Open-Ended Problems: A Future Chemical Engineering Education Approach. J. Patrick Abulencia and Louis Theodore.

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Applied Mathematics

This chapter is concerned with applied mathematics. As with all the chapters in Part II, there are several sections: overview several specific technical topics, illustrative open-ended problems, and, open-ended problems. The purpose of the first section is to introduce the reader to the subject of applied mathematics. As one might suppose, a comprehensive treatment is not provided, although several sections addressing additional specific technical topics are included. The section contains three open-ended problems; the authors' solutions (there may be other solutions) are also provided. The last section contains 45 problems; *no* solutions are provided here.

2.1 Overview

This overview section is concerned—as can be noted from its title—with applied mathematics. As one might suppose, it was not possible to address all topics directly or indirectly related to applied mathematics. However, additional details may be obtained from either the references provided at the end of this Overview section and/or at the end of the chapter.

Note: Those readers already familiar with the details associated with this subject may choose to bypass this overview.

The chemical engineer learns early in one's career how to use equations and mathematical methods to obtain exact answers to a large range of relatively simple problems. However, these techniques are often not adequate for solving real-world problems, although the reader should note that one rarely needs exact answers in technical practice. Most real-world engineering and, to a lesser degree, science applications are inexact because they have been generated from data or parameters that are measured, and thus represent only approximations. What one is likely to require and/or desire in a realistic situation is either an approximate answer or one having reasonable accuracy from an engineering point of view.

As noted above, the solution to a chemical engineering (or scientific) problem usually requires an answer to an equation or equations, and the answer(s) may be approximate or exact. Obviously an exact answer is preferred, but because of the complexity of some equations, exact solutions may not be attainable. Furthermore, an answer that is precise may not be necessary; for this condition, one may resort to another approach – a solution that has come to be defined as a *numerical method*. Unlike the exact solution, which is continuous and in closed form, numerical methods provide an inexact (but often reasonably accurate) solution.

Today's computers have had a tremendous impact on the chemical engineering profession, including engineering design, computation, and data processing. The ability of computers to handle large quantities of data and to perform mathematical operations described above at tremendous speeds permits the analysis of many more applications and more engineering variables than could possibly be handled on the slide rule – the trademark of chemical engineers (including one of the authors) of yesteryear. Scientific calculations previously estimated in lifetimes of computation time are currently generated in seconds and, in many occasions, microseconds, and in some rare instances, nanoseconds [1].

Although the chapter is titled "Applied Mathematics" the material presented is primarily concerned with numerical methods. This subject was taught in the past as a means of providing chemical engineers with ways to solve complicated mathematical expressions that they could not otherwise solve. A brief overview of the numerical methods below is given to provide the chemical engineer (as well as other engineers) with some insight into what many of the currently used software packages are actually doing. The authors have not attempted to cover all the topics of numerical methods.

Topics that traditionally fall in the domain of this subject and receive brief treatment include:

1. Differentiation and integration;
2. Simultaneous linear algebraic equations;
3. Nonlinear algebraic equations;
4. Ordinary and partial differential equations; and
5. Optimization.

Since a detailed treatment of each of the above topics is beyond the scope of this presentation, the reader is referred to the literature [2–4] for a more extensive analysis and additional information. The remainder of this section examines the five topics listed above.

2.2 Differentiation and Integration

Several differentiation methods are available to generate expressions for a derivative. One of the authors has provided information in an earlier work. Some useful *analytical* derivatives in engineering calculations are also provided [4].

Numerous chemical engineering and science problems require the solution of integral equations. In a general sense, the problem is to evaluate the function on the right hand side (RHS) of Equation 2.1:

$$I = \int_a^b f(x)\,dx \tag{2.1}$$

where I is the value of the integral. There are two key methods employed in their solution: analytical and numerical. If f(x) is a simple function, it may be integrated analytically. For example if f(x)= x^2

$$I = \int_a^b x^2 dx = \frac{1}{3}(b^3 - a^3) \tag{2.2}$$

If, however, $f(x)$ is a function too complex to integrate analytically; (e.g., $\log[\tanh\left(e^{x^3-2}\right)]$,one may resort to any of the numerical methods available. Two simple numerical integrations methods that are commonly employed in engineering practice are the *trapezoidal rule* and *Simpson's rule* [4].

