Chapter 4. Models

4.1. Reductionism

Rational human beings seek for order and control through understanding. Scientific knowledge falls broadly into categories, factual and conceptual. Alchemy grew into the science of chemistry when Lavoisier and Dalton began to study matter quantitatively. Similar to most intellectual efforts, science tries to understand systems through observation and speculation. These experimental and theoretical efforts complement each other: observations lead to generalizations (also called abstractions) which, in turn, suggest further testing. And so science marches on, at least in principle.

The first order of business is to identify the object of study, the area of investigation. A **system** is anything of interest. It may be tangible or intangible, real or imagined, stable or unstable, simple or complex. Tangible systems include persons, molecules and universes; intangible systems include ideas, feelings and mathematics. Objective reality requires independent existence; stability suggests persistence. Simplicity signals conciseness, while complexity connotes aggregation of subsystems. A description of a system requires a language to express its attributes and possibly how it differs from other systems. Components of the language are used to specify the **state** of the system, that particular set of values of its attributes which are subject to variation, called **variables**. Attributes which are needed for the description of the system, but which don't change are called **parameters**.[1] A **relationship** describes how the state variables of a system are connected. Some variables may be dependent or independent of others. A *causal system* is one for which there is a cause-and-effect relationship between its variables. Change one state variable and some other(s) respond by changing as well. Another term for causal relationship is *functional* relationship.

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[1] This definition differs from the common misuse of the term parameter to refer to a variable. The confusion arises since similar systems may differ only in the values of their parameters. Thus the parameters appear to vary, but only *between* different systems, not *within* a given system.

Causal relationships abound. "Pay your money, take your choice." Let go of an object near the surface of the earth and it responds to gravity. Apply resources to a project and it may achieve some goal. This last example shows that while a causal relationship may exist, it may be unknown, or unrecognized.

The way to bring order to the understanding of a system is to identify the relevant state parameters and variables, and (hopefully) discover relationships between the variables. This requires varying amounts of effort and insight and only approaches completeness for the simplest systems (by the definition of simple), but once accomplished, it becomes possible to predict future behavior. This is the essence of the scientific method. But scientists are not content with only describing behavior or even predicting behavior, they want to know *why* it behaves the way it does. This results in further probing of the underlying causes. Thus science proceeds in cycles of observation, description, explanation. The process leading from observation to description and from description to explanation is where the real work is done, where the real ingenuity comes in. It is not to be taken lightly, for it is the quintessence of science. For the sake of efficiency, or perhaps pride, tradition encourages reporting only the finished polished product of effort. In reality, the entire forrest often must be hacked down before the path through the forrest can be discovered.

4.2. Physical Models

A **model** *is a representation (real, abstract or imaginary) of an actual system*. It is in this generalized sense that we speak of model cities and economic theories, as well as fashion models and mathematical models. Chemistry and physics and many other areas make use of various models to represent their objects of interest.

Physical models are actual objects and may be used to simulate other objects. Miniature trains and planes are familiar examples. Under an assumption of *scaling*, namely that multiplying variables by a given amount doesn't alter relationships, inexpensive models may be constructed to study the properties of the more expensive objects they represent. Wind tunnels are used to study responses to changes in the hydrodynamic environment. Architectural models provide a visualization of the final product.

Models can assist in bridging the familiar to the unfamiliar. Bouncing billiard balls may be used to represent events at the molecular level. Lines of force between objects in space may be likened to elastic strings. The future behavior of an individual may be patterned after that of some "roll model".

Models may be used to simulate action and behavior. Analog computers use physical objects like fluids and gates to simulate mathematical operations such as arithmetic and logic. Digital computers use electrons and wires for the same purpose, and have the further advantage that the course of events may be "programmed" to simulate system behavior of arbitrary complexity.

Physical models have a place in science, but must be used with caution to the extent that they represent only an idealization or simplification of reality.

