ME 209
Numerical Methods

9. Numerical Differentiation

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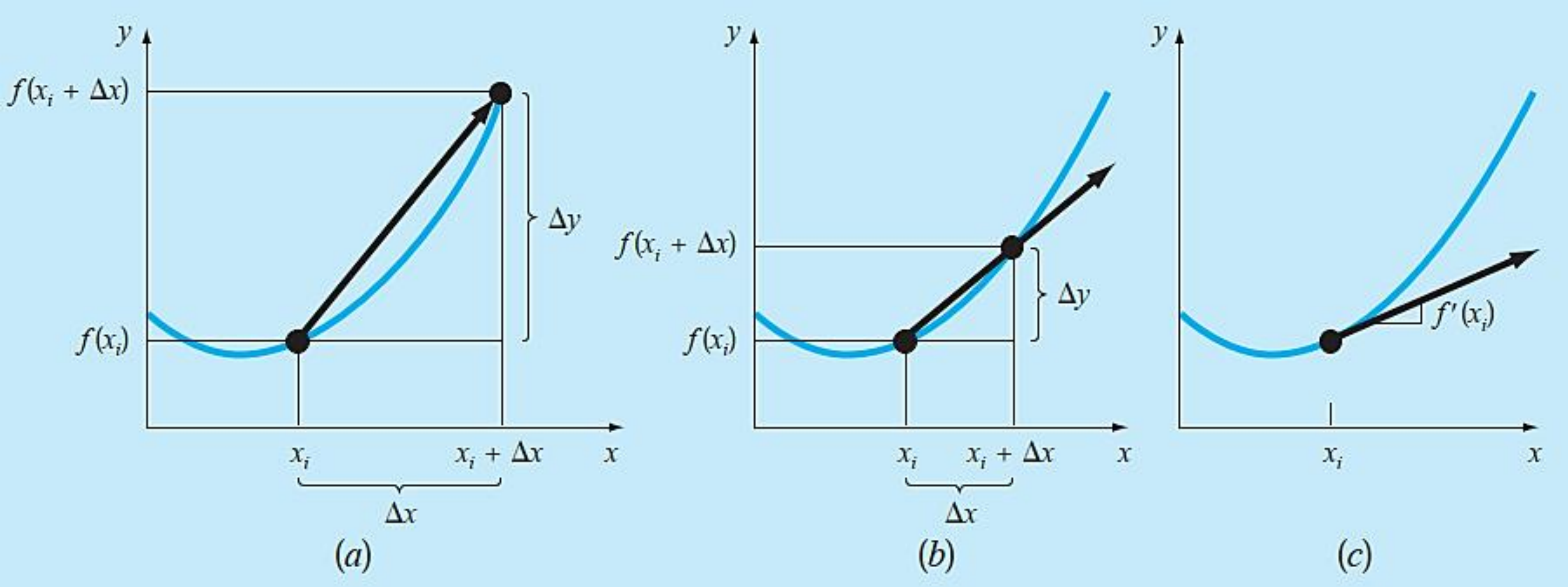
9.1. MOTIVATION

Calculus is the mathematics of change. Because engineers must continuously deal with systems and processes that change, calculus is an essential tool of our profession. Standing at the heart of calculus are the related mathematical concepts of differentiation and integration.