2.3 Simultaneous Linear Algebraic Equations

The chemical engineer often encounters problems that not only contain more than two or three simultaneous algebraic equations but also those that can be nonlinear as well. There is, therefore, an obvious need for systematic methods of solving simultaneous linear and simultaneous nonlinear equations [2,5]. This section will address the linear sets of equations; information on nonlinear sets is available in the literature [6].

Consider the following set of n equations:

$$\begin{aligned}
&a_{11}x_1 + a_{12}x_2 + \ldots + a_{1n}x_n = y_1 \\
&a_{21}x_1 + a_{22}x_2 + \ldots + a_{2n}x_n = y_2 \\
&\ldots \\
&\ldots \\
&a_{n1}x_1 + a_{n2}x_2 + \ldots + a_{nn}x_n = y_n
\end{aligned} \tag{2.3}$$

where a is the coefficient of the variable x and y is a constant. The above set is considered to be linear as long as none of the x-terms are nonlinear, e.g., x_2^2 or $ln\,x_1$. Thus, a linear system requires that all terms in x be linear. The system of linear algebraic equations may be set in *matrix* form:

$$\begin{bmatrix} a_{11} & a_{12} & \ldots & a_{1n} \\ a_{12} & a_{22} & \ldots & a_{2n} \\ \ldots & \ldots & \ldots & \ldots \\ a_{n1} & a_{n2} & \ldots & a_{nn} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ \ldots \\ x_n \end{bmatrix} = \begin{bmatrix} y_1 \\ y_2 \\ \ldots \\ y_n \end{bmatrix} \tag{2.4}$$

Methods of solution available for solving these linear sets of equations include:

1. Gauss-Jordan reduction;
2. Gauss elimination;
3. Gauss-Seidel;
4. Cramer's rule; and
5. Cholesky's methods.

Ketter and Prawler [3] provide several excellent illustrative examples.

2.4 Nonlinear Algebraic Equations

The subject of the solution to a nonlinear algebraic equation is considered in this section. Although several algorithms are available in the literature, the presentation will key on the Newton-Raphson (NR) method of evaluating the root(s) of a nonlinear algebraic equation.

The solution to the equation

$$f(x) = 0 \tag{2.5}$$

is obtained by guessing a value for x, i.e., x_{old}, that will satisfy the above equation. This value is continuously updated to x_{new} using the equation (the prime represents a derivative)

$$x_{new} = x_{old} - \frac{f(x_{old})}{f'(x_{old})} \tag{2.6}$$

$$\frac{x_{new} - x_{old}}{0 - f(x_{old})} = \frac{1}{f(x_{old})}$$

$$x_{new} = x_{old} - \frac{f(x_{old})}{f'(x_{old})}$$

until either little or no change in $(x_{new} - x_{old})$ or $(x_{new} - x_{old})/x_{old}$ is obtained. One can also express this operation graphically (see Figure 2.1). Noting that

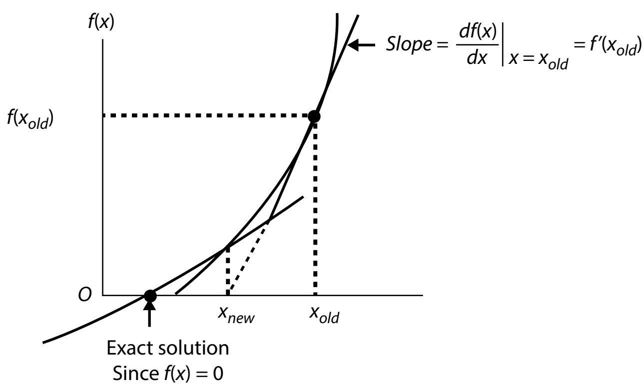

Figure 2.1 Newton-Raphson method for nonlinear equations.