4.3. Mathematical Models

Because mathematics provides a logical language for abstraction, physical science may be thought of as applied mathematics. Experiments are analyzed with statistics and theories are expressed by mathematical formulas. These mathematical procedures are called *mathematical modeling*, and the abstract mathematical entities and relationships which are supposed to represent real objects and their behavior are called **mathematical models**. Progression in understanding comes via the process experiments 〉 data 〉 relationships 〉 tables, graphs 〉 equations 〉 predictions, explanations.

Consider growth. Populations increase ("grow") with time, economies grow, as do energy consumption, bacterial colonies, living organisms, mountains and raindrops. If there are no constraints on the system, growth may continue indefinitely. But that is unrealistic; resources run out, competing factors may come into play and controlling influences may predominate. In the absence of such limiting factors, a reasonable model for growth assumes the amount of growth in a given time is proportional to the amount accumulated during past growth. Robert Malthus considered such a model for human population growth in the 18th Century. Mathematically, the model is described by an exponential function with P(t) representing the population at time t,[2]

$$P(t) = P(0)e^{kt} \tag{4.1}$$

and a "Malthusian" population "explosion" results as time progresses.

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[2] The model states that the rate of population growth is proportional to the population:

$$\frac{dP}{dt} = kP$$

where k is the proportionality constant ("growth constant"), a parameter for a given system. Rearranging to

While you were ‘‘growing up’’ your height and weight increased with time up to a certain point, where they began to level off. This is representative of constrained growth with growth-limiting factors taken into account. The relationships between height and weight and age are not necessarily simple. Let’s consider height as a function of age. Measurements of height *vs* age could be expressed in tabular form, and then converted to equivalent graphs or equations, as described in Section 3.3. We expect to see similar results for different individuals, but not necessarily exactly the same observations for all individuals. In making the transition between observations and models, time is treated as an independent variable, and height, which depends on time, is a dependent variable. Table 4.1 and Fig. 4.1 show some typical data.

Table 4.1 Average U.S. Male Height *vs* Age

Age (yr)	Height (cm)
0	51
2	88
4	80
8	130
12	150
16	173
18	175

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isolate (‘‘separate’’) the variables allows integration (of equal quantities) (cf. Table 3.1)

$$\frac{dP}{P} = d\ \ln(P) = kdt$$

$$\ln(P) - \ln(P_0) = k(t - t_0)$$

or

$$P = P_0 e^{kt}$$

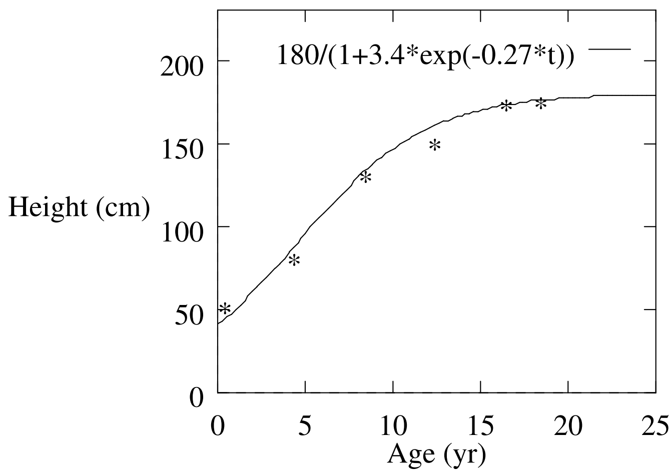

Fig. 4.1 Average U.S. Male Height as a Function of Age

The shape of the growth curve of Fig. 4.1 is not simple. It increases continuously (and eventually might decrease as well) but it is neither linear (except over a relatively small interval), quadratic (or some higher power) or exponential (except possibly in some restricted region). Whereas each of these functions might match (*fit*) the curve over some given interval, none passes through all of the points. A curve shaped like Fig. 4.1 is sometimes called "sigmoid" because it resembles the letter S. If we seek a mathematical formula to describe the data, how are we to proceed? First we need to recognize that the experimental process itself introduces uncertainties in values - no measurements are infinitely precise. So we may settle on some function which passes as close as possible to the points, if not through them. Matching experimental data to mathematical functions is called regression in statistical analysis. Closeness may be optimized by minimizing the distance between the experimental points and the curve. Least squares regression analysis is discussed in Section 3.4. The curve shown in Fig. 4.1 has the form $y = \frac{b}{1 + ae^{-kx}}$, with b = 180 (the maximum value), a = 3.4 y(0) = b/(1 + a) and k = 0.27. These parameter values were found empirically as discussed in the next paragraph.