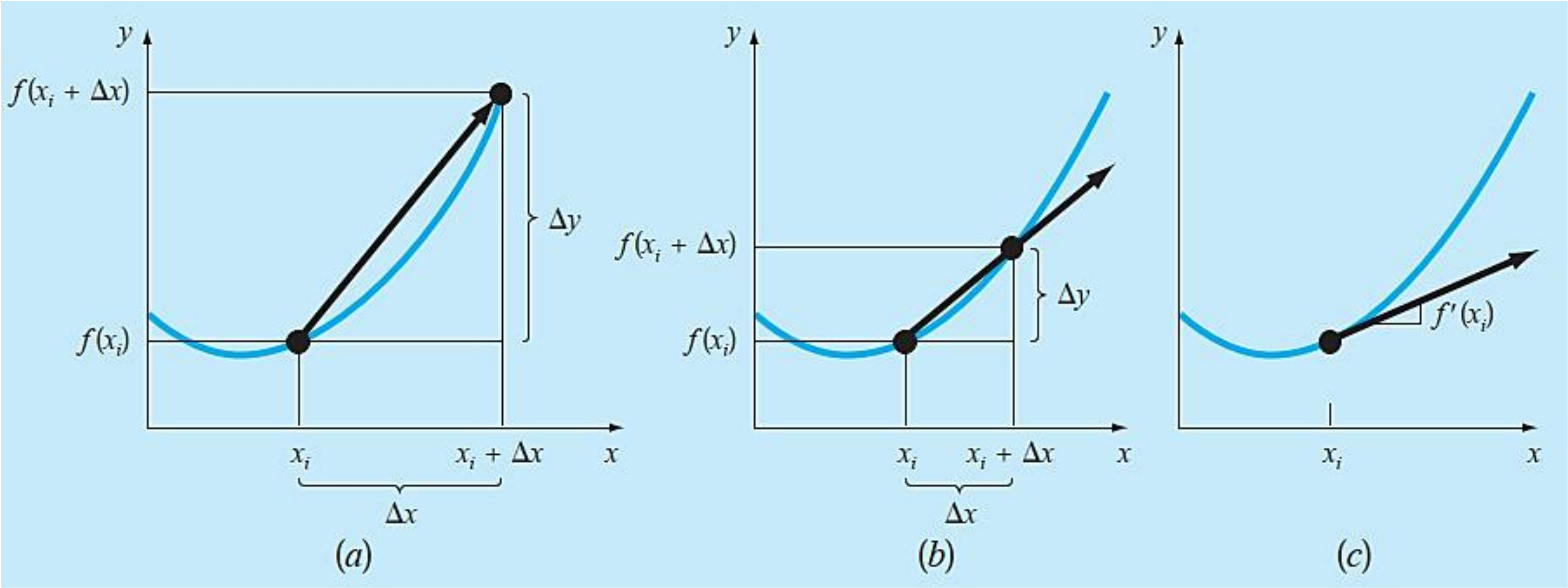
Mathematically, the *derivative*, which serves as the fundamental vehicle for differentiation, represents the rate of change of a dependent variable with respect to an independent variable.



As depicted in Figure, the mathematical definition of the derivative begins with a difference approximation:

$$\frac{\Delta y}{\Delta x} = \frac{f(x_i + \Delta x) - f(x_i)}{\Delta x}$$

where y and $f(x)$ are alternative representatives for the dependent variable and x is the independent variable.



If x is allowed to approach zero, as occurs in moving from Figure *a* to *c*, the difference becomes a derivative

$$\frac{dy}{dx} = \lim_{\Delta x \to 0} \frac{f(x_i + \Delta x) - f(x_i)}{\Delta x} \approx \frac{f(x_i + \Delta x) - f(x_i)}{\Delta x}$$

where dy/dx [which can also be designated as y' or $f'(x_i)$] is the first derivative of y with respect to x evaluated at x_i.

As seen in the visual depiction of Figure *c*, the derivative is the slope of the tangent to the curve at x_i.

The *second derivative* represents the derivative of the first derivative, $\frac{d^2y}{dx^2} = \frac{d}{dx}\left(\frac{dy}{dx}\right)$

Thus, the second derivative tells us how fast the slope is changing. It is commonly referred to as the *curvature*, because a high value for the second derivative means high curvature.

Partial Derivatives

- Finally, *partial derivatives* are used for functions that depend on more than one variable.
- Partial derivatives can be thought of as taking the derivative of the function at a point with all but one variable held constant. For example, given a function f that depends on both x and y, the partial derivative of f with respect to x at an arbitrary point (x, y) is defined as

$$\frac{\partial f}{\partial x} = \lim_{\Delta x \to 0} \frac{f(x + \Delta x, y) - f(x, y)}{\Delta x}$$

- Similarly, the partial derivative of f with respect to y is defined as:

$$\frac{\partial f}{\partial y} = \lim_{\Delta y \to 0} \frac{f(x, y + \Delta y) - f(x, y)}{\Delta y}$$

The function to be differentiated or integrated will typically be in one of the following three forms:

1. A simple continuous function such as a polynomial, an exponential, or a trigonometric function.

2. A complicated continuous function that is difficult or impossible to differentiate or integrate directly.

3. A tabulated function where values of x and $f(x)$ are given at a number of discrete points, as is often the case with experimental or field data.

