

12 Figures, 2 Tables, 0 Appendices, 0 Highlighted Boxes, 0 Footnote**Supplement 1. Mathematical Concepts****S.1. Linear Versus Quadratic Functions**

A linear function reflects constant proportionality between two variables and contains a constant offset of one variable relative to the other. Linear functions are written in the general form:

$$y = m x + b \quad (\text{S1})$$

where m represents the proportionality constant, or the slope, and b represents the offset constant, or the y-intercept. When plotted on a graph, Equation (S1) will reflect a straight line (Fig. S1). In a linear relationship, the slope of the line is the ratio of vertical distance to horizontal distance (often referred to as 'rise over run'). For a truly vertical line, the slope is ∞ . For a truly horizontal line, the slope is 0. The slope is the same for all points on the line. Linear functions are first-degree polynomials because the independent variable (in this case x) has an implied exponent of 1. (A polynomial is defined as an algebraic expression of the general form $y = ax^k$, where k is a positive integer and a is a real number.)

Quadratic functions are second-degree polynomials, meaning they describe a parabolic relationship between two variables (Fig. S2). Quadratic functions are written in the general form:

$$y = ax^2 + bx + c \quad (\text{S2})$$

where a , b , and c are constants. Different parabolic shapes, degrees of curvatures, and sizes can be defined by differences in the values of a , b and c . At $y = 0$, all values of x that satisfy the relationship:

$$ax^2 + bx + c = 0 \quad (\text{S3})$$

are referred to as the *roots of the quadratic*. At the roots, Equation (S3) can be rearranged to define x in terms of a , b and c :

$$x = \frac{-b \pm \sqrt{b^2 - 4ac}}{2a} \quad (\text{S4})$$

The \pm sign in Equation (S4) reflects the existence of two possible roots.

S.2 Exponents and Logarithms

An exponent (m) is defined as a positive integer indicating the factorial multiplication of a real number (a). Thus, a^m is defined as a multiplied by itself m times. By convention, a^{-m} represents $1/a^m$. Thus, $3^4 = 3*3*3*3 = 81$ and $3^{-4} = 1/(3^4) = 1/81$. From the last example, it is clear that $3^2*3^2 = 3^4 = 81$. Exponential terms can be combined according to a series of rules. Thus, $a^m * a^n = a^{m+n}$, $a^m/a^n = a^{m-n}$, and $a^m a^n/a^q = a^{(m+n)-q}$.

When present as a fraction, exponents reflect the root of a number as follows:

$$y = (a^{1/m}) = \sqrt[m]{a} \quad (\text{S5})$$

Thus, y is equal to the m^{th} root of a . As an example, $3^4 = 81$ can be rewritten as $81^{1/4} = 3$. Using Equation (S5) to define a root:

$$a^{m/n} = (\sqrt[n]{a})^m \quad (\text{S6})$$

Logarithms are defined with respect to the exponential series of base 10. Thus, $\log 100 = 2$ means that base 10 must be raised by the power of 2 to equal 100; taking the example further, $\log 10^2 = 2 \log 10$. (Note that the log of 10 is 1, since 10 raised to the power of 1 equals 10.) In general terms, if $\log a = b$, then $10^b = a$, and $\log a^b = b \log a$. Logarithms can be manipulated algebraically according to a series of rules. Thus, $\log^{(rs)} = \log r + \log s$ and $\log^{(r/s)} = \log r - \log s$.

To this point, we have only considered logarithms within the context of base 10. Such functions are often called *common logarithms*. In the application of calculus, the logarithm base is often expressed in terms of the irrational number 2.71828, which is designated as e . When expressed in base e , logarithmic functions are referred to as *natural logarithms* and denoted as \ln . This designation reflects the fact that e arises naturally from certain mathematical derivations, and can be applied effectively to the description of natural phenomena. Natural logarithms follow the same rules of algebra described above. Natural logarithms can be related to common logarithms by recognizing that $e^{\ln x} = x$, and taking the log of both sides of the equation:

$$\log(e^{\ln x}) = \ln x \log e = \log x \quad (\text{S7})$$

to derive the following relationship:

$$\ln x = \frac{\log x}{\log e} \quad (\text{S8})$$

S.3. Trigonometric Functions

Trigonometric functions relate the sides of a triangle to its angles. Three of the most useful trigonometric functions are the *sine*, *cosine*, and *tangent*. To illustrate, imagine angle θ which is formed as radius r , which is fixed to the vertex of a circle, and is rotated from the x axis in a counterclockwise direction (Fig. S3). Angle θ can be defined in units of *degrees* or *radians*, where a radian is defined as the length of arc q relative to radius r (1 radian = q/r). Trigonometric functions can be applied to the triangle that is formed by placing r within the context of x, y coordinates:

$$\sin \theta = y/r, \quad \cos \theta = x/r, \quad \tan \theta = y/x \quad (\text{S9})$$

Trigonometric functions are useful in quantifying the periodic phases of cyclic processes. Starting from the positive side of the x -axis and rotating the radius counterclockwise (through the

quadrant defined by $x, y > 0$), the sine function will progress through positive values to a maximum of 1 at $\theta=90^\circ$ (or $\theta = \pi/2$ radians). Continuing in the counterclockwise direction, the sine function will continue to reflect positive, but decreasing numbers to a value of 0 at $\theta = 180^\circ$ (or π radians). (Keeping in mind that $\sin \theta = y/r$, and noting that $y = 0$ at $\theta = 180^\circ$, it is clear why $\sin \theta = 0$ at $\theta = 180^\circ$.) As r is rotated still further in the counterclockwise direction, the sine function will reflect negative numbers (values of y are negative as r is rotated through the quadrant defined by $x, y < 0$), reaching a minimum of -1 at $\theta = 270^\circ$ (or $3\pi/2$ radians). Finally, as r is rotated back to the x axis, the sine function will progress through diminishing negative numbers to a final minimum of 0 at $\theta = 360^\circ$ (or 2π radians). The progression of the sine function through these cyclic phases can be represented by a periodic 'wave' pattern, with a periodicity of 360° (or 2π radians) (Fig. S4). Thus, cyclic processes can be described using trigonometric functions, and the trigonometric frequency (360° or 2π radians) can be calibrated to the frequency of cycles.

S.4. Differential Calculus

Differential calculus is the calculus of *derivative functions* – i.e., functions that define the rate of change in a dependent variable, as the span of the independent variable approaches an infinitesimally small value. Algebraically, the slope of a function is defined as $\Delta y/\Delta x$, given a function (f) that relates two variables as $y = f(x)$. For many functions, however, $f(x)$ cannot be defined at x . As an example consider the function:

$$y = f(x) = \frac{x^2 - 1}{x - 1} \quad (\text{S10})$$

In Equation (S10), $f(x)$ is undefined at $x = 1$. (At $x = 1$ the function yields a solution of $0/0$ which cannot be mathematically defined.) One means of solving this function is to let values of x get as close as possible to 1 without actually equaling 1. In other words, let $(x - 1)$ approach 0 [denoted as $(x - 1 \rightarrow 0)$]. For values of $x \neq 1$, $f(x)$ in Equation (S10) can be defined as:

$$y = f(x) = \frac{x^2 - 1}{x - 1} = \frac{(x+1)(x-1)}{(x-1)} = x + 1 \quad (\text{S11})$$

As values of x approach 1, $f(x)$ approaches 2. Thus, if we define $f(x)$ with the caveat that $(x - 1)$ approaches infinitesimally small values, then $f(x) = 2$. Under these conditions, $f(x)$ is said to be evaluated *within the limit* as $(x - 1) \rightarrow 0$. The evaluation of a function as the independent variable becomes infinitesimally small is defined mathematically as:

$$\lim_{x \rightarrow a} f(x) = M \quad (\text{S12})$$

which can be read, 'as the independent variable (x) approaches the value a , and the interval $(x-a)$ becomes infinitesimally small, the dependent variable will equal M '.

The requirement to evaluate functions as they approach their limit is particularly relevant to the study of biotic and abiotic fluxes. Flux (F) is defined as the product between a proportionality coefficient (K) and the space-dependent concentration gradient ($\Delta c/\Delta x$). Thus, $F = K (\Delta c/\Delta x)$. As long as c changes linearly as a function of x , $\Delta c/\Delta x$ can be evaluated algebraically. The evaluation becomes difficult, however, if c changes in a non-linear manner across distance Δx (Fig. S6). With such circumstances, it is often most meaningful to evaluate $\Delta c/\Delta x$ (and thus flux) at a specific point as $\Delta x \rightarrow 0$. Mathematically, flux at a specific point can be represented as:

$$F = K \lim_{x_2 \rightarrow x_1} \frac{c_2 - c_1}{x_2 - x_1} = K \lim_{\Delta x \rightarrow 0} \frac{\Delta c}{\Delta x} = K \frac{dc}{dx} \quad (\text{S13})$$

To appreciate the concept of a point-specific change in c , imagine a straight line drawn at a single point, A , whereby the *tangent* of that line represents the slope, or dc/dx at A (Fig. S6) In the language of differential calculus, point-specific slopes are denoted as dy/dx . This relationship reads that the *derivative* of y is evaluated with respect to x . Another way to refer to the derivative is to say that y is *differentiated* with respect to x .

It is important to keep in mind that in differential calculus, the dependent variable (y) is differentiated with respect to a function (f) defined in relation to the independent variable (x). The use of first principles to mathematically differentiate functions can be complex. Instead, most people use a series of rules that form a reliable foundation for differentiation problems. The simplest rule involves the function $f(x) = a$, where a is a constant. Imagine the graphical representation of this relationship – i.e., for all values of x , $y = a$. The slope of this relationship will be 0, leading to the formal statement:

$$\frac{dy}{dx} = \lim_{\Delta x \rightarrow 0} \frac{\Delta y}{\Delta x} = \lim_{\Delta x \rightarrow 0} 0 = 0 \quad (\text{S14})$$

Thus, the derivative of $f(x) = \text{constant}$ is 0. This result has an important implication – a constant can be added to any function without effect on the derivative of that function.

