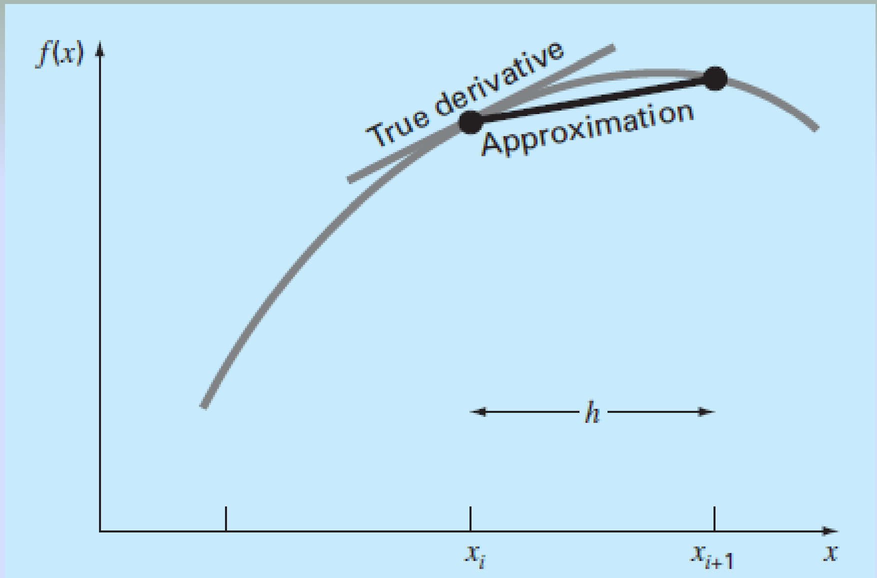
Solving for the first derivative term yields:

$$f'(x_i) = \frac{f(x_{i+1}) - f(x_{i-1})}{2h} - \frac{f^{(3)}(x_i)}{6}h^2 + \cdots$$

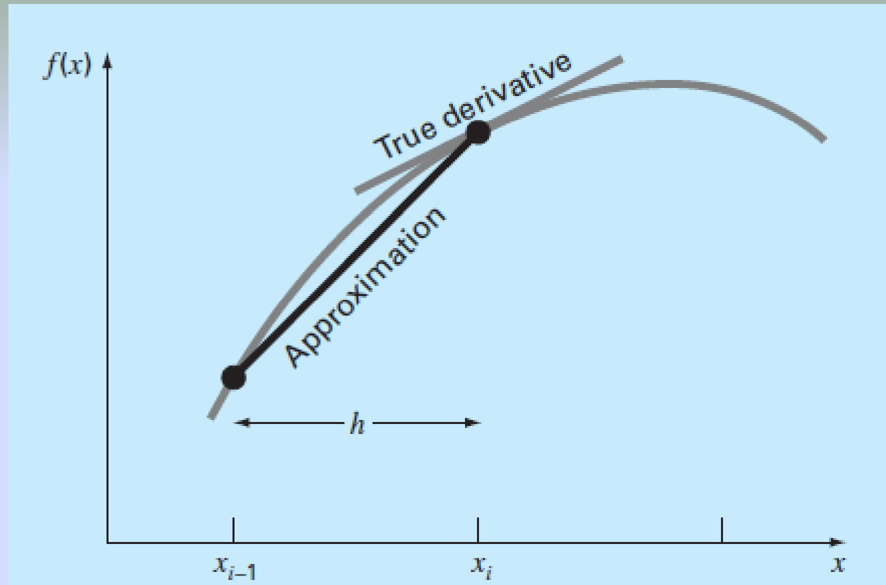
$$f'(x_i) = \frac{f(x_{i+1}) - f(x_{i-1})}{2h} - O\left(h^2\right)$$

This is a *centered difference representation* of the first derivative. Notice that the truncation error is of the order of h^2 in contrast to the forward and backward approximations that were of the order of h.