9.2. MATHEMATICAL BACKGROUND

- General rules are available for derivative of a function. For example, in the case of the monomial

$$y = x^n$$

the following simple rule applies ($n \neq 0$):

$$\frac{dy}{dx} = nx^{n-1}$$

which is the expression of the more general rule for

$$y = u^n$$

where $u =$ a function of x. For this equation, the derivative is computed via

$$\frac{dy}{dx} = nu^{n-1}\frac{du}{dx}$$

Two other useful formulas apply to the products and quotients of functions. For example, if the product of two functions of x(u and v) is represented as $y = uv$, then the derivative can be computed as

$$\frac{dy}{dx} = u\,\frac{dv}{dx} + v\,\frac{du}{dx}$$

For the division, $y = u/v$, the derivative can be computed as

$$\frac{dy}{dx} = \frac{v\,\dfrac{du}{dx} - u\,\dfrac{dv}{dx}}{v^2}$$

Other useful formulas are summarized in Table

Table Some commonly used derivatives.

$\frac{d}{dx}\sin x = \cos x$	$\frac{d}{dx}\cot x = -\csc^2 x$
$\frac{d}{dx}\cos x = -\sin x$	$\frac{d}{dx}\sec x = \sec x \tan x$
$\frac{d}{dx}\tan x = \sec^2 x$	$\frac{d}{dx}\csc x = -\csc x \cot x$
$\frac{d}{dx}\ln x = \frac{1}{x}$	$\frac{d}{dx}\log_a x = \frac{1}{x \ln a}$
$\frac{d}{dx}e^x = e^x$	$\frac{d}{dx}a^x = a^x \ln a$

9.3. NUMERICAL DIFFERENTIATION

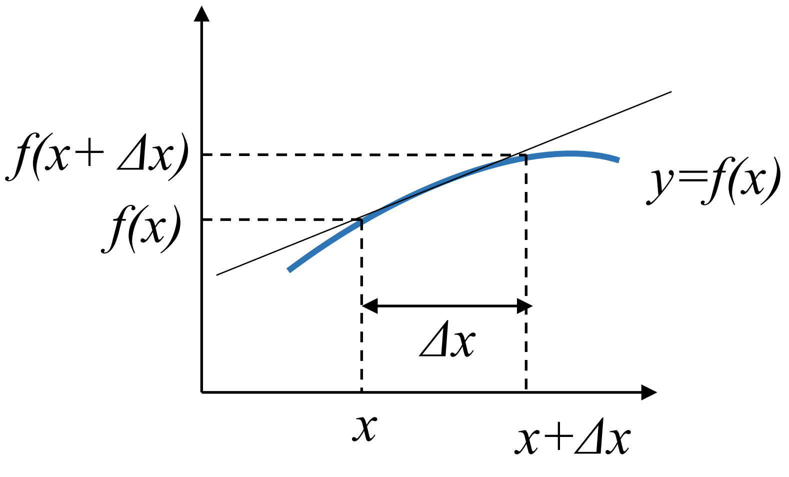
- As previously mentioned, a number of engineering problems require a numerically derived estimate of a derivative of a function $f(x)$, with two general approaches to the problem.
- First, if the function is known but the derivative cannot be computed analytically, the derivative can be estimated by computing the function for two values of the independent variable(s) separated by distance Δx and dividing the difference by Δx as follows:

$$\frac{dy}{dx} = \lim_{\Delta x \to 0} \frac{f(x_i + \Delta x) - f(x_i)}{\Delta x} \approx \frac{f(x_i + \Delta x) - f(x_i)}{\Delta x}$$

