# Derivatives and Integration



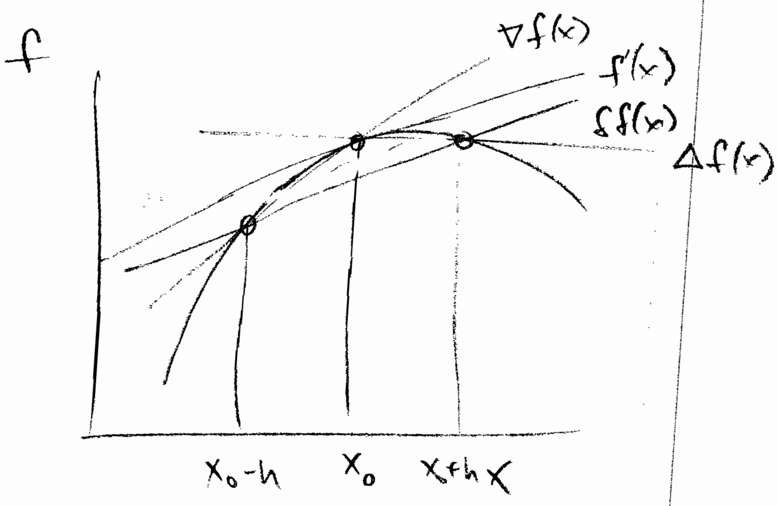
## (I) Numerical Derivatives (ch.3)

— Mathematical definition:

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

provided the limit exist!

☆ Graphically, it is the slope of tangent to graph $f(x)$ at $x_0$:




Draw & keep this graph

Numerically, we can't take $h \to 0$, we can only do finite differences

→ Then, there are three obvious implementation of Definition: (use previous graph)

1. Forward difference

$$\Delta f(x) \equiv \frac{f(x+h) - f(x)}{h}$$

2. Backward difference

$$\nabla f(x) \equiv \frac{f(x) - f(x-h)}{h}$$

3. Central difference

$$\delta f(x) = \frac{f(x+h) - f(x-h)}{2h}$$

In the limit $h \to 0$, all of these are equal

$$\Delta = \nabla = \delta = ' \quad !$$

- But, for finite difference $h$,

central difference is preferred over $\nabla$ or $\Delta$

To see that: Taylor's expansion.

$\Delta$:

(*) $f(x+h) = f(x) + h f'(x) + \frac{h^2}{2!} f''(x) + \frac{h^3}{3!} f'''(x) \dots$

Rearrange $\longrightarrow$

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

$$f'(x) = \Delta f(x) - O(h)$$

so, the estimate of $f'(x)$ by $\Delta f(x)$

is of order $h$!

$\nabla$: Similarly, we get

(**) $f(x-h) = f(x) - h f'(x) + \frac{h^2}{2!} f''(x) - \frac{h^3}{3!} f'''(x) + \dots$

This gives

$$f'(x) = \nabla f(x) + \frac{h}{2} f''(x) - \frac{h^2}{3!} f'''(x) + \dots$$

$$\boxed{f'(x) = \nabla f(x) + O(h) \quad \text{again!}}$$

However, if we now subtract (**) from (*), we have

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

$$\delta f(x) = f'(x) + \underbrace{\frac{h^2}{3!} f'''(x) + \dots}_{O(h^2)}$$

$$\boxed{\text{So, } \delta f(x) \text{ \& } f'(x) \text{ differs by terms of order } h^2 \text{ !}}$$

Thus, $\delta f(x)$ in general will give more accurate results than $\nabla$ or $\Delta$!

* "Rule of Thumb" $\rightarrow$ symmetric method is better!

# Numerical Derivative & Subtractive Cancellation

☆ Classic Numerical Derivatives are subspectible to subtractive cancellation if step size $h$ is too small!

→ compromise between truncation error ($h$ smaller) & potential subtractive cancellation error ($h$ too small).

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# USING COMPLEX VARIABLES TO ESTIMATE DERIVATIVES OF REAL FUNCTIONS*

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**Abstract.** A method to approximate derivatives of real functions using complex variables which avoids the subtractive cancellation errors inherent in the classical derivative approximations is described. Numerical examples illustrating the power of the approximation are presented.