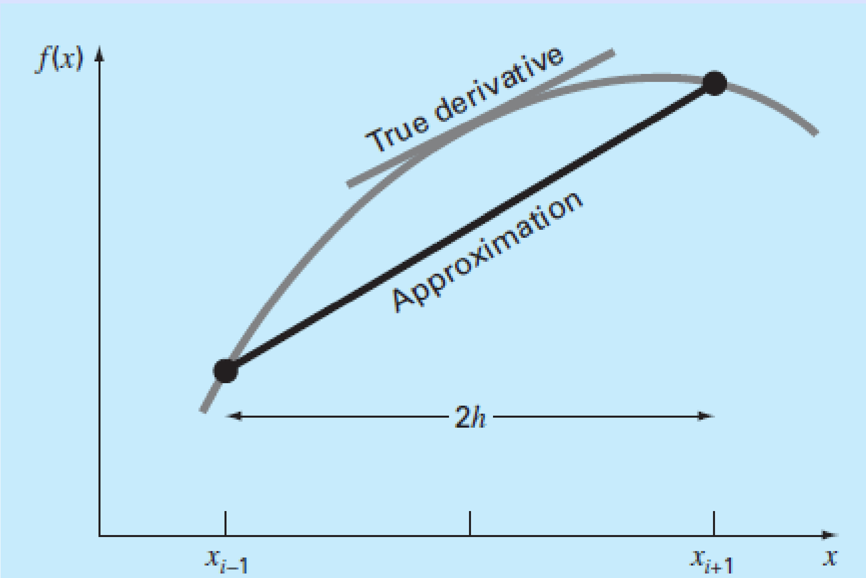
- Forward and backward difference formulas are first order, $O(h)$, accurate. That is the error drops approximately by a factor of 2 as the step size h drops to $h/2$.
- Centered difference formula is second order, $O(h^2)$. Error drops by a factor of 4 as h drops to $h/2$.
- Centered difference formula uses the same number of arithmetic operations as forward and backward formulas, and it offers better accuracy. Therefore it is more efficient.



(*a*) forward



(*b*) backward



(*c*)

(*c*) centered finite-divided-difference approximations of the first derivative.

Example-1:

Finite-Divided-Difference Approximations of Derivatives

Problem Statement. Use forward and backward difference approximations of $O(h)$ and a centered difference approximation of $O(h^2)$ to estimate the first derivative of

$$f(x) = -0.1x^4 - 0.15x^3 - 0.5x^2 - 0.25x + 1.25$$

at $x = 0.5$ using a step size $h = 0.5$. Repeat the computation using $h = 0.25$. Note that the derivative can be calculated directly as

$$f'(x) = -0.4x^3 - 0.45x^2 - 1.0x - 0.25$$

and can be used to compute the true value as $f'(0.5) = -0.9125$.

Let's use MATLAB for the calculations and let's calculate errors in each case.

```
clear all

f=@(x) -0.1*x^4-0.15*x^3-0.5*x^2-0.25*x+1.25; % function f
f_d=@(x) -0.4*x^3-0.45*x^2-x-0.25; %derivative of the function f

xi=0.5;
h=0.5;

% Forward difference approximation:
f_d_a=(f(xi+h)-f(xi))/(h);
err_a=((f_d(xi)-f_d_a)/f_d(xi))*100; %relative error (%)

% Backward difference approximation:
f_d_b=(f(xi)-f(xi-h))/(h);
err_b=((f_d(xi)-f_d_b)/f_d(xi))*100;%relative error (%)

% Centered difference approximation:
f_d_c=(f(xi+h)-f(xi-h))/(2*h);
err_c=((f_d(xi)-f_d_c)/f_d(xi))*100;%relative error (%)

tablo=[f_d(xi) f_d_a f_d_b f_d_c;0 err_a err_b err_c]
% First line of tablo is derivatives; the second line are errors
```

Answer table:

	err_a	err_b	err_c
***h*=0.5**	-58.9041	39.7260	-9.5890
***h*=0.25**	-26.5411	21.7466	-2.3973

Example-2: Homework

The following table is the data given for some x and $f(x)$. Approximate the derivative of the function at all points by using forward difference method at the first point, backward difference method at the last point and centered difference method at any middle point.

x	$f(x)$
0	0
0.1	0.15
0.2	0.47
0.3	0.62
0.4	0.84
0.5	0.98

Answer table:

1.5000
2.3500
2.3500
1.8500
1.8000
1.4000

Higher order formulas for the first derivative

- Proper combinations of Taylor series expansions of $f(x_{i+1})$, $f(x_{i-1})$, $f(x_{i+2})$, $f(x_{i-2})$ can also be used to obtain the first derivative.