Forward Difference Equation

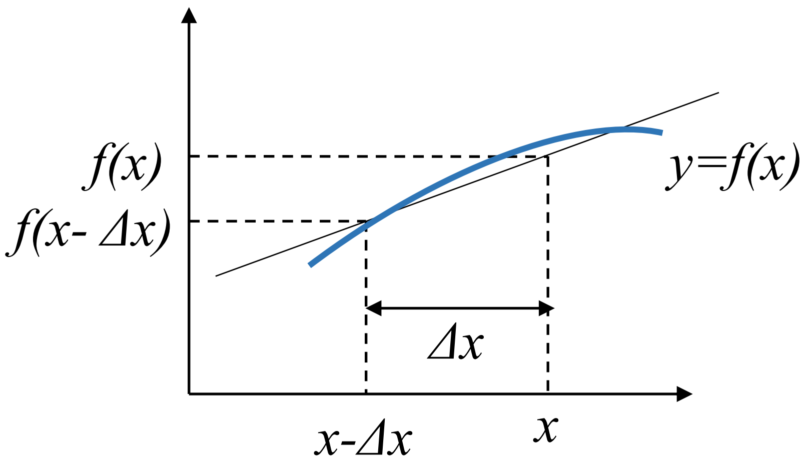
- The second approach to numerical differentiation is to fit a function to a set of points that describes the relationship between the dependent and independent variables and then differentiate the fitted function.
- Specifically, an interpolation polynomial of order n could be fit to the data and the derivative of the polynomial used as the estimate of the derivative.
- The selection of one of the two methods depends on the form in which the data are presented and the desired level of accuracy.

9.3.1. Finite-Difference Differentiation



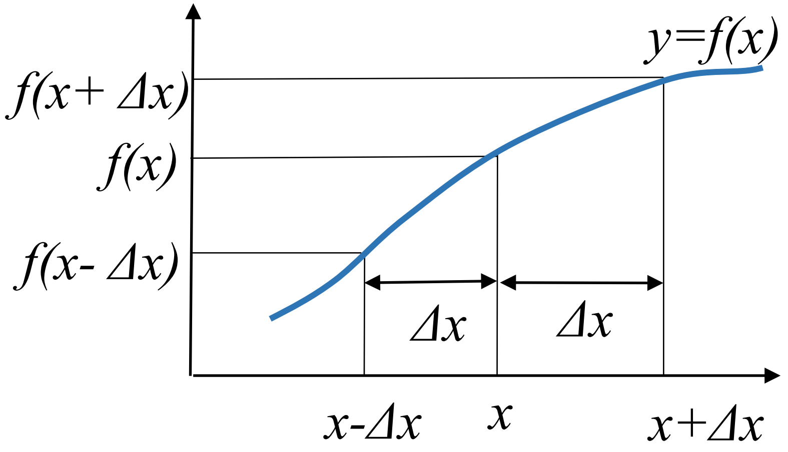
$$\frac{df(x)}{dx} \approx \frac{f(x+\Delta x) - f(x)}{\Delta x}$$

Forward Difference Equation



$$\frac{df(x)}{dx} \approx \frac{f(x) - f(x-\Delta x)}{\Delta x}$$

Backward Difference Equation



$$\frac{df(x)}{dx} \approx \frac{f(x+\Delta x) - f(x-\Delta x)}{2\Delta x}$$

Two-step Method

Example

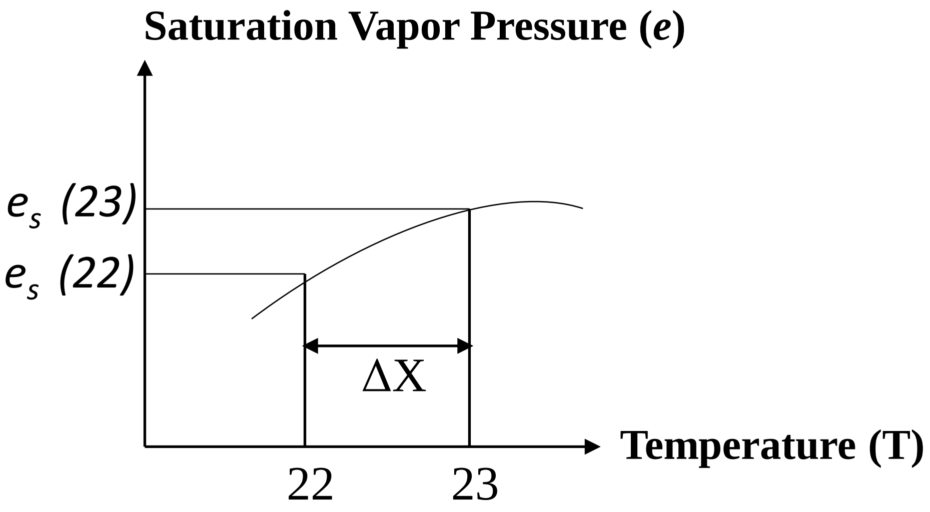
A design engineer must make estimates of evaporation rates when the amount of water needed to meet irrigation demands is required. One input to a frequently used formula for estimating evaporation rates is the slope of the saturation vapor pressure curve at air temperature *T*. A small part of the table that is used to make such estimates is given in Table.