$$\frac{df(x)}{dx} \approx \frac{\Delta f(x)}{\Delta x} = \frac{f(x_{old}) - 0}{x_{old} - x_{new}} = f'(x_{old}) \tag{2.7}$$

one may rearrange Equation 2.7 to yield Equation 2.8 below. The x_{new} then becomes the x_{old} in the next calculation.

$$x_{new} = x_{old} - \frac{f(x_{old})}{f'(x_{old})} = f(x)/dx \tag{2.8}$$

This method is also referred to as Newton's Method of Tangents (NMT), and is a widely used method for improving a first approximation of a root via the aforementioned equation of the form $f(x)= 0$.

2.5 Ordinary and Partial Differential Equation

The Runge-Kutta (RK) method is one of the most widely used techniques in chemical engineering practice for solving first-order differential equations. For the equation

$$\frac{dy}{dx} = f(x, y) \tag{2.9}$$

the solution takes the form

$$y_{n+1} = y_n + \frac{h}{6}(D_1 + 2D_2 + 2D_3 + D_4) \tag{2.10}$$

where

$$\begin{aligned} D_1 &= hf(x, y) \\ D_2 &= hf\left(x_n + \frac{h}{2}, y_n + \frac{D_1}{2}\right) \\ D_3 &= hf\left(x_n + \frac{h}{2}, y_n + \frac{D_2}{2}\right) \\ D_4 &= hf\left(x_n + h, y_n + D_3\right) \end{aligned} \tag{2.11}$$

The term h represents the increment in x. The term y_n is the solution to the equation x_n, and y_{n+1} is the solution to the equation at x_{n+1} where $x_{n+1} = x_n + h$. Thus, the RK method provides a straightforward means for developing expressions for Δy; i.e., $y_{n+1} - y_n$, in terms of the function $f(x,y)$ at various "locations" along the interval in question.

The RK method can also be applied if the function in question also contains the independent variable or more than one differential equation or to treat higher-order differential equations.

Many practical problems in chemical engineering applications involve at least two independent variables; i.e., the dependent variable is defined in terms of (or is a function of) more than one independent variable. The derivatives describing these independent variables are defined at *partial* derivatives. Differential equations containing partial derivatives are referred to as partial differential equations (PDEs).

The three main PDEs encountered in chemical engineering practice are briefly introduced below employing T (e.g., the temperature as the dependent variable), t (time) and x,y,z (position) as the independent variables. Note that any dependent variable; e.g., pressure, concentration, etc., could also have been selected in Equations 2.12 to 2.14 below.

The parabolic equation:

$$\frac{\partial T}{\partial t} = a\,\frac{\partial^2 T}{\partial z^2} \tag{2.12}$$

The elliptical equation:

$$\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} = 0 \tag{2.13}$$

The hyperbolic equation:

$$\frac{\partial^2 T}{\partial t^2} = a\,\frac{\partial^2 T}{\partial x^2} \tag{2.14}$$

The preferred numerical method of solutions of PDEs involve finite differences [3].

2.6 Optimization

Optimization has come to mean different things to different people. However one might offer the following generic definition for many chemical engineers: "Optimization is concerned with determining the 'best' solution to a given problem". Alternatively, a dictionary would offer something to the effect: "to make the most of… develop or realize to the utmost extent… often the most efficient or optimum use of…". This process or operation in chemical engineering practice is required in the solution of problems that involve the maximization or minimization of a given function.

A significant number of optimization problems challenge the practicing chemical engineer. The optimal design of process equipment as well as industrial processes has been an ongoing concern to the practicing chemical engineer, and for some, might define the function and goal of applied engineering. The practical attainment of an optimum design is generally a result of factors that include mathematical analysis, empirical information, and both the subjective and objective experiences of the chemical engineer.