$$f(x_{i+1}) = f(x_i + h) = f(x_i) + f'(x_i)h + \frac{f''(x_i)}{2}h^2 + \cdots$$

$$f(x_{i+2}) = f(x_i + h + h) = f(x_i) + f'(x_i)(2h) + \frac{f''(x_i)}{2}(2h)^2 + \cdots$$

$$f(x_{i-1}) = f(x_i - h) = f(x_i) + f'(x_i)(-h) + \frac{f''(x_i)}{2}(-h)^2 + \cdots$$

$$f(x_{i-2}) = f(x_i - h - h) = f(x_i) + f'(x_i)(-2h) + \frac{f''(x_i)}{2}(-2h)^2 + \cdots$$

Higher order formulas for the first derivative

• Proper combinations of Taylor series expansions of $f(x_{i+1})$, $f(x_{i-1})$, $f(x_{i+2})$, $f(x_{i-2})$ can also be used to obtain the first derivative.

Forward differencing:

$$f(x_{i+2}) = f(x_i) + f'(x_i)(2h) + \frac{f''(x_i)}{2!}(2h)^2 + \cdots$$

$$f(x_{i+1}) = f(x_i) + f'(x_i)(h) + \frac{f''(x_i)}{2!}h^2 + \cdots$$

$$f(x_{i+2}) - 4f(x_{i+1}) = -3f(x_i) - 2f'(x_i)h + \cdots$$

$$f'(x_i) = \frac{-f(x_{i+2}) + 4f(x_{i+1}) - 3f(x_i)}{2h} - O(h^2)$$

Higher order formulas for the first derivative

- Proper combinations of Taylor series expansions of $f(x_{i+1})$, $f(x_{i-1})$, $f(x_{i+2})$, $f(x_{i-2})$ can also be used to obtain the first derivative.

Backward differencing:

$$f(x_{i-2}) = f(x_i) - f'(x_i)(2h) + \frac{f''(x_i)}{2!}(2h)^2 + \cdots$$

$$f(x_{i-1}) = f(x_i) - f'(x_i)(h) + \frac{f''(x_i)}{2!}h^2 + \cdots$$

$$f(x_{i-2}) - 4f(x_{i-1}) = -3f(x_i) + 2f'(x_i)h + \cdots$$

$$f'(x_i) = \frac{f(x_{i-2}) - 4f(x_{i+1}) + 3f(x_i)}{2h} + O(h^2)$$

Higher order formulas for the first derivative

• Proper combinations of Taylor series expansions of $f(x_{i+1})$, $f(x_{i-1})$, $f(x_{i+2})$, $f(x_{i-2})$ can also be used to obtain the first derivative.

Centered differencing:

$$f(x_{i+2}) = f(x_i) + f'(x_i)(2h) + \frac{f''(x_i)}{2!}(2h)^2 + \frac{f'''(x_i)}{3!}(2h)^3 + \frac{f^{(4)}(x_i)}{4!}(2h)^4 + \cdots$$

$$f(x_{i+1}) = f(x_i) + f'(x_i)h + \frac{f''(x_i)}{2!}h^2 + \frac{f'''(x_i)}{3!}h^3 + \frac{f^{(4)}(x_i)}{4!}h^4 + \cdots$$

$$f(x_{i-2}) = f(x_i) - f'(x_i)(2h) + \frac{f''(x_i)}{2!}(2h)^2 - \frac{f'''(x_i)}{3!}(2h)^3 + \frac{f^{(4)}(x_i)}{4!}(2h)^4 - \cdots$$

$$f(x_{i-1}) = f(x_i) - f'(x_i)h + \frac{f''(x_i)}{2!}h^2 - \frac{f'''(x_i)}{3!}h^3 + \frac{f^{(4)}(x_i)}{4!}h^4 - \cdots$$

$$-f(x_{i+2}) + f(x_{i-2}) + 8f(x_{i+1}) - 8f(x_{i-1}) = 12f'(x_i)h$$

$$f'(x_i) = \frac{-f(x_{i+2}) + 8f(x_{i+1}) - 8f(x_{i-1}) + f(x_{i-2})}{12h} + O(h^4)$$

Higher order formulas for the first derivative

- Proper combinations of Taylor series expansions of $f(x_{i+1})$, $f(x_{i-1})$, $f(x_{i+2})$, $f(x_{i-2})$ can also be used to obtain the first derivative.