As another example, consider $f(x) = ax$. Graphically, this function would depict a straight line with slope a and y -intercept = 0. Conceptually, it is clear that if dy/dx reflects the slope of a function and if the slope of this function is a , then:

$$\frac{dy}{dx} = \lim_{\Delta x \rightarrow 0} \frac{\Delta y}{\Delta x} = \lim_{\Delta x \rightarrow 0} \frac{a\Delta x}{\Delta x} = a \quad (\text{S15})$$

Thus, the derivative of $f(x) = ax$ is a .

Several additional rules of differentiation are commonly used to solve differential equations. Some of these rules are listed in Table S1. A more complete discussion of the rules of differentiation can be found in a basic calculus book. One rule that is worth considering in more detail is the chain rule, one of the most commonly used tools in differential calculus. The chain rule is stated as:

$$\frac{df}{dx} = \frac{df}{du} \frac{du}{dx} \quad (\text{S16})$$

The chain rule is especially useful in the differentiation of functions that can be factored into separate entities, but linked with related variables. An example is presented in Appendix 9.1 (Chapter 9). In the latter case, $f(x) = e^{-GL/\cos \theta}$, and $f(x)$ is differentiated with respect to L . The resultant derivative is not straightforward because of the complexity of carrying multiple variables in the exponent, only one of which (L) is the independent variable driving the differentiation. If we let $c = -G/\cos \theta$, and $u = cL$, the chain rule can be applied as:

$$\frac{de^u}{dL} = \frac{de^u}{du} \frac{du}{dL} = \frac{de^u}{du} \frac{d(cL)}{dL} = c e^{cL} \quad (\text{S17})$$

It is worth considering two additional types of derivatives. Higher-order derivatives are derivatives of a derivative. Thus, the derivative of dx/dy is referred to as a second derivative and is denoted as:

$$\frac{d^2y}{dx^2} = \frac{d}{dx} \left(\frac{dy}{dx} \right) \quad (\text{S18})$$

A second derivative can be thought of as the slope of a slope. Recall that flux reflects a derivative function (i.e., $K dc/dx$). The second derivative of a flux reflects the rate by which the flux changes with respect to the x coordinate (in this case distance in the x spatial coordinate). Higher-order derivatives can be solved using the same rules for derivatives. First, the primary derivative is solved, and then the primary solution is differentiated to obtain the second derivative.

Partial derivatives refer to the case when a dependent variable is defined by a function with two or more independent variables. When a derivative function is evaluated with regard to its partial derivatives, it is first evaluated with respect to one independent variable, then the other variables in their turn, in each case with all other independent variables held constant. Thus:

$$\frac{dy}{dx} = \left(\frac{\partial y}{\partial x} \right)_{m,n} dx + \left(\frac{\partial y}{\partial m} \right)_{x,n} dm + \left(\frac{\partial y}{\partial n} \right)_{x,m} dn \quad (\text{S19})$$

where the *total derivative* (dy/dx) is broken into its partial derivatives. (The symbol " ∂ " is used to denote partial derivatives.) The subscripts in each term refer to the independent variables that are held constant while the function represented in the numerator is evaluated with respect to the function represented in the denominator. Partial derivatives are solved using the same rules that apply to total derivatives.

S.5 Integral Calculus

Whereas differential calculus has as its focus the instantaneous slope of functions, integral calculus focuses on determination of the area beneath the curve defined by a function. The process of determining the area beneath curves is called *integration*. In the case of fluxes, integration yields the total flux with respect to a definitive span of the independent variable. To illustrate the concept of integration, imagine a function $f(x)$ that produces the curve presented in Figure S7. The area (A) beneath the designated portion of the curve will be defined by the distance along the x -axis ($x_2 - x_1$) at one boundary and $f(x)$ at the other boundary. Now imagine a change in x ($x_2 + \Delta x$), with an accompanying change in the area beneath the curve (ΔA). The value for ΔA will reflect Δx at one boundary and $f(x)$ at the other boundary [i.e., $\Delta A = f(x)(\Delta x)$]. As was the case for determining the slope of complex functions, determination of the area beneath the curve can be difficult. The task is made easier as $\Delta x \rightarrow 0$. In that case, $\Delta A \rightarrow dA/dx$, and $dA/dx \rightarrow f(x)$. Stated formally:

$$\frac{dA}{dx} = \lim_{\Delta x \rightarrow 0} \frac{f(x)\Delta x}{\Delta x} = f(x) \quad (\text{S20})$$

The aim of integration is to find the function that when differentiated equals $f(x)$. This function will equal A, the area beneath the curve represented by $f(x)$ when determined as $\Delta x \rightarrow 0$. The area under the curve at values outside the limit can be determined by multiplying the integration by dx . This is represented by:

$$A = \int f(x) dx \quad (\text{S21})$$

Equation (S21) reads: the area beneath the curve (A) equals the integral of $f(x)$ determined across dx . The area defined in Equation (S21) is called the *indefinite integral*. As for the case of differentiation, integration is often done using a series of rules. Some of the more commonly used rules for indefinite integrals are listed in Table S2.

To gain a better conceptual grasp of integration, imagine finding the area beneath a curve by using a series of progressively smaller rectangles, all positioned next to each other, with the sum of their independent areas representing the total area beneath the curve (Fig. S8). The greater the number of rectangles that is squeezed under the curve, the more accurate the estimate of the area beneath the curve, since each rectangle has a flat upper boundary, and is thus only an approximation of its representative area beneath the curve. Using the concept of a limit, the area beneath the curve can be determined as:

$$A = \lim_{\Delta x \rightarrow 0} \sum_{i=1}^N f(x_i) \Delta x \quad (\text{S22})$$

where N is the number of rectangles squeezed into the area beneath the curve and Δx is the thickness of each rectangle. Thus, within the limit as the thickness of each rectangle approaches 0 and the number of rectangles approaches ∞ , the sum of the independent areas of all of the rectangles should equal the area beneath the curve. The limit defined in Equation (S22) is called the *definite integral*. The definite integral is related to the indefinite integral – i.e., the definite integral is the indefinite integral defined at its limits. The definite integral is simply another way of defining the area under a curve, in this case by quantification of the area of a simpler geometric relation defined within its limit. The definite integral is written as:

$$\int_a^b f(x) dx = \lim_{\Delta x \rightarrow 0} \sum_{i=1}^N f(x_i) \Delta x \quad (\text{S23})$$

where a and b on the left side of Equation (S23) define the points on the x -axis bounding the curve of interest.

Current computers make integration easy through a process known as *numerical integration*. Numerical integration involves an estimate of the integral between two points (b –

a) after arbitrarily choosing some number N of rectangular areas. Using a computer, $y_i = f(x_i)$ is evaluated for each interval ($b - a/N = \Delta x$) and multiplied by the total distance of the integral ($b - a$). The accuracy of the integral estimate will depend on the thickness of each rectangular area (i.e., how well the assumption $\Delta x \rightarrow 0$ is satisfied).

Occasionally, a variable is dependent on two or more separate independent variables, rather than one variable as has been assumed to this point. Integration of the relationship between these multiple variables requires use of a *multiple integral*. As an example, take the relationship $z = f(x, y)$, where z is a variable dependent on the values of x and y . Because there are two independent variables, integration is determined within the bounds of a curve defined in two-dimensions (x and y), rather than one (x alone). The formal definition of a multiple integral in two dimensions is:

$$\iint f(x, y) dA = \lim_{\Delta A \rightarrow 0} \sum_{i=1}^N f(x_i, y_i) \Delta A_i \quad (\text{S24})$$

Note that in Equation (S24) the relevant variable upon which the integration is based is change in area (dA), a two-dimensional variable, not change in Δx alone.

S.6 Polynomial Approximations of Elementary Functions (The Taylor Polynomial Theorem)

In some cases, complex functions that are not resolvable by simple computational methods, are more easily evaluated by a polynomial approximation. The polynomial model will not be an exact solution, and the degree of error in the representation must be evaluated and minimized in order to control the approximation. To illustrate the polynomial approximation, let $f(x)$ represent an exact function, and let $P_n(x)$ represent the polynomial approximation of $f(x)$. Accordingly:

$$f(x) = P_n(x) + R_n(x) \quad (\text{S25})$$

where $R_n(x)$ represents the error (or remainder) between the approximation and the exact function. The polynomial expansion and resulting error can be quantified using the Taylor Polynomial Theorem:

$$f(x) = f(c) + \frac{f'(c)}{1!}(x-c) + \dots + \frac{f^{(n)}(c)}{n!}(x-c)^n + R_n(x) \quad (\text{S26})$$

where:

$$R_n(x) = \frac{f^{(n+1)}(\xi)}{(n+1)!}(x-c)^{n+1} \quad (\text{S27})$$

and ξ represents a number in the interval between c , the value for the polynomial approximation, and x , the value for the exact function, and f represents a differentiable function through $n + 1$ derivatives.

Polynomial approximation is especially useful in dealing with the many non-linearities that emerge during the derivation of flux and energy-balance relationships. A non-linear function relating two variables can be approximated as a first-degree (linear) polynomial using the Taylor expansion theorem. The error in making the approximation (R_n) will be minimized if the relationship is applied across a small interval for the two variables. [The difference between a non-linear function $f(x)$ and linear approximation $P_n(x)$ will decrease as Δx decreases, minimizing the degree of non-linearity in $f(x)$.] A good example of use of the Taylor Polynomial Theorem is found in Appendix 6.1 (Chapter 6) in which linear approximations greatly facilitates derivation of the Penman-Monteith relation, which describes surface evaporation.