An analytic function which describes a realistic growth curve requires some mathematical model. One model based on competitive growth was proposed by P. Verhulst in 1845, which he referred to as the ‘‘logistic’’ equation. The model is of constrained growth, where growth is limited by some feedback phenomena, such as disease, resources, competition, etc. If the total population is P, the mathematical model states that the rate of growth is proportional both to the population P at that time and to the residual population (L - P) from some limiting amount L:

$$\frac{dP}{dt} = kP(L - P) \tag{4.2}$$

L plays the roll of a limiting feedback parameter. Note that if $P < L$, the population increases, while it decreases if $P > L$, and $P = L$ represents a ‘‘stable’’ population (P constant with time, no change). The equation is expressed in simpler form if it is transformed such that p represents the fractional population relative to a limit L (i.e. P/L is replaced by p) and the proportionality constant k is replaced with $k' = kL$

$$\frac{dp}{dt} = k'p(1 - p) \tag{4.3}$$

This equation may be solved by standard differential equation techniques with the result

$$p(t) = \frac{1}{1 + ae^{-kt}} \tag{4.4}$$

where the parameter a is related to the initial population, $a = \frac{1 - p_0}{p_0}$. Since p is a fraction, it ranges between zero and unity.

A discrete logistic equation would model generations of periodic growth. The discrete analogue to the (continuous) differential logistic equation (Eq. (4.3)) is a difference equation with discrete unit time steps of the form

$$p_{n+1} = kp_n(1 - p_n) \tag{4.5}$$

This equation has been extensively explored and has very interesting behavior. For certain values of the parameter k, p_n converges to a constant value. For other values, the population oscillates with various periodicity (period two bounces between two values, period three between three, etc.). For particular values of k the periodicity becomes infinite, meaning p_n

does not return to a previous value until it has visited an infinite number of other values. Such a system is called ‘‘chaotic’’. It is a remarkable recent discovery to find simple models (equations) with such complex behavior.

As the analysis of the logistic model shows, behavior depends on the values of parameters, and can change qualitatively with small changes in parameters. No model analysis is complete without some exploration of the dependence on parameters. Such analysis is called ‘‘sensitivity analysis’’ in numerical analysis. Since parameters are supposed to represent measurable properties of systems, values which produce unusual behavior are particularly interesting.

4.4. Wave Models

Cyclic motion is one of the fundamental themes of nature. Ultimately periodic (recurrent) motion is the only possible final destiny of a system. Two extreme forms are a static (fixed) state of period one, and chaotic (random) behavior of infinite periodicity.[3] Cyclic motion is seen in water ripples, undulating flags, seasons, and phases of the moon. Vibration models have been used to describe the behavior of springs (Robert Hooke, 1678), fluids (James Bernoulli, 1738), light (Thomas Young, 1802), electricity and magnetism (James Clerk Maxwell, 1856), and sound (Lord Rayleigh, 1877).