If it is necessary to make design estimates at a temperature of 22 °C, then the slope of the saturation vapor pressure curve at 22 °C could be estimated using, as follows, the forward, backward, or two-step method:

TABLE 7.1 Saturation Vapor Pressure (e_s) in mm Hg as a Function of Temperature (T) in °C

T(°C)	e_s (mm Hg)
20	17.53
21	18.65
22	19.82
23	21.05
24	22.37
25	23.75

Solution (Forward Difference Equation)



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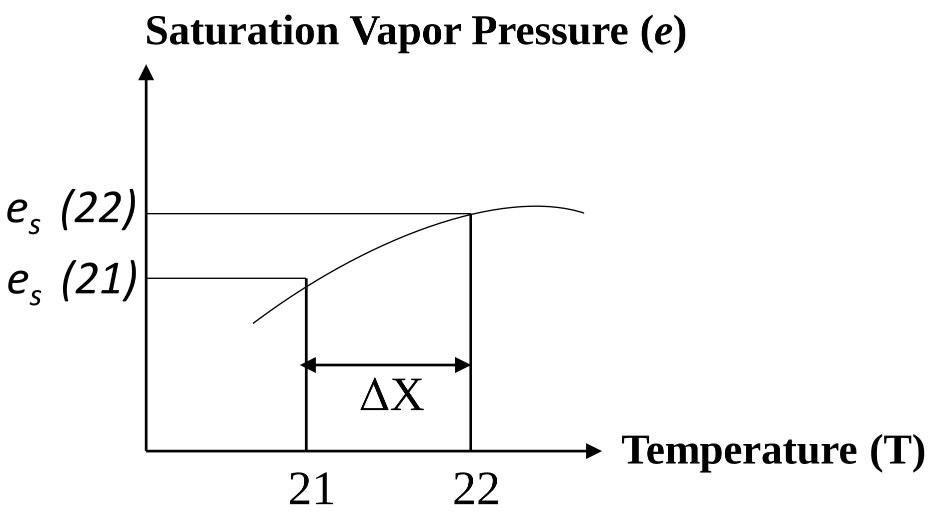
24	22.37
25	23.75

$$\frac{df(x)}{dx} \approx \frac{f(x+\Delta x) - f(x)}{\Delta x}$$

$$\frac{de_s}{dT} = \frac{e_s(23) - e_s(22)}{23 - 22} = \frac{21.05 - 19.82}{1} = 1.23 \text{ mm Hg/°C}$$

Solution (Backward Difference)Equation



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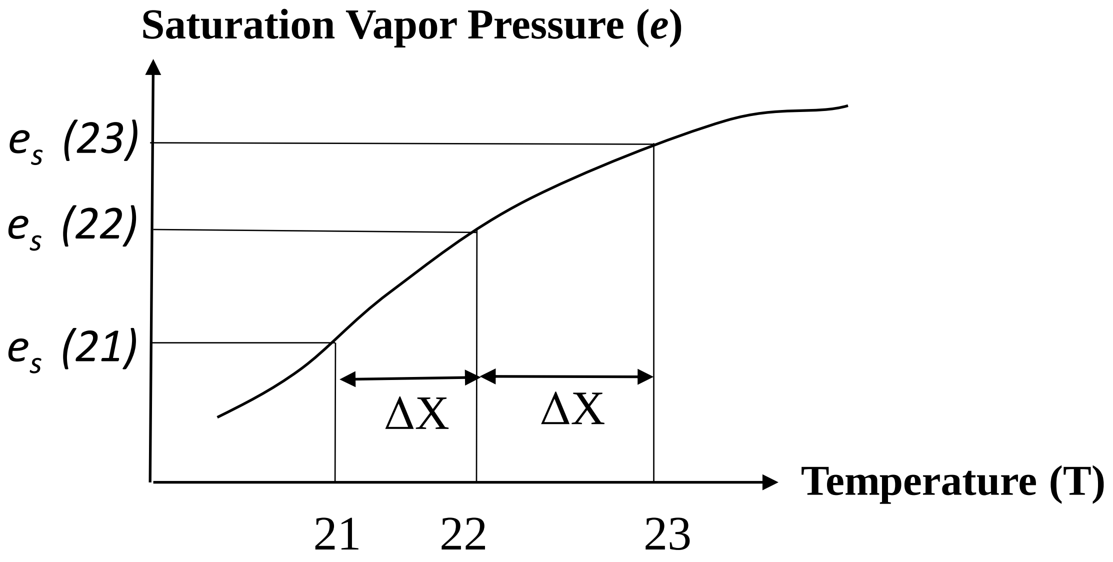
24	22.37
25	23.75