S.7 Probability Density Functions

The statistical foundation for many of the models used in predicting ecosystem-atmosphere fluxes is based on the probability of an event occurring. Probability (P) refers to the fractional number of successes in making an observation or predicting an event. Thus, $P = \text{number of successes} / \text{total number of attempts}$, where $0 \leq P \leq 1$. When P is expressed as a function of an

independent variable [e.g., number of attempts, time (t), distance (x), etc.], a probability density function (pdf) and its associated graph can be described (Fig. S9).

Derivation of the pdf is essentially a problem in integral calculus. Given the distribution of probabilities across a defined interval of values for the independent variable, the total probability can be described by:

$$P = \int_a^b f(x) dx \quad (\text{S28})$$

where a and b define the interval bounds and $f(x)$ represents the pdf. Given that P is defined as a fractional variable and has an upper limit of 1, we can write:

$$P = \int_0^{+\infty} f(x) dx = 1 \quad (\text{S29})$$

To explore the relevance of pdf's, let's address the question as to why so many flux equations have a similar mathematical form. Why does the equation describing the velocity of a chemical reaction ($v = k [A][B]$) look so similar to the equation describing diffusive flux [$F = K_d (\partial c / \partial x)$]? The answer lies in the fact that both are statistical models predicting the probability distribution of an event happening as a function of an independent variable. In the case of reaction velocity, the statistical function [$f(x)$] predicts the probability of reactants A and B combining to form a product (with reactant concentration being the independent variable). In the case of diffusive flux, the function is predicting the probability of a scalar moving from one position to another along the x coordinate (with the scalar concentration gradient being the independent variable). The ' k ' coefficients are simply proportionality factors used to quantify probability within the context of $f(x)$ (which in both of these cases is a first-order linear function).

One of the most fundamental pdf's is the Gaussian (normal) distribution (Fig. S10). The Gaussian distribution requires only two parameters for definition; the mean (μ), which is the central tendency of the distribution of events, and the standard deviation (σ), which is the

tendency for dispersion about the mean. In formal terms, the Gaussian probability distribution is defined as:

$$f(x) = \frac{1}{\sqrt{(2\pi\sigma)}} e^{-[(x-\mu)^2/2\sigma^2]} \quad (\text{S30})$$

where σ^2 is the variance.

Statistical moments of a pdf are expressions of dispersion about the mean; they define the symmetry of the pdf. Mathematically, statistical moments are stated as:

$$\mu_n = (x - \mu)^n \quad (\text{S31})$$

where μ_n denotes the order of the moment (e.g., μ_1 is the first moment and μ_2 is the second moment). The first moment is defined as the mean itself. The second moment is defined as the variance (σ^2). Thus, to define a Gaussian distribution, one only needs the first and second moments. The third moment, which is defined as the third power deviation $[(x - \mu)^3]$ is often used to evaluate skewness, which reflects asymmetry in the distribution around the mean (Fig. S10). The fourth moment is the fourth power deviation $[(x - \mu)^4]$, and is often used to evaluate kurtosis, the tendency for peakedness in the distribution.

Skewness in the distribution of x (Sk_x) is defined as:

$$Sk_x = \frac{\overline{x'^3}}{\sigma_x^3} \quad (\text{S32})$$

where x' is the deviation from the mean (i.e., $x - \mu$) and σ is the standard deviation of x . A Gaussian distribution would exhibit skewness equal to 0. When deviations from the mean are multiplied to the third power, the extremes become weighted most heavily. If the most extreme deviations tend to be negative more frequently than positive, a third-moment analysis will reveal negative skewness, and vice versa if the most frequent extreme deviations are positive. If the

positive and negative deviations are evenly distributed (i.e., a Gaussian distribution), a third-power product will equal σ_x^3 . Kurtosis in the distribution of x (Kr_x) is defined as:

$$Kr_x = \frac{\overline{x^4}}{\sigma_x^4} \quad (\text{S33})$$

Expressing deviations as the fourth power causes the distribution to flatten. This flattened condition is ideal for analyzing aspects of peakedness. A Gaussian distribution will reveal a Kr_x of 3. *Leptokurtic* distributions have $Kr_x > 3$, and exhibit "fatter" tails in the distribution (i.e., there is a higher probability of an event occurring in the tails), compared to a Gaussian distribution. *Platykurtic* distributions have $Kr_x < 3$, and refer to the case where the flanks of the distribution are heavier, but the tails are thinner. The peak of a platykurtic distribution is flatter than the Gaussian case. In general, pdf's with significant skewness and/or kurtosis are referred to as *non-Gaussian*. Models of non-Gaussian functions are complex given the difficulty of predicting third and fourth moment terms.

In the statistical analysis of turbulence, *covariances* are frequent. A covariance is a 'double correlation'; i.e., two independent variables are multiplied together to reveal correlated patterns of variance. An example, is the eddy flux which consists of the covariance between the fluctuating components of vertical wind velocity (w') and scalar concentration (c'). (The term 'fluctuating components' is derived from Reynolds averaging, which is defined in Appendix 10.1, Chapter 10.) In formal terms, the time-averaged eddy-flux ($\overline{w'c'}$) is a second-order statistical moment (a variance). When models are derived to predict $\overline{w'c'}$, skewness emerges as a required term. In the case of eddy flux, skewness emerges as a *mixed third-order moment*. A mixed third-order moment refers to a 'triple correlation' among mixed variables. The mixed third-order moment that often emerges in modeling the eddy flux is $\overline{w'w'c'}$. In order to define this third-order moment, kurtosis emerges as a required term. Thus, models of pdf's typically require that lower-order moments be defined in terms of higher-order moments. This exemplifies a problem in statistical modeling known as the *closure problem*; attempts to define statistical moments in terms of higher-order moments lead to more unknowns than equations, preventing complete mathematical closure.

S.8 Scalars, Vectors and Tensors

Mathematical approaches in the field of physics often require that variable quantities be defined with regard to a coordinate system. Coordinate systems allow objects or points of reference to be explicitly defined in space. The most common coordinate system used in atmospheric physics is the Cartesian coordinate system; a system of coordinate axes that are mutually perpendicular and, by convention, referred to as the x , y and z coordinates. A fourth coordinate that is often referenced in the field of atmospheric physics is time, t . In fact, several models that are used in both diagnostic and prognostic roles in atmospheric physics are referred to as 4-dimensional models, meaning that they include the Cartesian spatial coordinates and time as fundamental reference frames. Variables that are independent of a coordinate system are called scalars. Examples of scalars include mass, molecular density, temperature and humidity. These variables are represented by a single number that has magnitude, but is independent of direction in space or time. Variables that are defined within the context of a coordinate system, and thus have dimensions of *both* magnitude and direction, are called vectors. Examples of vectors include wind velocity, force and acceleration. Vectors represent quantitative entities that can be mathematically manipulated to provide the sum influence of a variable with contributions from different coordinate axes. Vectors are geometrically summed, when defined by the same coordinate axis, by placing them head to tail. When defined by different coordinate axes, the gross contributions of each vector quantity to a net vector quantity can be determined within a geometric framework (e.g., Pythagorean geometry).

The derivation and expression of equations to represent physical processes that involve vectors becomes complicated when forced to deal with multiple coordinates. In order to simplify such derivations, they are often written in vector notation, a type of 'shorthand' wherein the coordinates attached to a vector quantity are represented as subscript indices. Thus, velocity (v) can be represented in vector notation as v_i , where the subscript "i" represents the three coordinate components of the vector, $i = 1, 2$ and 3 (or x , y and z in the Cartesian coordinate system). Using summation notation, equations can be developed for the single variable v_i , with the understanding that behind the equation is an expansion of the relationship into all three component coordinates.

Most fluxes that are relevant to ecosystem-atmosphere interactions are defined with respect to a vector field, a field of vector quantities associated with each point in a defined spatial domain. The vector field will define the *net* coordinate components to any given flux. For example, the flux of heat across a surface will have components in the x , y and z directions that, when summed, provide a net heat flux from one side of the surface to the other. Some variables cannot be derived in only three coordinates. An example is momentum flux. Momentum is defined as mass times velocity, a scalar quantity times a vector quantity. Momentum flux is defined as momentum transferred across some surface area (m^2) per unit time (s), so that momentum flux has combined units of $(\text{kg m s}^{-1}) (\text{m}^{-2} \text{s}^{-1})$; these units condense to N m^{-2} (force per unit area), the same units as stress. Momentum, being the product of a scalar and a vector, can be defined in the three Cartesian coordinates, x , y and z which, for the case of wind, are identified as u , v and w , respectively. Momentum flux, has the additional quality of being able to transfer these three wind coordinates in one of three different Cartesian directions, x , y and z . Thus, momentum flux has nine components, rather than the three typically used for vector quantities (Fig. S.11). Momentum flux is an example of a tensor quantity. (Technically, one can equate the concepts of scalars, vectors and tensors by recognizing that a scalar is actually a zero-order tensor, a vector is a first-order tensor and momentum flux is a second-order tensor.)

Once again, in the spirit of trying to simplify the derivation of equations for tensor quantities such as momentum flux, we often rely on a type of shorthand, in this case referred to as Einstein's summation notation. In this case, a tensor quantity (F) is represented as F_{ij} , where the two subscript indices represent $i = 1, 2$ and 3 , $j = 1, 2$ and 3 . In matrix algebra, these indices represent the cross multiplication of all nine coordinates.

Vector algebra is often written with special operators which define specific functions. One example that is particularly relevant to atmospheric physics is the gradient operator, ∇ . The gradient operator defines the divergence or convergence in a vector field, for example:

$$\nabla \cdot \mathbf{v} = \frac{\partial v_x}{\partial x} + \frac{\partial v_y}{\partial y} + \frac{\partial v_z}{\partial z} = \frac{\partial v_i}{\partial x_i} \quad (\text{S34})$$

where the right-hand side of Equation S34 represents the divergence or convergence written in vector notation. In this case, the divergence or convergence is an expression of how much the

velocity vectors (v_i) spread apart or come together, respectively, around a single point in Cartesian space.