In a general sense, optimization applications can be divided into four categories:

1. The number of independent variables involved;
2. Whether the optimization is "constrained";
3. Time-independent systems; and
4. Time-dependent systems.

In addition, if no unknown factors are present, the system is defined as *deterministic*, while a system containing experimental errors and/or other random factors is defined as *stochastic*.

Formal optimization techniques have as their goal the development of procedures for the attainment of an optimum in a system that can be characterized mathematically. The mathematical characterization may be:

1. partial or complete;
2. approximate or exact, and/or;
3. empirical or theoretical.

The resulting optimum may be a final implementable design or a guide to a practical design and a criterion by which practical designs are to be judged. In either case, the optimization techniques should serve as an important part of the total effort in the design of the units, structure, and control of not only equipment but also industrial process systems.

Optimization is qualitatively viewed by many as a tool in decision-making. It often aids in the selection of values that allow the chemical engineer to better solve a problem. In its most elementary and basic form, one may say—as noted above—that optimization is concerned with the determination of the "best" solution to a given problem. As noted, optimization is required in the solution of many general problems in chemical engineering and applied science—in the maximization (or minimization) of a given function(s); in the selection of a control variable to facilitate the realization of a desired condition; in the scheduling of a series of operations or events to control completion dates of a given project; and, in the development of optimal layouts of organizational units within a given design space, etc. [4]

The optimization problem has been described succinctly by Aris [7] as "getting the best you can out of a given situation." Problems amenable to solution by mathematical optimization techniques have these general characteristics:

1. One or more independent variables whose values must be chosen to yield a viable solution; and
2. Some measure of "success" is available to distinguish between the viable solutions generated by different choices of these variables.

Mathematical optimization techniques are used for guiding the problem solver to that choice of variables that maximizes the goodness measure (profit, for example) or that minimizes some badness measure (cost, for example).

One of the most important areas for the application of mathematical optimization techniques is in engineering design. Applications include [8]:

1. The generation of the "best" functional representations (e.g. curve fitting);
2. The design of optimal control systems;
3. Determining the optimal height (or length) of a mass transfer unit;
4. Determining the optimal diameter of a unit;
5. Finding the best equipment materials of construction;
6. Generating operating schedules; and
7. Selecting operating conditions.

A detailed and expanded treatment of applied mathematics is available in the following two references:

1. R. Ketter and S. Prawler, *Modern Methods of Engineering Computations*, McGraw-Hill, New York City, NY, 1969 [3].
2. L. Theodore, *Chemical Engineering: The Essential Reference*, McGraw-Hill, New York City, NY, 2014 [9].

2.7 Illustrative Open-Ended Problems

This section provides open-ended problems. However, solutions *are* provided for the three problems in this section in order for the reader to hopefully obtain a better understanding of these problems, which differ from the traditional problems/illustrative examples. The first problem is relatively straightforward, while the third (and last problem) is somewhat more difficult and/or complex. Note that solutions are not provided for the 45 open-ended problems in the next Section.

Problem 1: Provide a general description in layman terms of optimization methods.

Solution: The optimization problem has been described by some (see pervious section) as "getting the best you can out of a given situation." Problems amenable to solution by mathematical optimization techniques are those that generally have one or more independent variables whose values must be chosen to yield a viable solution; and possess some measure of *success* to distinguish between the many viable solutions generated by different choices of these variables. Mathematical optimization techniques are used for guiding the problem-solver to that choice of variables that *maximizes* the *approximation measure* (profit, for example) or that *minimizes* some *approximation measure* (cost, for example). In addition, one of the most important areas for the application of mathematical optimization techniques is in engineering design; and, these methods have wide applicability for large classes of problems involving the search for extreme functional values. Applications vary from the generation of "best" functional representations (curve fitting, for example) to the design of optimal operating conditions.

Problem 2: Define the Laplace Transform and provide several transforms of some elementary functions.