$$\frac{df(x)}{dx} \approx \frac{f(x) - f(x - \Delta x)}{\Delta x}$$

$$\frac{de_s}{dT} = \frac{e_s(22) - e_s(21)}{22 - 21} = \frac{19.82 - 18.65}{1} = 1.17 \text{ mm Hg/°C}$$

Solution (Two-step Method)



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$$\frac{df(x)}{dx} \approx \frac{f(x+\Delta x) - f(x-\Delta x)}{2\Delta x}$$

$$\frac{de_s}{dT} = \frac{e_s(23) - e_s(21)}{23-21} = \frac{21.05 - 18.65}{2} = 1.20 \text{ mm Hg/°C}$$

The true value is 1.20 mm Hg/°C, so the two-step method provided the most accurate estimate.

9.3.2. Differentiation Using Taylor Series Expansion

The forward Taylor series expansion can be written as $f(x+\Delta x)=f(x)+\frac{df(x)}{dx}\Delta x+\frac{df^2(x)}{dx^2}\frac{(\Delta x)^2}{2!}+\frac{df^3(x)}{dx^3}\frac{(\Delta x)^3}{3!}+\ldots$

Truncated this result by excluding the second- and higher-derivative terms and were thus left with a final result of

$$\frac{df(x)}{dx}\approx\frac{f(x+\Delta x)-f(x)}{\Delta x}$$

The equation above represents first-order approximation of the first derivative of *f(x)*. We can also derive the second-order approximation of *f(x)* by including higher order terms in Taylor's expansion.

$$\frac{df(x)}{dx}\approx\frac{f(x+\Delta x)-f(x)}{\Delta x}-\frac{df^2(x)}{dx^2}\frac{\Delta x}{2!}$$

Second-order approximation of the first derivative

The second-order approximation requires knowledge of the second derivative of $f(x)$.

The finite-difference approximation can also be used to compute higher order derivatives. For example, if we let $f'(x)$ be the first derivative of $f(x)$ with respect to x, then the forward difference approximation of the second derivative is given by

$$\frac{d^2 f(x)}{dx^2} \approx \frac{f'(x+\Delta x) - f'(x)}{\Delta x}$$

Substituting the first-order approximation of $f'(x)$ in the equation above produces the following equation for the second order derivative:

$$\frac{d^2 f(x)}{dx^2} \approx \frac{f(x+2\Delta x) - 2f(x+\Delta x) + f(x)}{(\Delta x)^2}$$

First-order approximation of the second derivative

$$\frac{df(x)}{d(x)} \approx \frac{-f(x+2\Delta x) + 4f(x+\Delta x) - 3f(x)}{2\Delta x}$$

Second-order approximation of the first derivative

Similarly, the first-order estimate of the second derivative can be revised by including a second-order term from the Taylor series expansion to obtain its second-order approximation as

$$\frac{d^2 f(x)}{dx^2} \approx \frac{-f(x+3\Delta x)+4f(x+2\Delta x)-5f(x+\Delta x)+2f(x)}{(\Delta x)^2}$$

Second-order approximation of the second derivative

Using *backward difference* in the Taylor series expansion, the following first- and second-order estimates, respectively, for the first derivative of $f(x)$ can be obtained:

$$\frac{df(x)}{dx} \approx \frac{f(x)-f(x-\Delta x)}{\Delta x}$$

$$\frac{df(x)}{dx} \approx \frac{3f(x)-4f(x-\Delta x)+f(x-2\Delta x)}{2\Delta x}$$

Using *backward difference* in the Taylor series expansion, the following first- and second-order estimates, respectively, for the second derivative of *f(x)* can be obtained:

$$\frac{d^2 f(x)}{dx^2} \approx \frac{f(x) - 2f(x-\Delta x) + f(x-2\Delta x)}{(\Delta x)^2}$$

$$\frac{d^2 f(x)}{dx^2} \approx \frac{2f(x) - 5f(x-\Delta x) + 4f(x-2\Delta x) - f(x-3\Delta x)}{(\Delta x)^2}$$