S.9 Coordinate rotation

When considering the role of wind in transporting scalar quantities to produce a flux, we often run into a problem when undulating terrain forces the various wind vectors to take on differential importance. For example, when the wind is forced over an upward-oriented slope, even though the net direction of the wind remains predominantly horizontal (in the x coordinate), the vertical component of the wind (in the z coordinate) increases in importance. When the wind is forced down the other side of the slope, the vertical coordinate remains important, but the mathematical sign of the important component will be reversed. Thus, in situations where wind-driven processes are considered (as in many studies of turbulent flux) we rotate the 'local' coordinate system to provide a consistent, or standardized, frame of reference. In other words, we rotate the coordinate system to reflect ideal, perfectly flat terrain, irrespective of the nature of the real terrain.

To understand coordinate rotation, imagine a wind vector (v) with three orthogonally-oriented, Cartesian vectors (v_x , v_y and v_z) above flat terrain (Fig. S.12). Now, imagine that we need to rotate the coordinate system to define a new vector (v'), accounting for the up-and-down undulations (in the z -coordinate) above sloped terrain. In this case, we need to rotate the system within vertical space, through angle θ , which defines the angle of the undulation. The result will be two new coordinate axes, x' , z' , formed from the original axes, x , z . Vector v' can be defined in the new coordinate frame by drawing perpendiculars from the tail of the vector through the x -axis (Fig. S.12). In geometric terms, we can define v' with respect to axis x' as:

$$\begin{aligned}
 v_x' &= OA + AB \\
 &= \frac{v_x}{\cos \theta} + (v_z - v_x \tan \theta) \sin \theta \\
 &= \frac{v_x}{\cos \theta} (1 - \sin^2 \theta) + v_z \sin \theta \\
 &= v_x \cos \theta + v_z \sin \theta
 \end{aligned}
 \tag{S35}$$

A similar approach can be taken to define v_z' as:

$$v_z' = -v_x \sin \theta + v_z \cos \theta \quad (\text{S36})$$

In the rotation described above, the side-stream, lateral component (v_y) is unaffected. However, for situations where the terrain undulates laterally a similar rotation can be performed to define v_y' .

Table S1. Some of the most commonly used relationships for differentiation.

$$(1) \frac{d(a)}{dx} = 0, \text{ where } a \text{ is a constant}$$

$$(2) \frac{d(ax)}{dx} = a, \text{ where } a \text{ is a constant}$$

$$(3) \frac{d(x^m)}{dx} = mx^{(m-1)}$$

$$(4) \frac{d(e^m)}{dx} = e^m$$

$$(5) \frac{d \ln x}{dx} = \frac{1}{x}$$

$$(6) \frac{d(au)}{dx} = a \frac{du}{dx}, \text{ where } u = f(x)$$

$$(7) \frac{d(e^u)}{dx} = e^u \frac{du}{dx}, \text{ where } u = f(x)$$

Table S2. Some of the most commonly used relationships for integration.

(1) $\int a \, dx = ax$, where a is a constant

(2) $\int \frac{dx}{x} = \ln x$

(3) $\int (r + s) \, dx = \int r \, dx + \int s \, dx$

(4) $\int a f(x) \, dx = a \int f(x) \, dx$

(5) $\int e^x \, dx = e^x$

(6) $\int \sin x \, dx = -\cos x$

(7) $\int \cos x \, dx = \sin x$.

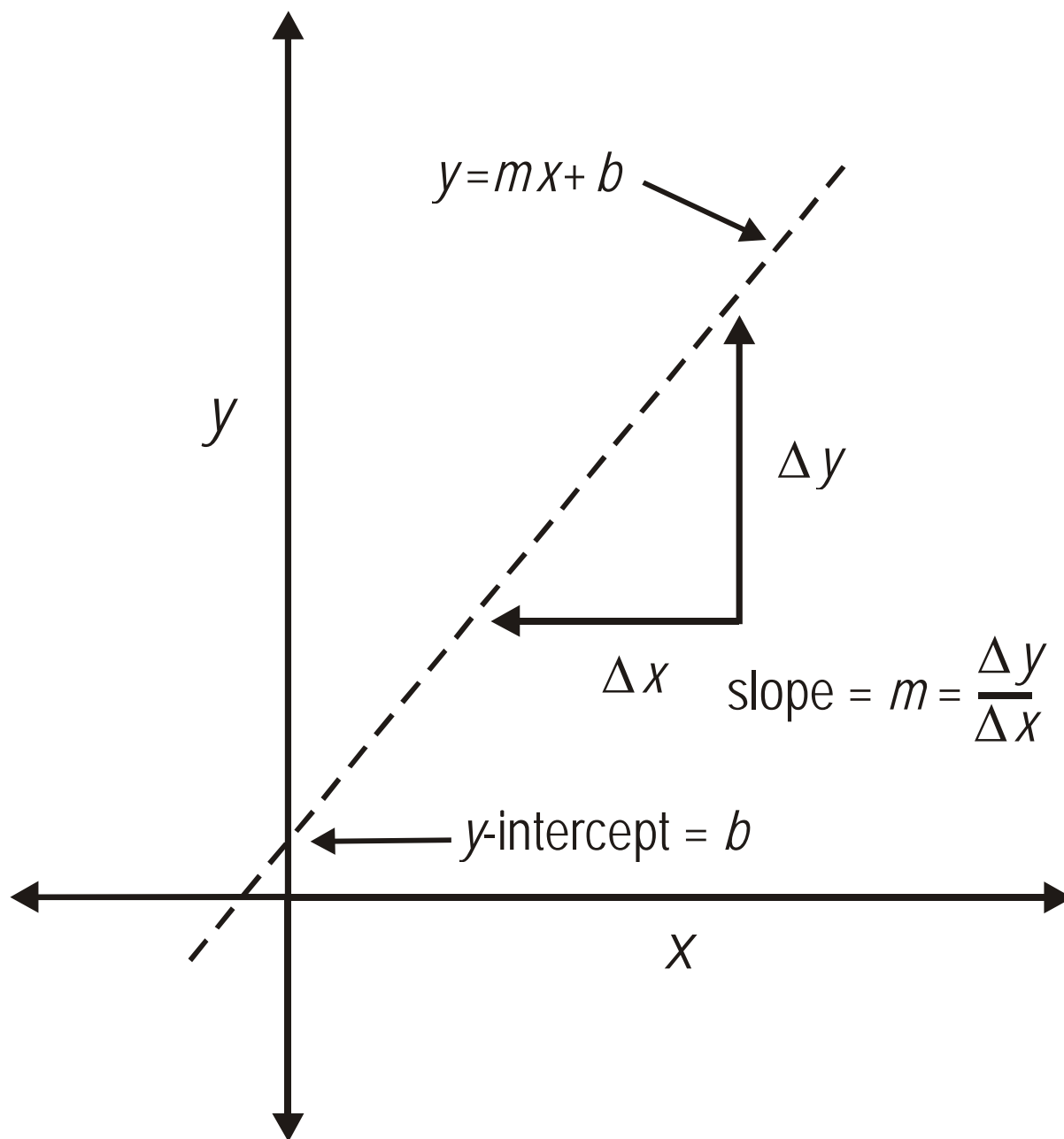


Figure S1. A linear relationship between independent (x) and dependent (y) variables.