**Key words.** divided difference, subtractive cancellation

**AMS subject classifications.** 65D25, 30E10, 65-04

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**1. Overview.** A standard method to approximate the derivative of a real valued function $F(x)$ at the point $x_0$ is to use the central difference formula

$$F'(x_0) \sim (F(x_0+h) - F(x_0-h))/2h. \tag{1}$$

The truncation error is $O(h^2)$. With most derivative approximations one is faced with the dilemma of using a small $h$ to minimize the truncation error vs. avoiding a small $h$ because of the subtractive cancellation error. Work has been done to improve the answer obtained using equation 1 by analyzing its monotonic behavior as $h$ goes to zero. It turns out that when the roundoff error becomes significant, the estimate from equation (1) oscillates around the correct answer, and this behavior can be used to select an optimal $h$; see [1, 5]. This approach provides only marginal improvement, whereas allowing $h$ to take on a complex value results in an entirely different approximation with unexpected properties.

Using complex variables to develop differentiation formulas originated with Lyness and Moler [2] and Lyness [3]. Since most current numerical analysis textbooks do not normally cover complex variables, we thought a sample of this work with representative computations would be of interest.

In equation (1) we replace $h$ with $ih$ ($i = \mathrm{sqrt}(-1)$). If $F$ is analytic then, letting $Im(F)$ represent the imaginary part of the function $F$, the approximation in (1) can be rewritten

$$\boxed{F'(x_0) \sim Im(F(x_0+ih))/h.} \tag{2}$$

Formula (2) involves the evaluation of the function at a complex argument, but it eliminates the subtractive cancellation error. One way to understand the approximation in (2) is to recast the problem in terms of functions of a complex variable. Let $F(z)$ be an analytic function of the complex variable $z$; also assume that $F$ is real on the real axis. $F$ may be expanded in a Taylor series about the real point $x_0$ as follows:

$$F(x_0+ih) = F(x_0) + ihF'(x_0) - h^2F''(x_0)/2! - ih^3F^{(3)}(x_0)/3! + \cdots. \tag{3}$$

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★ Note:

- If $f(x)$ is known, $f'(x)$ can generally be found analytically. Numerical methods are not needed. This is not the case for integration (which will come next), in which analytic solns only exist for a few limited classes

- However, numerical differentiation is needed if $f(x)$ is sampled from experiments!

- Numerical Methods for diff is in general less accurate than Intergation.

[redacted]

∵ it involves ratios of small #s

$$\frac{f(x+h)-f(x-h)}{2h}$$

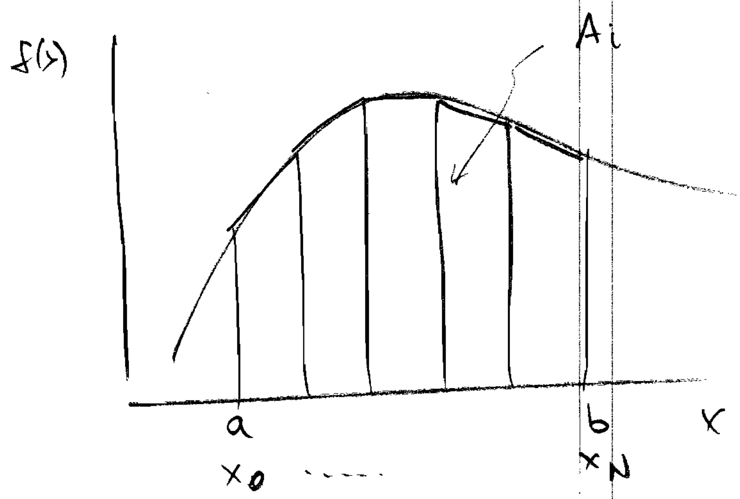
If $\delta f(x) \ll f(x)$, then #SF in

[redacted]

$\delta f(x)$ could be much less th #SF in $f(x)$ (original data)!

# II Integration : Quadrature

$$I = \int_a^b f(x)\, dx$$




$$I \approx \sum_{i=0}^{N} A_i$$

__Main idea:__ To find a collection of simple "four-sided" shapes with area $A_i$s such that the sum of them will best approximate the area under the curve!