Solution: Assume $F(t)$ is a function of t specified for $t > 0$. The Laplace transform of $F(t)$ is usually denoted by $L[F(t)]$ and is defined by

$$L\left[F(t)\right] = f(s) = \int_0^\infty e^{-st} F(t)\,dt \tag{2.15}$$

where the parameter t is usually considered to be real; however, it can also be complex. In addition, $L[F(t)]$ exists if it *converges* for some value of s; otherwise it does not exist.

The Laplace transforms of some simple functions are provided in Table 2.1. The reader may choose to refer to Chapter 9, Illustrative open-ended Problem 1.

Problem 3: Discuss the subject of regression analysis as it applies to *scatter diagrams*.

Solution [10]: It is no secret that many statistical calculations are now performed with the help of spreadsheets or packaged programs. This statement is particularly true for regression analysis. Often, the use of packaged programs reduces or eliminates one's fundamental understanding of regression analysis.

Chemical engineers encounter applications that require the need to develop a mathematical relationship between data for two or more variables. For example, if y (a dependent variable) is a function of or depends on x (an independent variable) i.e., $y = f(x)$, one may be required to express this (x,y) data in equation form. This process is referred to as *regression analysis*, and

Table 2.1 Laplace Transforms of Simple Functions

F(t)	$L[F(t)]$
1	$\frac{1}{s}$; $s > 0$
t	$\frac{1}{s^2}$; $s > 0$
e^{at}	$\frac{1}{s-a}$; $s > a$
sin at	$\frac{a}{s^2+a^2}$; $s > 0$
cos at	$\frac{s}{s^2+a^2}$; $s > 0$

the regression method most often employed is the method of *least squares*. An important step in this procedure—which is often omitted—is to prepare a plot of y vs. x. The result, referred to as a *scatter diagram*, could take on any form. Three such plots are provided in Figure 2.2 (a to c).

The first plot (a) suggest a linear relationship between x and y; i.e.,

$$Y = a_o + a_1 X \tag{2.16}$$

The second graph (b) appears to be represented by a second order (or parabolic) relationship:

$$Y = a_o + a_1 X + a_2 X^2 \tag{2.17}$$

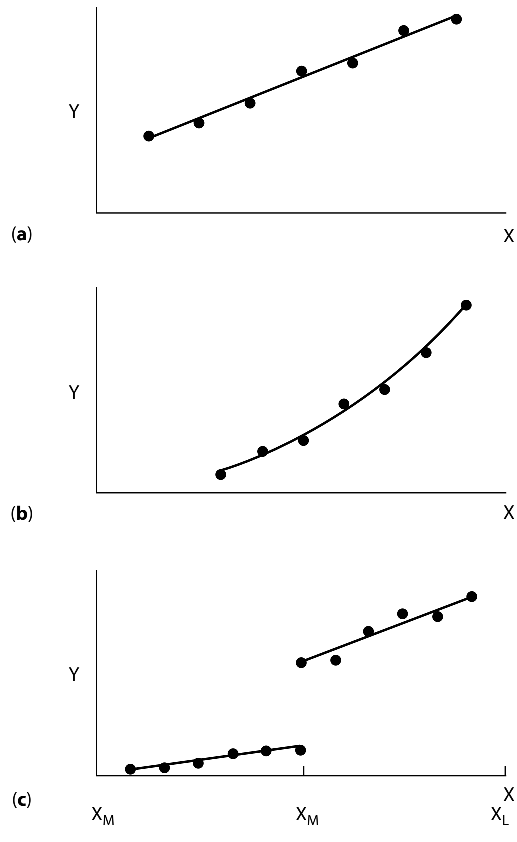

Figure 2.2 Scatter diagrams: (a) linear relationship, (b) parabolic relationship, and (c) dual-linear relationship.