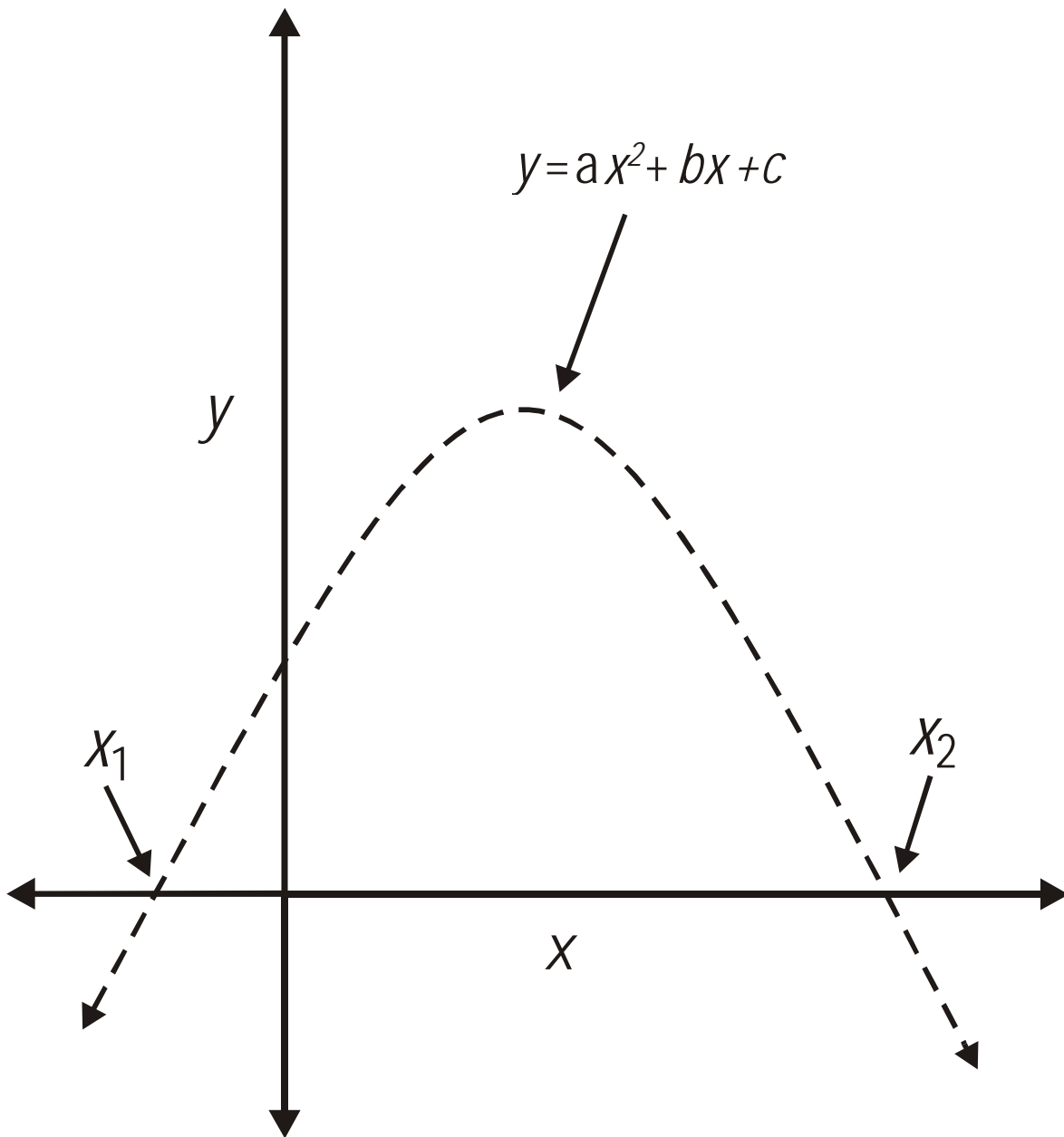


Figure S.2. A quadratic relationship between independent (x) and dependent (y) variables. The minimum and maximum roots are indicated as x_1 and x_2 , respectively.

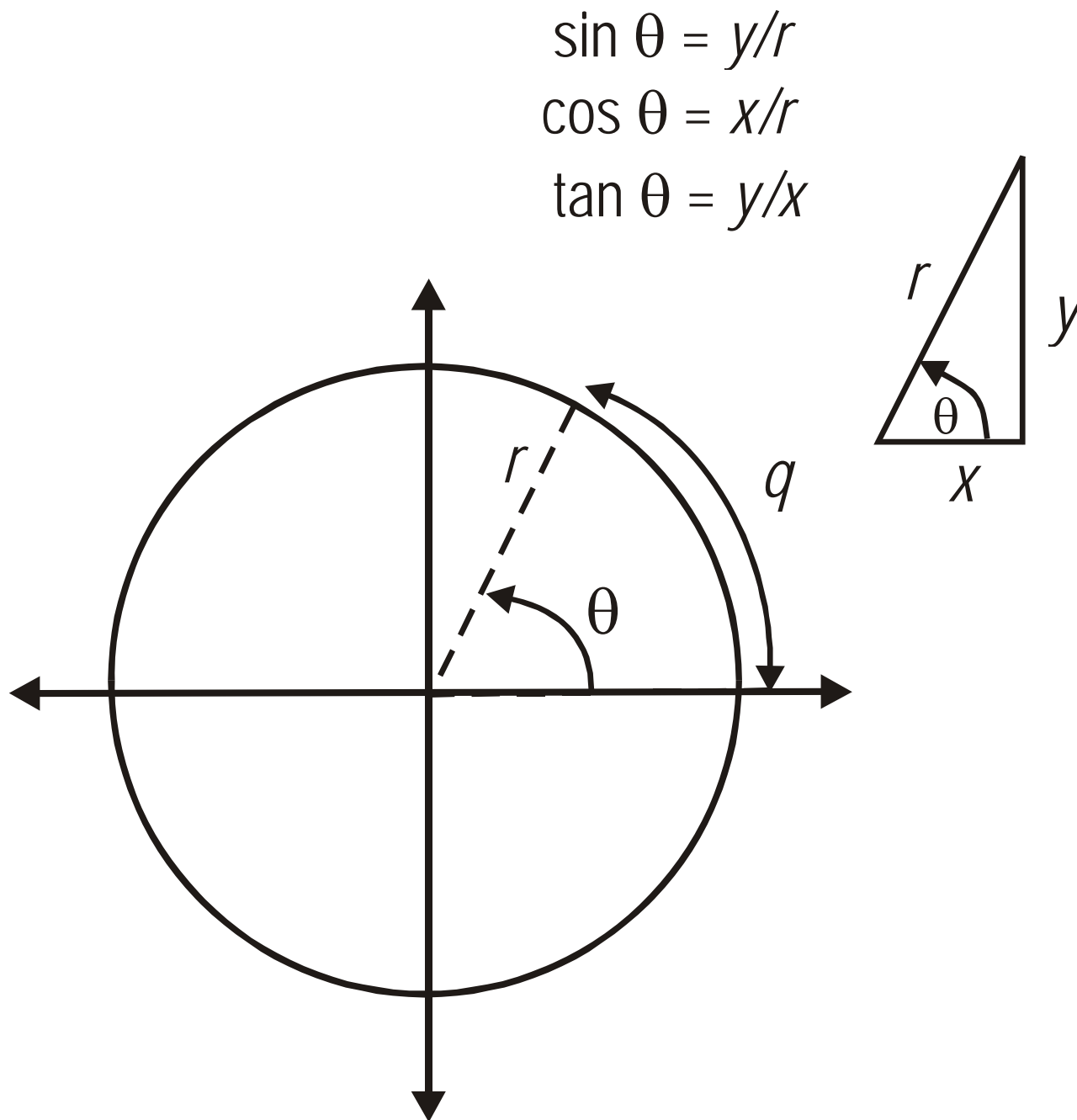


Figure S.3. The cyclic foundation for three of the primary trigonometric functions determined from triangular ratios. The triangle formed from the counterclockwise rotation of radius r and defined around angle θ is used to determine the \sin , \cos and \tan according to the ratio of sides.

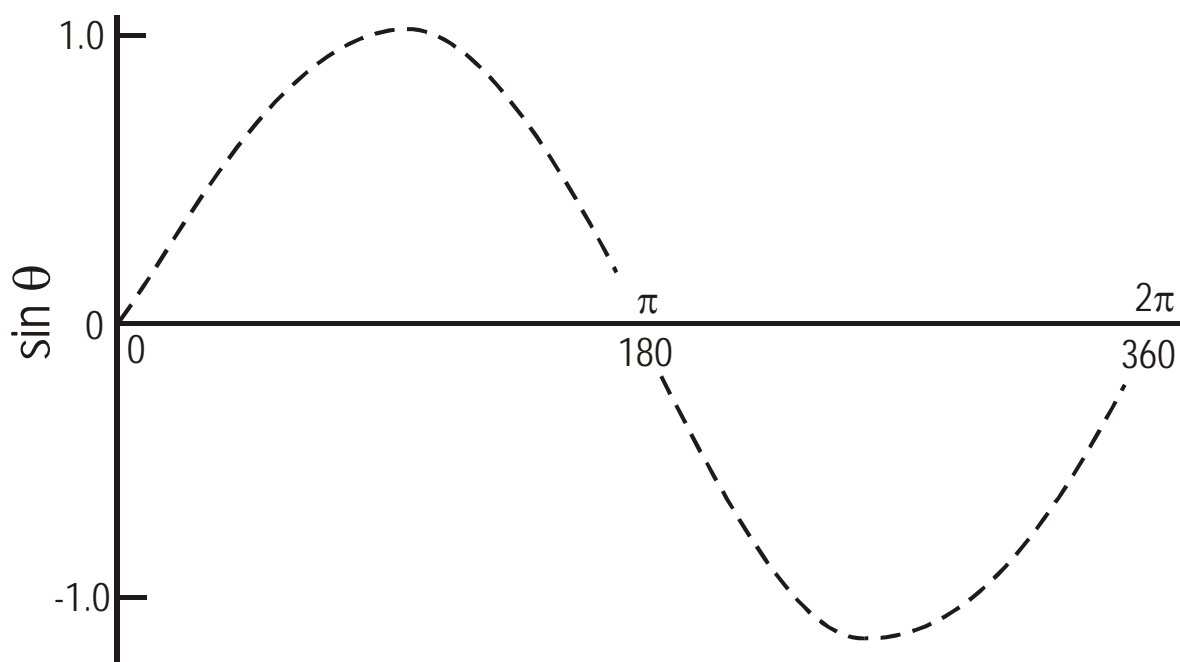


Figure S.4. The sine wave pattern formed from the progressive counterclockwise rotation of radius r plotted according to the angle θ in degrees and radians.