Forward differencing: $\Rightarrow f'(x_i) = \dfrac{-f(x_{i+2}) + 4f(x_{i+1}) - 3f(x_i)}{2h} + O(h^2)$

Bacward differencing: $\Rightarrow f'(x_i) = \dfrac{3f(x_i) - 4f(x_{i-1}) + f(x_{i-2})}{2h} + O(h^2)$

Centered differencing: $\Rightarrow f'(x_i) = \dfrac{-f(x_{i+2}) + 8f(x_{i+1}) - 8f(x_{i-1}) + f(x_{i-2})}{12h} + O(h^4)$

Derivative estimates are improved if small h or higher order approximation is used.

Example-3:

High-Accuracy Differentiation Formulas

Problem Statement. Recall that in Example 4.4 we estimated the derivative of

$$f(x) = -0.1x^4 - 0.15x^3 - 0.5x^2 - 0.25x + 1.2$$

at $x = 0.5$ using finite divided differences and a step size of $h = 0.25$,

	Forward $O(h)$	Backward $O(h)$	Centered $O(h^2)$
Estimate	−1.155	−0.714	−0.934
ε_t (%)	−26.5	21.7	−2.4

where the errors were computed on the basis of the true value of −0.9125. Repeat this computation, but employ the high-accuracy formulas from Figs. 23.1 through 23.3.

```
clear all

f=@(x) -0.1*x^4-0.15*x^3-0.5*x^2-0.25*x+1.25; % function f
f_d=@(x) -0.4*x^3-0.45*x^2-x-0.25; %derivative of the function f

xi=0.5;
h=0.25;

% Forward difference approximation O(h^2):
f_d_a=(-f(xi+h+h)+4*f(xi+h)-3*f(xi))/(2*h);
err_a=((f_d(xi)-f_d_a)/f_d(xi))*100;

% Backward difference approximation O(h^2):
f_d_b=(3*f(xi)-4*f(xi-h)+f(xi-h-h))/(2*h);
err_b=((f_d(xi)-f_d_b)/f_d(xi))*100;

% Centered difference approximation O(h^2):
f_d_c=(-f(xi+h+h)+8*f(xi+h)-8*f(xi-h)+f(xi-h-h))/(12*h);
err_c=((f_d(xi)-f_d_c)/f_d(xi))*100;

tablo=[f_d(xi) f_d_a f_d_b f_d_c;0 err_a err_b err_c]
```

	1	2	3	4
1	-0.9125	-0.8594	-0.8781	-0.9125
2	0	5.8219	3.7671	-2.4334e-14

Richardson Extrapolation

- There are two ways to improve derivative estimates when employing finite divided differences:
  - Decrease the step size, or
  - Use a higher-order formula that employs more points.
- A third approach, based on *Richardson extrapolation*, uses two derivative estimates to compute a third, more accurate approximation.

Recall that Richardson extrapolation provided a means to obtain an improved integral estimate *I* :

$$I \cong I(h_2) + \frac{1}{(h_1/h_2)^2 - 1}[I(h_2) - I(h_1)]$$

$$h_2 = h_1/2$$

$$I \cong \frac{4}{3}I(h_2) - \frac{1}{3}I(h_1)]$$

$$D \cong \frac{4}{3}D(h_2) - \frac{1}{3}D(h_1)]$$

A similar fashion can be written for derivatives as well

- For centered difference approximations with $O(h^2)$. The application of this formula yield a new derivative estimate of $O(h^4)$.

Derivatives of Unequally Spaced Data

- Data from experiments or field studies are often collected at unequal intervals. One way to handle such data is to fit a second-order Lagrange interpolating polynomial.

$$f'(x) = f(x_{i-1})\frac{2x - x_i - x_{i+1}}{(x_{i-1} - x_i)(x_{i-1} - x_{i+1})} + f(x_i)\frac{2x - x_{i-1} - x_{i+1}}{(x_i - x_{i-1})(x_i - x_{i+1})} +$$
$$f(x_{i+1})\frac{2x - x_{i-1} - x_i}{(x_{i+1} - x_{i-1})(x_{i+1} - x_i)}$$

x is the value at which you want to estimate the derivative.