Using the *two-step method* in the Taylor series expansion, the following first- and second-order estimates, respectively, for the first derivative of *f(x)* can be obtained:

$$\frac{df(x)}{dx} \approx \frac{f(x+\Delta x) - f(x-\Delta x)}{2\Delta x}$$

$$\frac{df(x)}{dx} \approx \frac{-f(x+2\Delta x) + 8f(x+\Delta x) - 8f(x-\Delta x) + f(x-2\Delta x)}{12\Delta x}$$

Using the *two-step method* in the Taylor series expansion, the following first- and second-order estimates, respectively, for the second derivative of *f(x)* can be obtained:

$$\frac{d^2 f(x)}{dx^2} \approx \frac{f(x+\Delta x) - 2f(x) + f(x-\Delta x)}{(\Delta x)^2}$$

$$\frac{d^2 f(x)}{dx^2} \approx \frac{-f(x+2\Delta x) + 16f(x+\Delta x) - 30f(x) - 16f(x-\Delta x) - f(x-2\Delta x)}{12(\Delta x)^2}$$

Example

Forward Difference Method

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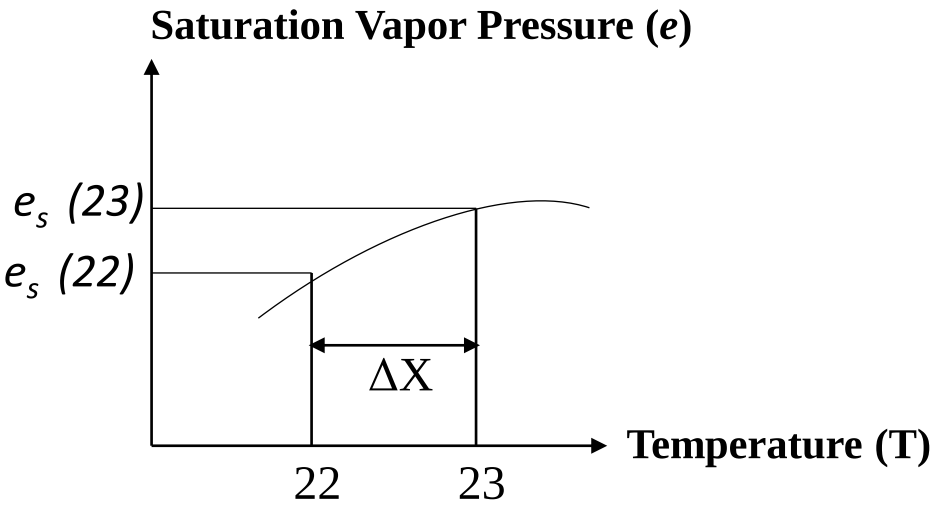

(7.33)

$$\frac{df(x)}{d(x)} \approx \frac{-f(x+2\Delta x)+4f(x+\Delta x)-3f(x)}{2\Delta x}$$

(7.43)

$$\frac{df(x)}{dx} \approx \frac{-e_s(24)+4e_s(23)-3e_s(22)}{2(1)}$$

$$\approx \frac{-22.37+4(21.05)-3(19.82)}{2(1)} = 1.185 \text{ mm Hg/°C}$$

Backward Difference Method

TABLE 7.1 Saturation Vapor Pressure (e_s) in mm Hg as a Function of Temperature (T) in °C