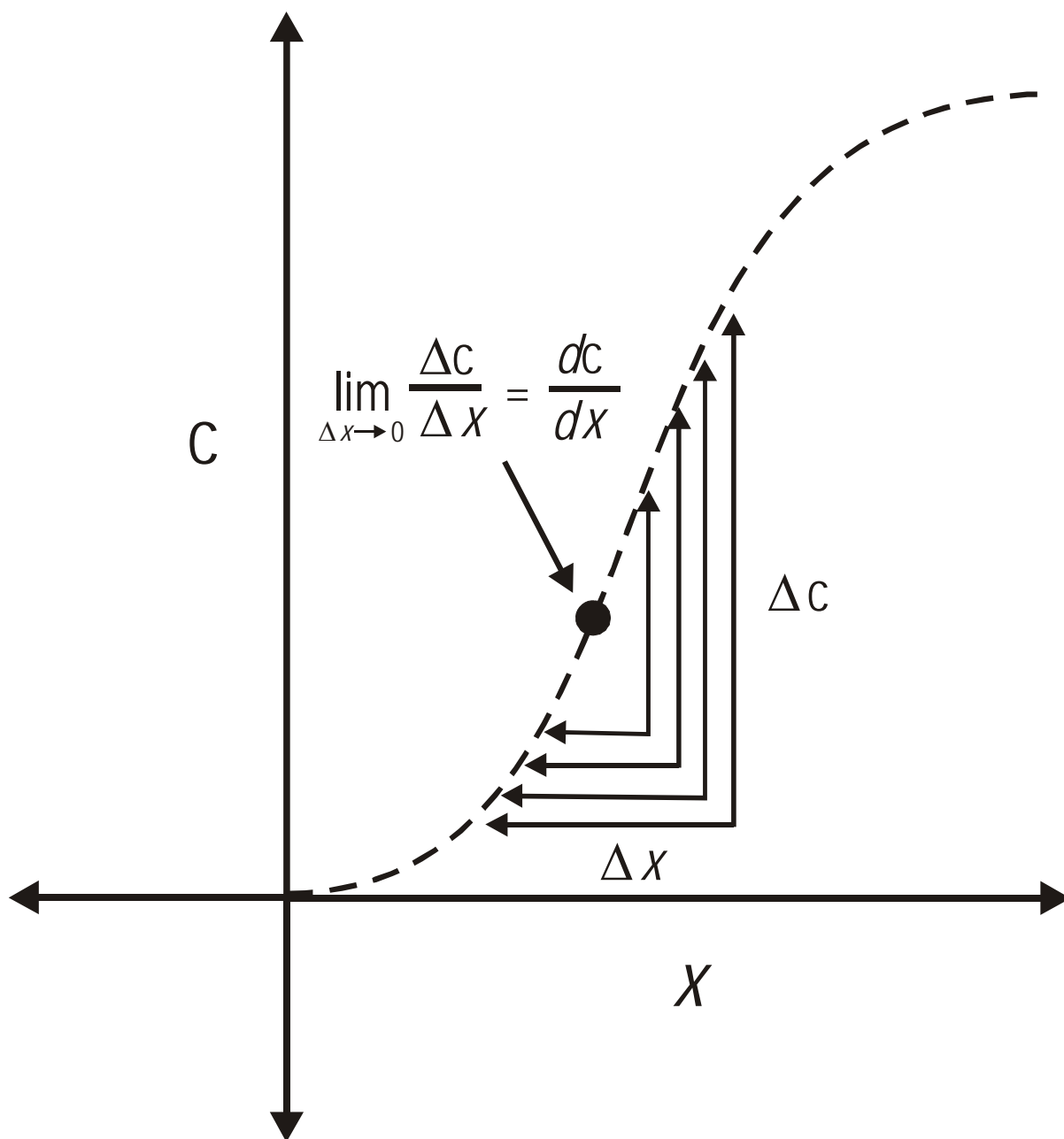


Figure S.5. The graphical representation of a limit in the relationship between scalar concentration (c) and distance (x). As Δx gets progressively smaller and eventually approaches 0 (i.e., $\Delta x \rightarrow 0$) the limit is reached.

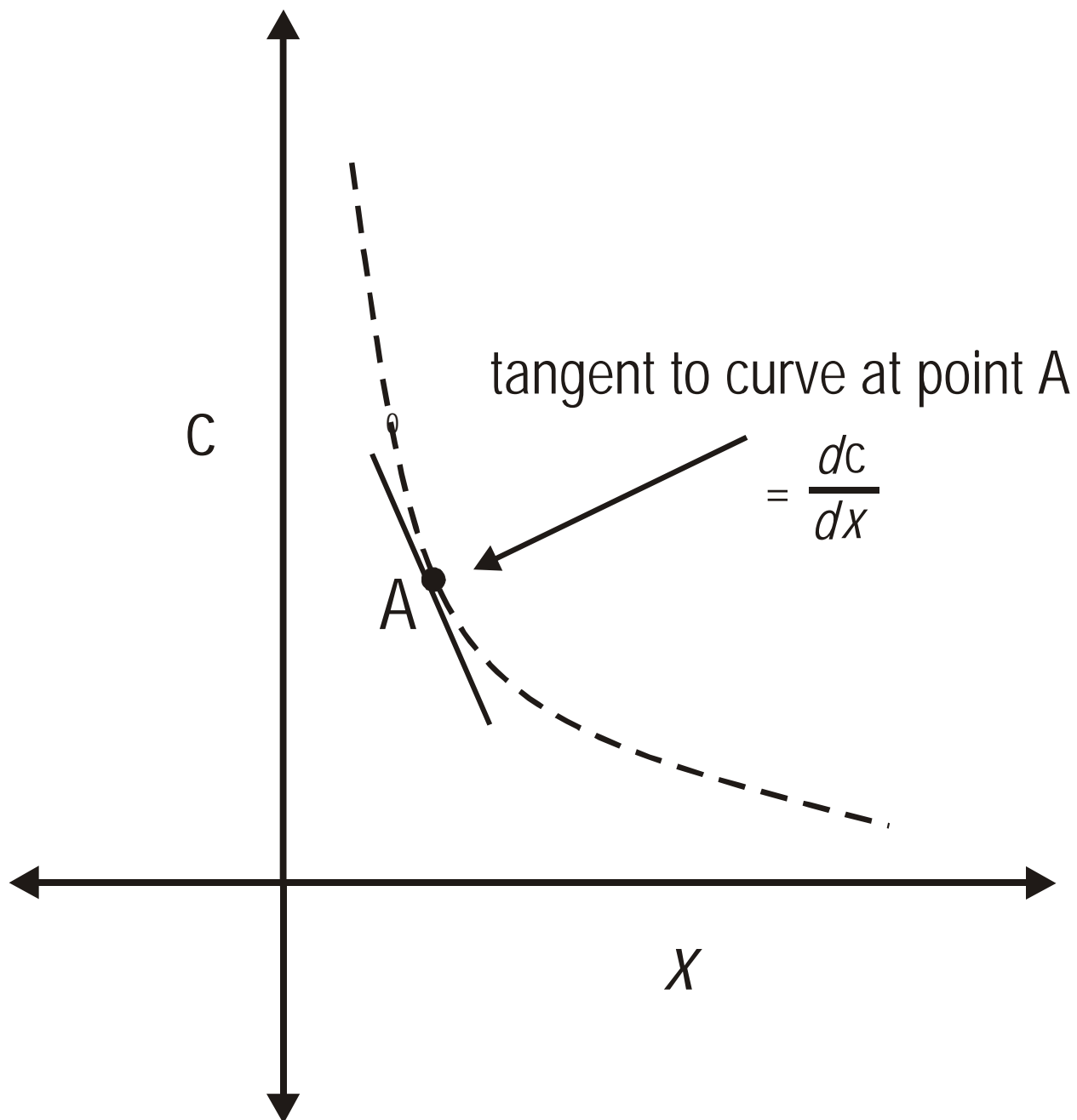


Figure S.6. The graphical representation of a point-specific slope illustrating the concept of the derivative of c with respect to x (dc/dx) as the tangent located at point A .

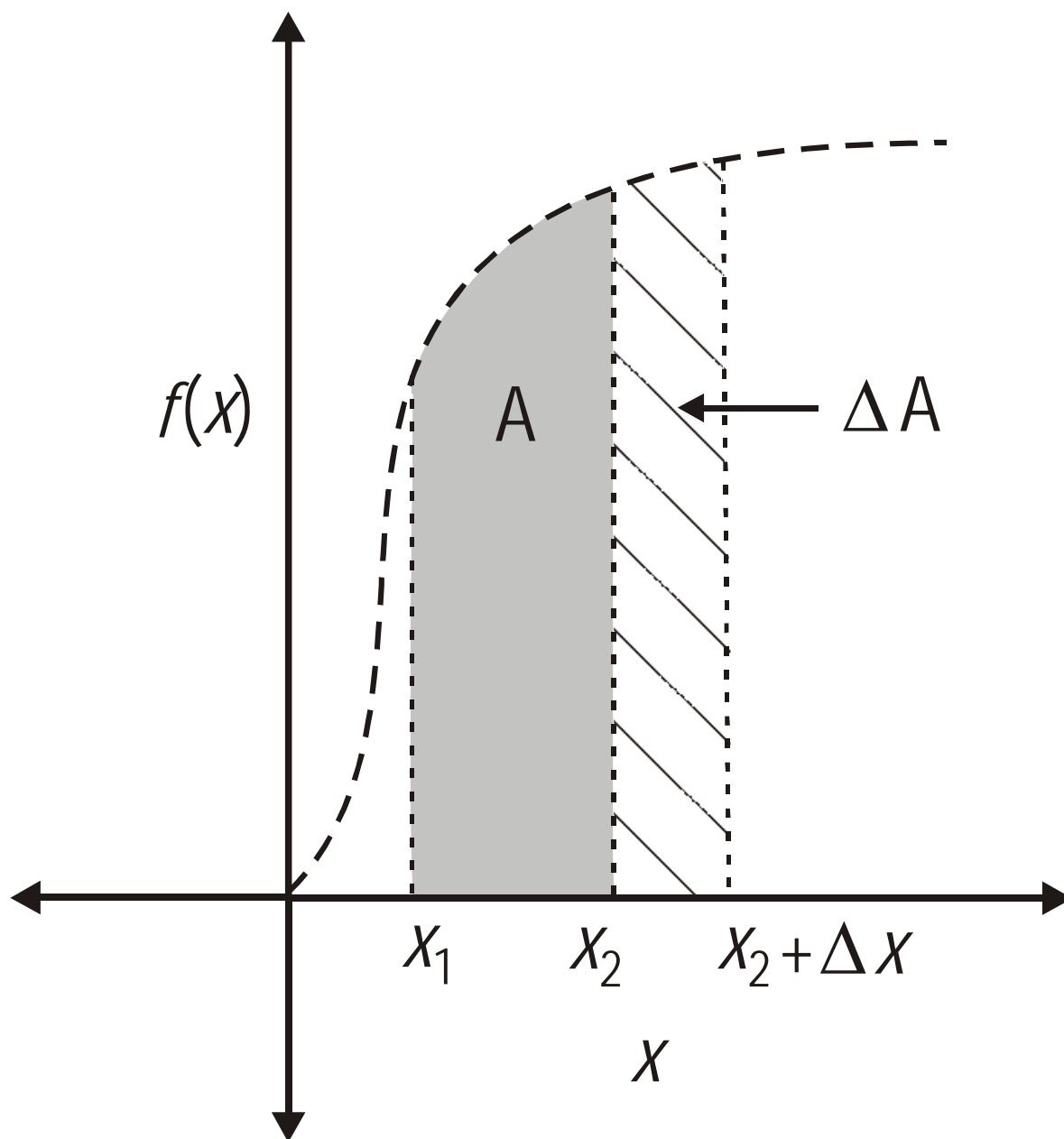


Figure S.7. The graphical representation of integration. The aim of integration is to find the area beneath the curve (A) defined by the interval between two values of the independent variable [i.e., bounded by $f(x_1)$ and $f(x_2)$]. This is accomplished by determining the function that when differentiated (i.e., as $\Delta x \rightarrow 0$) equals $f(x)$. The necessity to integrate within the limit is illustrated by designation of a change in area (ΔA), which approaches dA/dx as $\Delta x \rightarrow 0$.