- The advantages of this equation are
  - It can be used to estimate the derivative anywhere within the range prescribed by the three points.
  - The points do not have to be equally spaced.
  - The derivative estimate is of the same accuracy as the centered difference.

Derivatives and Integrals for Data with Errors

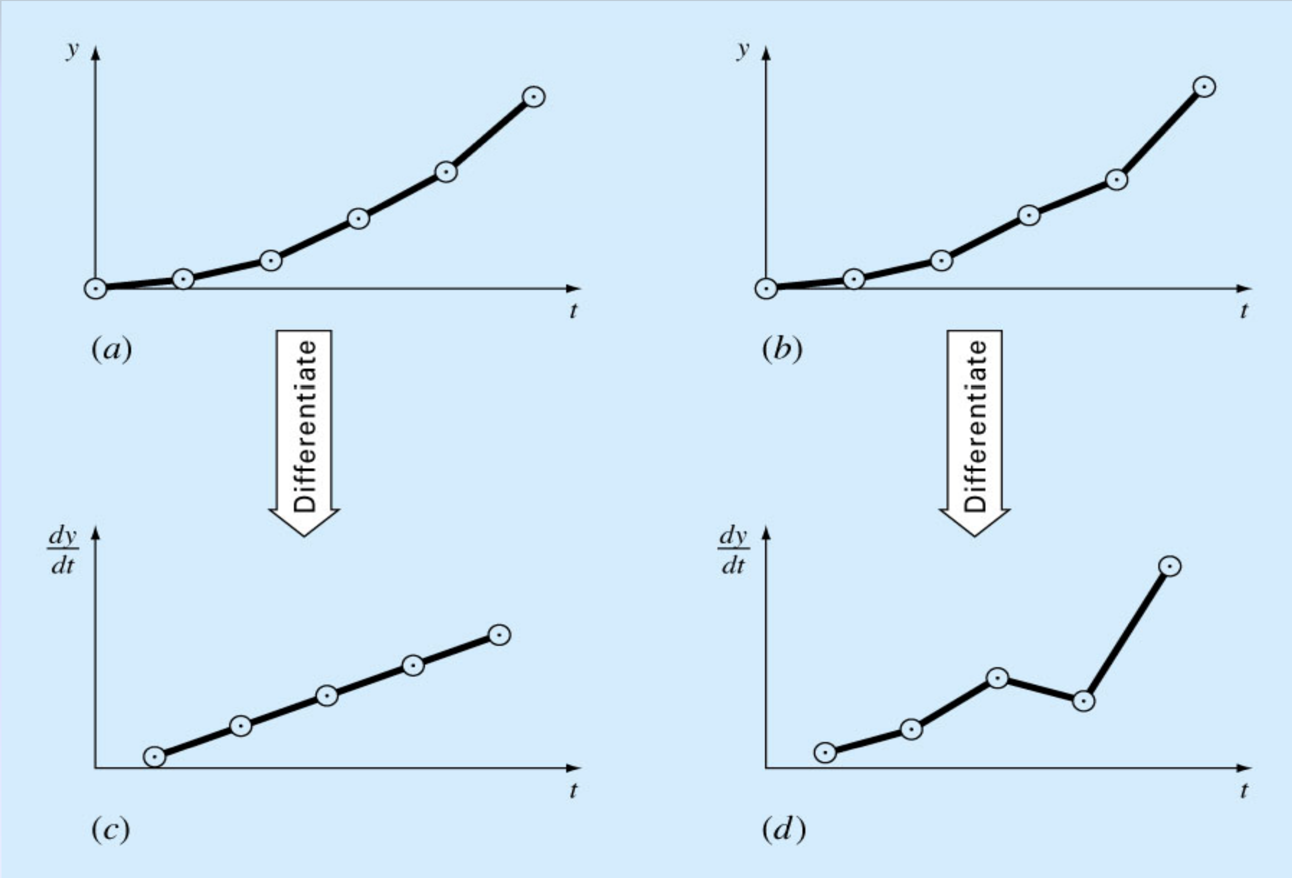


Illustration of how small data errors are amplified by numerical differentiation: (a) data with no error, (b) data modified slightly, (c) the resulting numerical differentiation of curve (a), and (d) the resulting differentiation of curve (b) manifesting increased variability. In contrast, the reverse operation of integration [moving from (d) to (b) by taking the area under (d)] tends to attenuate or smooth data errors.