Anyone who has played with a rope, water in a bathtub, or a musical instrument knows something about waves. Holding a rope at one end and ‘‘waving’’ it produces bumps that propagate along the rope. How can this phenomenon be described mathematically? The bump can be described in terms of a function, f called the *wave function*, that represents the displacement of the rope from its resting (equilibrium) state. The function describes how the bump travels down the rope, and so should be a function of space, or distance along the rope, x, and time, t. To understand the dependence on space and time, consider how the system behaves for each variable separately. Take a snapshot of the rope at any instant. At that time the hump is somewhere on its journey along the rope. At a later time it has moved a distance given by the product of the velocity of propagation of the hump, v and the time, t. Now chose some point along the rope and visualize its motion. As waves pass by this point the

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[3] That is, never returning to a former state until all other possible states have been ‘‘visited’’. (We will pass on the discussion of what the possible states are and how they may be determined.)

rope oscillates with time. A mathematical function which combines these behaviors is the *sine* function:

$$f(x, t) = A \sin[\frac{2\pi}{\lambda} (\alpha + x - vt)], \tag{4.6}$$

where A, α and λ are *parameters*, or constants characteristic of the system. A graph of the sine function shows a characteristic wavy curve for the displacement f as a function of distance or time, with the value of the function at any point on an axis repeated λ units further ahead (i.e. the function is *periodic*). A is the maximum displacement, or *amplitude* of the wave, λ is the distance between points having equal displacement, or *wavelength*, and α is the initial *phase*, determining the displacement at zero time and distance. Where the motion starts is not important, and α can be set to 0 for convenience. Fig. 4.2 shows a plot of sin(x), which represents Eq. (4.6) at time t = 0 for the case phase $\alpha = 0$, wavelength $\lambda = 2\pi$ and amplitude A = 1.

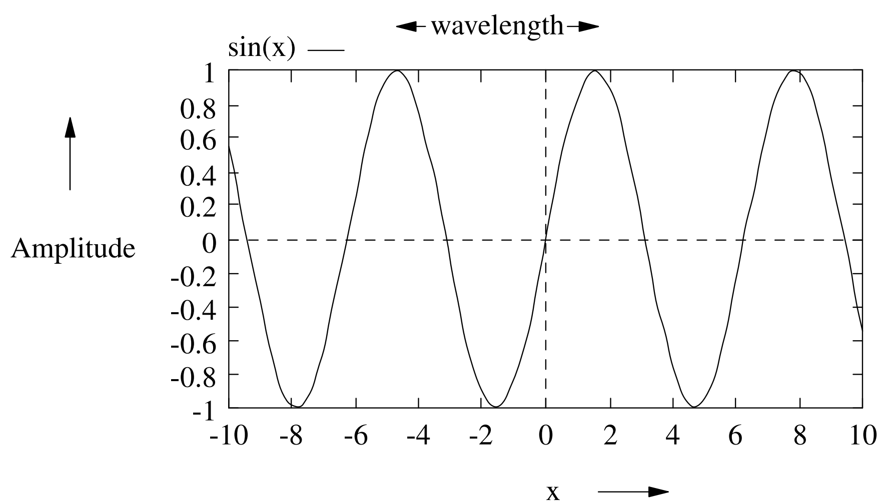

Fig. 4.2 The Sine Wave

More complicated wave forms can be described with a sum of trigonometric functions. Such a sum is called a *linear combination*, or "superposition" of functions. In fact, restricting our discussion for the moment to a single independent variable x (which could represent space or time), there is a theorem which states that any arbitrary periodic function may be expressed as a (possibly infinite) sum of sine and/or cosine functions.[4]

$$f(x) = \sum_{n=0}^{\infty} [A_n \sin(nx) + B_n \cos(nx)] \tag{4.7}$$

Now consider two people generating waves from each end of a rope. The function describing the motion from one end is Eq. 4.6 and that for the other end is the same with the minus sign replaced with a plus sign for motion in the opposite direction. There will be an interaction of the two waves and the displacement at any point will be the *sum* of the two separate displacements. If the parameters (amplitudes, phases, wavelengths and velocities) are equal from both sources, the combined function can be shown from trigonometry (using the expansion for the sine of the sum or difference of two arguments) to have the form

$$f(x, t) = 2A \sin(\frac{2\pi x}{\lambda}) \cos(2\pi \nu t), \tag{4.8}$$

where the frequency of oscillation, ν is related to wavelength by

$$\lambda \nu = v. \tag{4.9}$$

Such separation of motion into two factors is characteristic of *standing waves*, consisting of a basic wave form which does not move along the system but oscillates in a direction perpendicular to the system.