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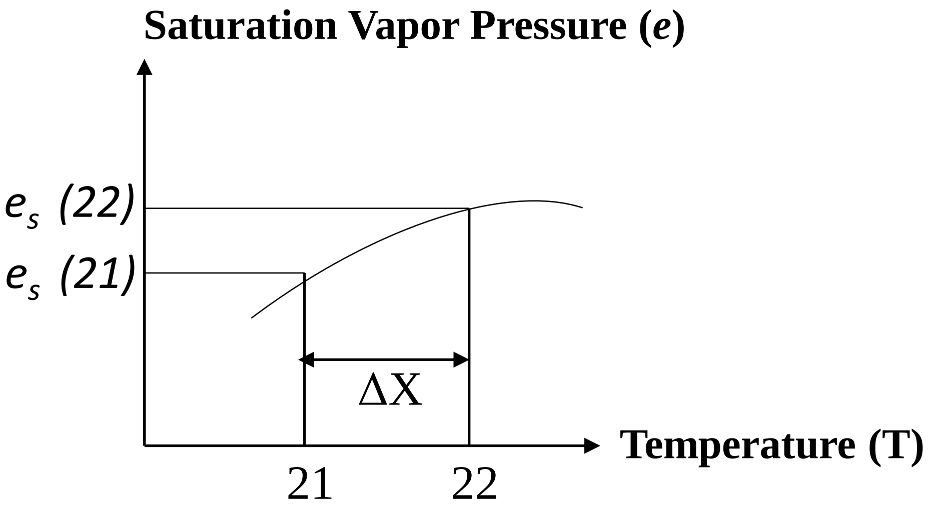

$$\frac{df(x)}{dx} \approx \frac{3f(x) - 4f(x-\Delta x) + f(x-2\Delta x)}{2\Delta x} \tag{7.36}$$

$$\frac{df(x)}{dx} \approx \frac{3e_s(22) - 4e_s(21) + e_s(20)}{2(1)}$$

(7.44)

$$\approx \frac{3(19.82) - 4(18.65) + 17.53}{2(1)} = 1.195 \text{ mm Hg/°C}$$

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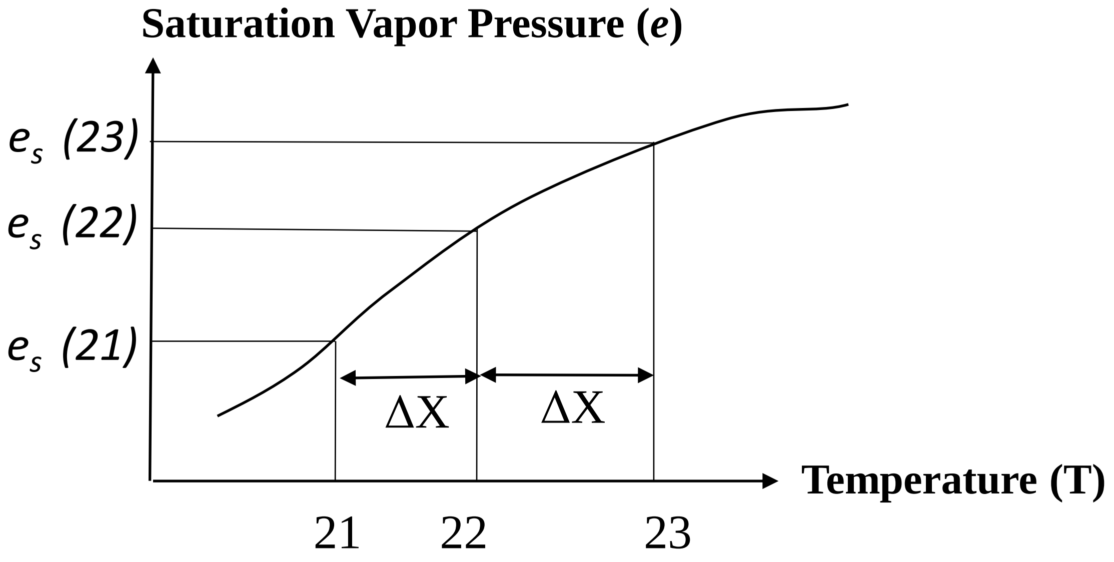
Two-step Method



$$\frac{df(x)}{dx} \approx \frac{-f(x+2\Delta x)+8f(x+\Delta x)-8f(x-\Delta x)+f(x-2\Delta x)}{12\Delta x} \quad (7.40)$$

$$\frac{df(x)}{dx} \approx \frac{-e_s(24)+8e_s(23)-8e_s(21)+e_s(20)}{12(1)}$$

$$\approx \frac{-(22.37)+8(21.05)-8(18.65)+(17.53)}{12(1)} = 1.19667 \text{ mm Hg/°C}$$

(7.45)

The accuracy of the three methods is improved by using the second-order approximation. The two-step method still provides the best estimate, since the true value at T = 22°C is 1.2 mm Hg/°C.

NEXT WEEK
NUMERICAL INTEGRATION