Note: This is a classic problem. __Quadrature__: Find a square which has the same area as a circle!

★ Since $f(x)$ must be measured at discrete points $\{x_i\}$, the shape must be chosen so that the area $A_i$ can be directly calculated from $(x_i, f(x_i))$!

## The problem statement:

What are the possible choices of a set of evaluation points $\{x_i\}$ and weights $\{w_i\}$ such that

$$I \simeq \sum_{i=0}^{N} w_i f(x_i)$$

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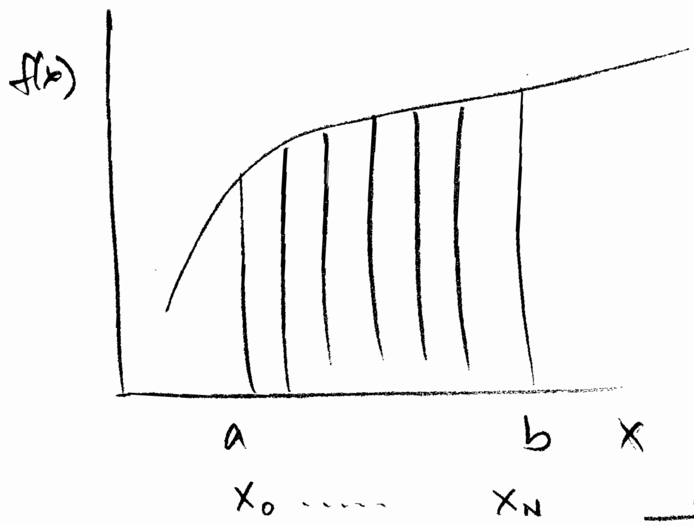
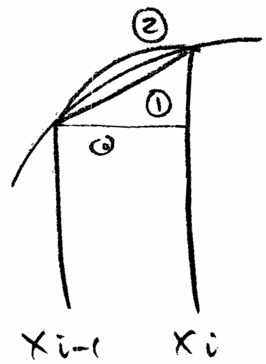
- In general, we have two sets of degrees of freedom:
  - the spacing of the evaluation pts (abscissas)
  - the weighted importance of each pts.
- we will also see how the choice for $\{x_i\}$ & $\{w_i\}$ correspond to the shapes of $A_i$
- advantages & disadvantages for the different choices.

# A Newton - Cotes Formulas

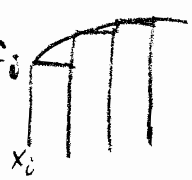
★ $\{x_i\}$ are evenly spaced! ← one of the simplest choice




choice of weights $\{w_i\}$ → shape of fit curve

(0) Rect rule : $f_i$




$$\{w_i\}=\begin{cases}1 & 0\le i<N\\ 0 & i=N\end{cases}$$

(1) Trapezoidal rule (1st order)

— app. $f(x) \in [x_{i-1}, x_i]$ by a straight line starting at $f(x_{i-1})$ and ending at $f(x_i)$ (see graph.)

$$I_{[i-1,i]} = \text{area of trap} = \tfrac{1}{2}h(f_{i-1}+f_i)$$

$$h = x_i - x_{i-1} \quad ; \quad f_i = f(x_i)$$

$$I_{[a,b]} = \sum_{i=1}^{N} I_{[i-1,i]} = \frac{h}{2}\sum_{i=1}^{N}(f_{i-1}+f_i)$$

$$= \frac{h}{2}(f_0+f_1) + \frac{h}{2}(f_1+f_2) + \dots + \frac{h}{2}(f_{N-1}+f_N)$$

$$= h\left(\frac{f_0}{2} + f_1 + f_2 + \dots + f_{N-1} + \frac{f_N}{2}\right)$$

So, in this case we have

$$\boxed{\{w_i\}_{i=0}^{N} : \quad w_i = \begin{cases} \frac{1}{2} & , i=0,N \text{ (end pts)} \\ 1 & , \text{otherwise} \end{cases}}$$

Error estimates:

$[x_{i-1}, x_i]$ : error in one interval

$$E = \int_{x_{i-1}}^{x_i} f(x)\,dx - \frac{h}{2}(f_{i-1}+f_i)$$

☆ Let Taylor expand 1st & 2nd terms around the mid-pt & compare their diff