Now consider a string of length L firmly attached at the ends, such as a guitar string. The requirement that it have no displacement at the ends generates a constraining condition on the allowed wavelengths. The condition $f(0, t) = 0$ is satisfied by zero phase. The condition $f(L, t) = 0$ requires $\frac{2\pi L}{\lambda} = n\pi$, or $\lambda = \frac{2L}{n}$, where $n = 0, 1, 2, \cdots$. $n = 0$ describes the system at rest (no vibrational motion), $n = 1$ corresponds to a musical fundamental and $n > 1$ to

[4] Commonly called Fourier series for the French mathematician Jean Baptiste Joseph Baron Fourier (1768-1830) who employed them to study the propagation of heat, although used earlier by Daniel Bernoulli (1700-1782) in connections with vibrating strings.

harmonic overtones. The wave form has zero displacement at n + 1 places (including the two end points), called *nodes*. *Constrained* systems in general result in constrained *values* of the variables, called **eigenvalues**, and constrained *forms* of the wave function, called **eigenfunctions**.

We have described only one-dimensional idealized waves, without friction and sinusoidal in shape. What about more general waves? *Sinusoidal oscillation in time is assumed to be the same for all waves* (the cosine part of Eq. 4.8), but *the space part differs for each system, and is assumed to obey a general governing equation called the space wave equation*. In one dimension the space wave function looks like this:

$$\frac{d^2f}{dx^2} = -\left(\frac{2\pi}{\lambda}\right)^2 f \tag{4.10}$$

This equation differs from ordinary algebraic equations in that the term on the left is a *derivative operation*, which roughly means in this case (second derivative), compute the curvature of the function f.[5] Equations involving derivatives are called *differential equations*. Fortunately we do not have to know how to solve differential equations to discuss their results, the most important of which is that their solutions yield *functions and values*, whereas algebraic equations yield only *values*. Eq. 4.10 seeks, in effect, those functions whose curvatures are proportional to their value at each point. Those familiar with calculus can verify (by differentiating twice with respect to t) that the sine function of Eq. 4.8 satisfies Eq. 4.10, and therefore is a solution of the one-dimensional wave equation.

Wave motion in three dimensions is described by an equation similar to Eq. 4.10 with the wave function extended to three variables, traditionally given the Greek letter ψ (pronounced "sigh"), and the operator extended to three dimensions, traditionally given the Greek letter ∇^2 (pronounced "del squared"), and called the *Laplacian operator* in honor of the Eighteenth Century mathematician Pierre Simon Le marquis de Laplace:

$$\nabla^2\psi = \frac{d^2\psi}{dx^2} + \frac{d^2\psi}{dy^2} + \frac{d^2\psi}{dz^2} \tag{4.11}$$

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[5] Derivative operations are treated in calculus (cf. Section 3.11) and represent limiting slopes of curves (Section 3.3).

Curvature of a function at a point can be measured in terms of the inverse of the radius of a circle tangent to the function. (Straight lines have zero curvature, circles constant curvature.) The sign of the curvature deter-

The general space wave equation in terms of these quantities is:

$$\nabla^2 \psi = -\left(\frac{2\pi}{\lambda}\right)^2 \psi \tag{4.12}$$

4.5. Matter Models

A law of nature is an universal fundamental relationship. Laws of nature describe behavior, and by extension may be said to explain behavior and to direct behavior. Explanation is simplification - the behavior of the more complex is described in terms of the behavior of the simpler. This idea is called *reductionism*. For example, certain physiological or psychological behaviors may be explained in terms of a particular genetic and environmental makeup, which in turn may be determined by a set of molecular sequences and compounds. Molecular structure and behavior may be described by various physical theories. Broadly, biology builds on chemistry which builds on physics which builds on the foundation of mathematics. To the degree that complex systems are more than the sum of their parts however, this is but a limited model of reality.