The third plot (c) suggests a linear model that applies over two different ranges; i.e., it could represent the data:

$$Y = a_o + a_1 X;\ X_o < X < X_M \tag{2.18}$$

and

$$Y = a_o' + a_1' X;\ X_M < X < X_L \tag{2.19}$$

This multiequation model finds application in representing adsorption equilibria, multiparticle size distributions, quantum energy relationships, etc. In any event, a scatter diagram and individual judgment can suggest an appropriate model at an early stage in the analysis.

2.8 Open-Ended Problems

This last Section of the chapter contains open-ended problems as they relate to applied mathematics. No detailed and/or specific solution is provided; that task is left to the reader, noting that each problem has either a unique solution or a number of solutions or (in some cases) no solution at all. These are characteristics of open-ended problems described earlier.

There are comments associated with some, but not all, of the problems. The comments are included to assist the reader while attempting to solve the problems. However, it is recommended that the solution to each problem should initially be attempted *without* the assistance of the comments.

There are 45 open-ended problems in this Section. As stated above, if difficulty is encountered in solving any particular problem, the reader should next refer to the comments if any are provided with the problem. The reader should also note that the more difficult problems are generally located at or near the end of the Section.

1. Describe the early history associated with the general subject of mathematics.
2. Discuss the recent advances in applied mathematics.
3. Select a refereed published article on applied mathematics from the literature and provide a review.
4. Provide some normal everyday domestic applications involving the general topic of mathematics.
5. Develop an original problem in applied mathematics that would be suitable as an illustrative example in a book.

6. Prepare a list of the various books that have been written on applied mathematics. Select the three best and justify your answer. Also select the three weakest books and justify your answer.
7. Describe the term "machine language program" in layman terms.
8. Chemical engineers are aware that most numerical calculations are, by their very nature, inexact. The errors are primarily due to one of three sources:
   - inaccuracies in the original data;
   - lack of precision in carrying out elementary operations; and
   - inaccuracies introduced by approximate method(s) of solution.

   Of particular significance are the errors due to the *roundoff* and the inability to carry more than a certain number of significant figures in a given calculation. Terms such as *absolute error*, *relative error*, and *truncation error* have a very real meaning. And frequently, an analysis parallel to this question must be carried out to establish the reliability of a given answer. Describe the above four italicized terms in layman terms.
9. Error due to roundoff was not considered to be too difficult when calculations were carried out by hand or by desk calculators. Added places and/or error terms could be introduced with little additional work. However, there is evidence that available elementary "error theories" do not seem to be adequate for estimation, with any real degree of certainty, of the roundoff and truncation errors that result when modern high-speed digital computers are used. Develop an improved method to quantify errors that can arise in those numerical calculations.
10. There are a host of topics that reside under the applied mathematics umbrella. List these topics in order of importance and justify your answer.
11. Discuss the difference(s) between analytical mathematics and numerical methods. Which is most important? Explain your choice.
12. Discuss the difference between analog and digital computers.
13. Provide, in technical detail, the various methods for solving simultaneous linear algebraic equations.

14. Provide, in technical detail, the various methods for solving nonlinear equations.
15. Provide, in technical detail, the various methods for solving ordinary differential equations.
16. Provide, in technical detail, the various methods for solving partial differentiation equations.
17. Provide, in technical detail, the various methods for solving optimization problems.
18. Refer to Problem 2 in the previous section. Provide a short paragraph describing how differential equations can be solved by intuition.
19. Refer to Problem 2 in the previous section. Provide a short paragraph describing how differential equations can be solved by analytical methods.
20. Refer to Problem 2 in the previous section. Provide a short paragraph describing how differential equations can be solved by analytical numerical methods.
21. Refer to Problem 2 in the previous Section. Discuss how separation of variables is employed in the analytical solution of differential equations.
22. Refer to Problem 2 in the previous Section. Discuss how the Fourier Series is employed in the analytical solution of differential equations.
23. Refer to Problem 2 in the previous Section. Discuss how Bessel functions are employed in the analytical solution of differential equations.
24. Refer to Problem 2 in the previous Section. Discuss how the Error function is employed in the analytical solution of differential equations.
25. A $10,000 penalty is imposed on an oil service company every time the sulfur (S) content of a 20,000-gallon delivery of oil to an industrial facility is in excess of *one half percent*. Comment on whether the oil company should be penalized if the percent sulfur content is:
    - 0.5
    - 0.55
    - 0.546
    - 0.545
    - 0.51
    - 0.505
    - 0.50001