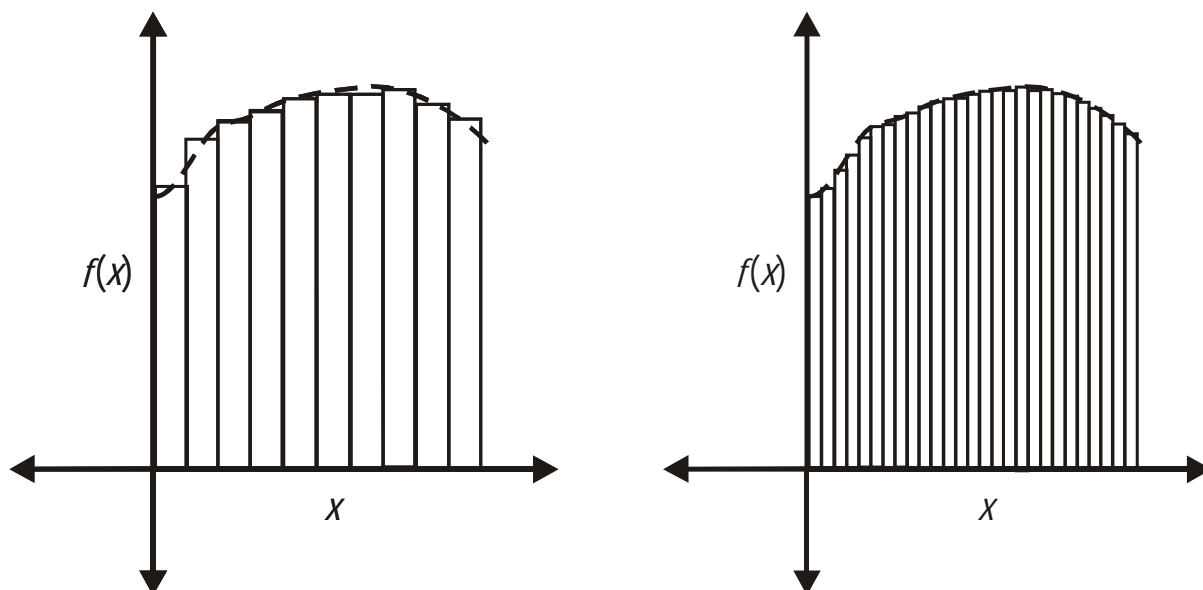


Figure S.8. An alternative perspective on integration. Integration can be thought of as the cumulative sum of areas for a series of rectangles arranged beneath the curve of interest. As the width (Δx) of the rectangles becomes smaller, the accuracy of the integration improves. The true area beneath the curve is determined within the limit as $\Delta x \rightarrow 0$.

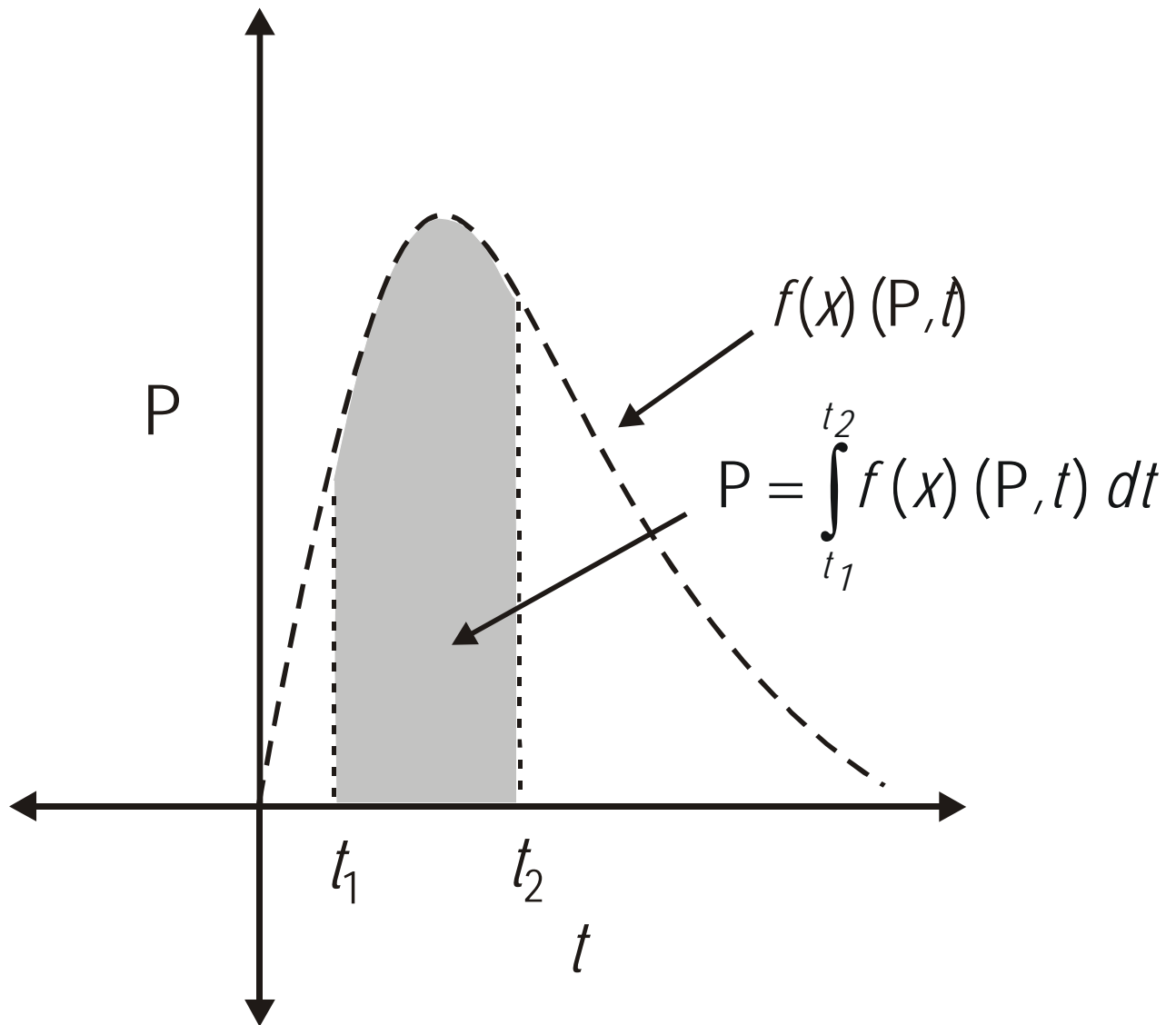


Figure S.9. Graphical representation of a probability density function $[f(x)(P,t)]$ expressed in relation to time (t). The probability of a successful event at any point in time can be estimated by the function. The total probability of a successful event within the time interval $t_2 - t_1$ can be evaluated as the definite integral as shown.