The process of seeking the simplest description of nature has led to the quest for "The Theory (model) of Everything", a single statement with the capacity to explain all physical objects and behavior. Along that quest physicists have developed what they refer to as the "Standard Model" to describe the current understanding of the fundamental nature of matter and energy. The smallest particles of matter are classified into two groups, quarks and leptons, each containing six types distinguished by their mass (rest energy) and charge.[6] Combinations of these fundamental particles make larger particles such as protons (two *up* quarks plus one *down* quark) and neutrons (two *down* quarks plus one *up* quark). The forces which hold the fundamental particles are carried ("mediated") by three classes of other fundamental quantities called *gluons* (for strong nuclear attractions), *photons* and *W and Z bosons* (for weak electromagnetic attractions), and *gravitons* (for very weak gravitational attractions). The search is still on for a unified theory of force.

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mines whether the curve bends *upward* (positive) or *downward* (negative).

[6] All have spin 1/2, a quantum property. For the curious, the names (masses in electron volts, charges in atomic charge units) of the quarks are *up* (360 MeV, +2/3e), *down* (360 MeV, -2/3e), *charmed* (1500 MeV, +2/3e), *strange* (540 MeV, -2/3e), *top* (100 GeV, +2/3e) and *bottom* (5 GeV, +2/3e). The leptons are comprised of *electrons* (e), *muons* (μ), *tauons* (τ) and *neutrinos* (ν): e^- (511 keV, -e), μ^- (107 MeV, -e), τ^- (1784 MeV, -e), ν_e (<30 eV, 0), ν_μ (<0.5 MeV, 0), ν_τ (<250 MeV, 0).

4.6. Reality

Models are not reality, but merely representations of reality. They may be useful or even essential to apprehending reality, but they cannot substitute for it. In this sense they are idealizations, abstractions. Yet models have a valid existence of their own, even when they have no analogue in experience. This leads to an interesting dilemma. Consider mathematical models. Not all phenomena are describable by mathematics and not all mathematics describe phenomena for that matter. The fact that there exists any overlap at all is extraordinary. Einstein once said, ‘‘The fact that the universe is comprehensible at all is the most incomprehensible thing.’’

Philosophical questions arise from this line of reasoning. Is mathematics absolute or relative? Is it the language of nature, or only one of many possible languages? Or is it the invention of humans, which, in turn, are products of nature? Will it possible to discover an ultimate theory, a ‘‘theory of everything’’, or are there phenomena for which there can be no explanation, problems for which no solution can exist? Is the universe deterministic, chaotic, or some combination? Can free will be exercised without imposition? In science, we are beginning to appreciate the distinction between simple phenomena with simple descriptions and explanations, and complex phenomena which do not lend themselves to simple analysis. Yet we cannot seem to resist the temptation to seek for the simplest explanations, structures and models to explain existence.

Summary

Models are used as representations to explain phenomena. The principle of economy, referred to as the law of parsimony or Occam’s ‘‘razor’’ leads to a reductionist view of properties and behavior. Complex systems resist simple analysis.

MODELS EXERCISES

1. Describe the state variables, parameters and functional relationships of biological systems.
2. Discuss some economic models.
3. Which parameter in the growth model equation Eq. (4.2) determines the maximum size?
4. Use a computer mathematics program like *Maple* to integrate Verhulst's growth differential equation.
5. Iterate the discrete logistic equation, Eq. (4.5), for k =0, 1, 2, 3, and 4, starting $p_0 = 0.1$. and 1.
6. What would the plot of the wave function Eq. (4.6) look like for varying time and fi xed space?

MODELS EXERCISE HINTS

1. Do you know the difference between *genotypes* and *phenotypes*?
2. For starters, consider the "law of supply and demand".
3. What happens to the growth function when the parameters vary?
4. For *Maple*, read the on-line manual and study the examples on `dsolve`.
5. You can demonstrate this even with a pocket calculator (although a computer might be more convenient).
6. Refer to Fig. 4.2.