26. Use any suitable method to linearize the following equations

$$ae^{y} = lnx + bx \tag{2.20}$$

$$\ln y = a + \frac{b}{x^2} + \frac{c}{x} \tag{2.21}$$

$$cy = \frac{1}{\ln(ax - b)} \tag{2.22}$$

27. Fluid is flowing from a storage tank 10 ft in diameter. The drop in the tank level was observed at various times as follows (see Table 2.1). Develop an equation describing the instantaneous flow rate in gal/min as a function of time, by any graphical method.
28. Refer to the previous problem. Select an equation to describe the displacement as a function of time, and use this equation to solve the problem.
29. Develop another (and hopefully improved) method of numerically evaluating an integral.
30. Develop another (and hopefully improved) method of numerically evaluating a derivative.
31. Develop another (and hopefully improved) method of solving an ordinary differential equation.
32. Develop another (and hopefully improved) method of solving a nonlinear algebraic equation.

Table 2.1 Storage Tank Problem

Displacement from top, ft	Time, min
0.0	0
3.9	30
5.9	60
7.5	90
8.9	120

33. Develop another (and hopefully improved) method of solving a set of linear algebraic equations.
34. Develop another (and hopefully improved) method of solving an optimization problem.
35. Monte Carlo simulation is a procedure for mimicking observations of a random variable that permits verification of results that would ordinarily require difficult mathematical calculations or extensive experimentation. The method normally uses computer programs called *random number generators*. A random number is a number selected from the interval (0,1) in such a way that the probabilities that the number comes from any two subintervals of equal "length". For example, the probability that the number is in the subinterval (0.1, 0.3) is the same as the probability that the number is in the subinterval (0.5, 0.7). Thus, random numbers are observations on a random variable x having a uniform distribution in the interval (0,1). This means that the probability distribution function (PDF)—defined in the Probability and Statistics Chapter in Part II—of x is specified by

$$f(x) = 1; \quad 0 < x < 1 \tag{2.23}$$

$$f(x) = 0; \quad \text{elsewhere} \tag{2.24}$$

The above PDF assigns equal probability to subintervals of equal length in the interval (0,1). Using random number generators, Monte Carlo simulation can generate observed values of a random variable having any specified PDF. For example, to generate observed values of t, the time to failure, when t is assumed to have a pdf specified by $f(t)$, one first uses the random number generator to generate a value x between 0 and 1. The solution is an observed value of the random variable t having a PDF specified by $f(t)$ [8].

The above provides a technical definition of Monte Carlo simulation. Your task is to describe the Monte Carlo simulation in layman terms.
36. Is Monte Carlo simulation a topic that should be addressed as a mathematics operation?

37. Describe the various searching schemes that are employed in optimization.
38. Develop a general procedure to employ to determine the optimum operating conditions in a plant.
39. Develop an optimum design for a new plant.
40. Develop the optimum design of a plant retrofit.
41. Describe advances in numerical methods this century.
42. Discuss the role the weighted-sum method of analysis in optimization studies.
43. In an attempt to mathematically describe the behavior of an operating system, a young engineer discovers that he/she has generated six equations that contain five variables. Suggest some *simple* approaches that the youngster can employ to best describe the system of concern.
44. In an attempt to mathematically describe the behavior of an operating system, the same young engineer discovers that he/she has generated five equations that contain six variables. Suggest some *simple* approaches that the youngster can employ to best describe the system of concern.
45. Develop a simplified manual procedure (not employing a computer) to generate, for any number, its:
    - square root
    - cube root
    - n^{th} root

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