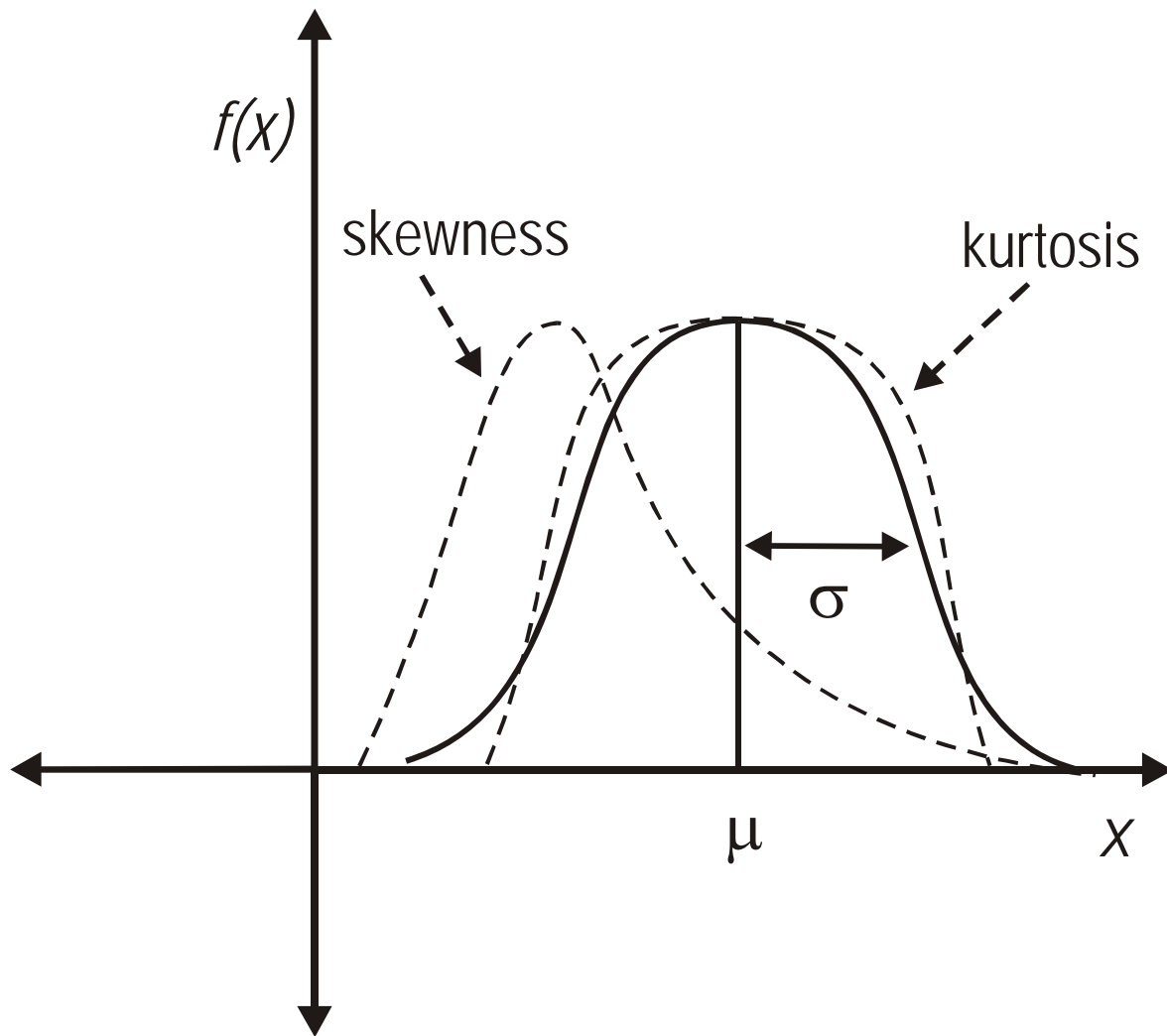


Figure S.10. A Gaussian probability distribution (shown as the solid curve) with the mean (μ) and standard deviation (σ) indicated. Distributions displaying significant kurtosis (platykurtosis) and negative skewness are also shown.

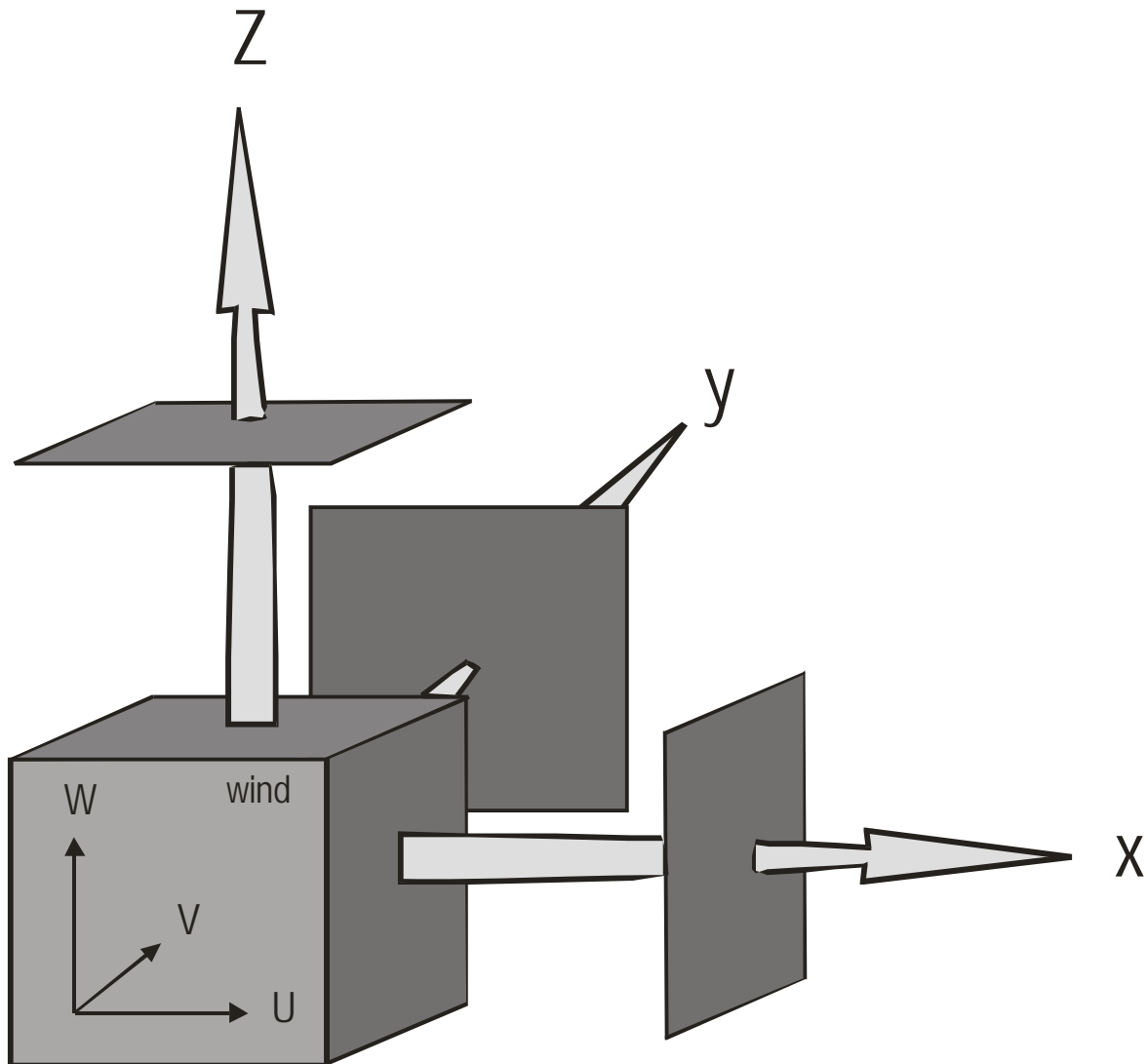


Figure S.11. Momentum flux occurs when wind, with its three Cartesian coordinates (u , v and w), is transferred in three possible Cartesian directions (x , y and z), yielding nine possible vector components. (Redrawn from Stull 1988).

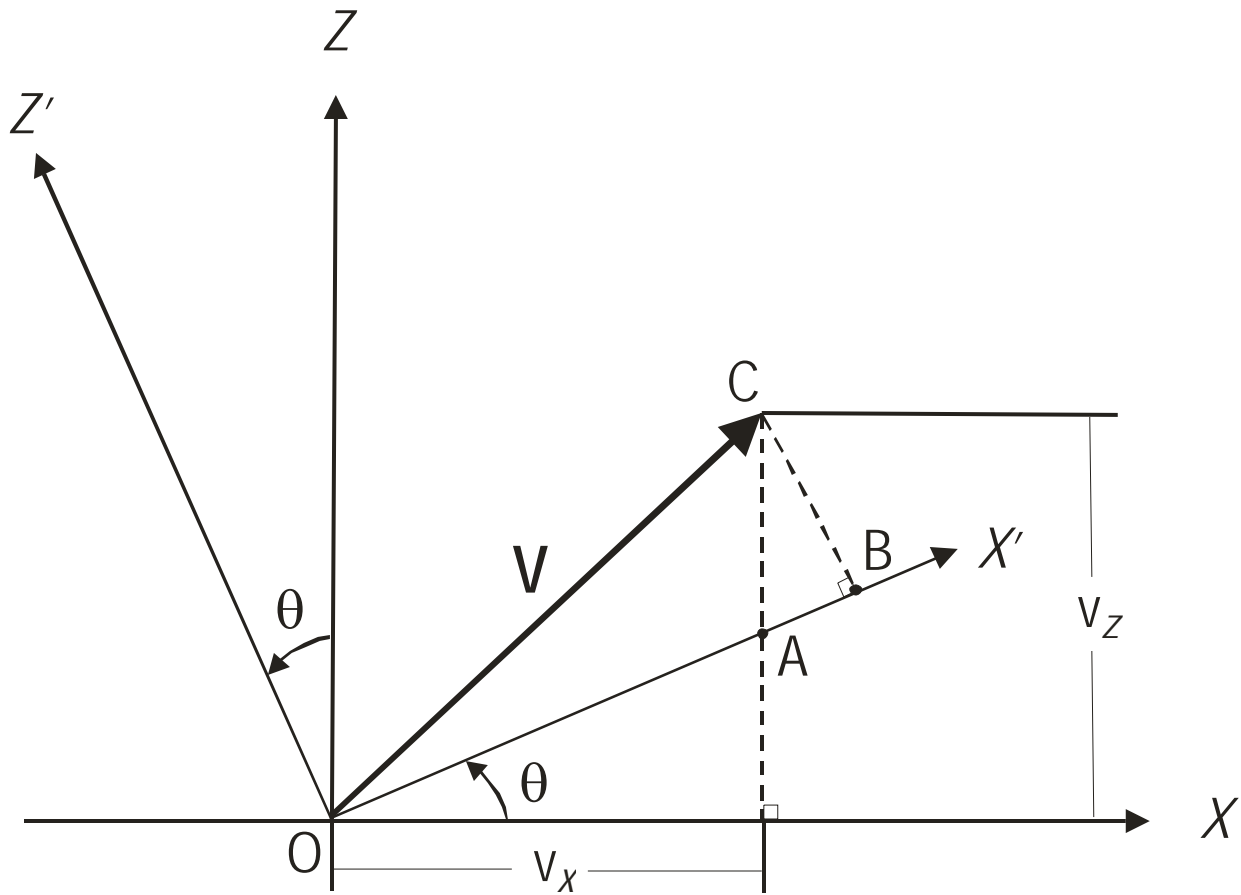


Figure S12. Rotation of Cartesian axes around the y-axis. The original vector (v) is drawn relative to the original x, z axes. The rotation is intended to redefine v relative to the new, rotated x', z' axes. See text for more details. (Redrawn from Lea 2004).