

Chapter 2

Mathematical Models: A First Look

In the second chapter, we want to look more closely at mathematical models with which we can describe natural systems. Our aim is first and foremost to familiarize ourselves with a model's basic components, as well as with different types of models. We will learn how to construct a model on the basis of examples. For this, we will not yet need complex mathematics.

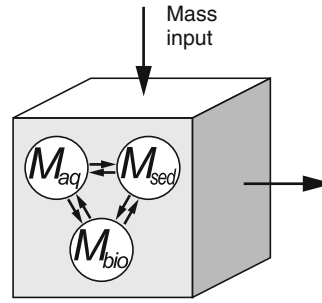
2.1 From System to Model

Before forming a model, we should think carefully about what we need the model for. What questions do we want to examine with it? Our research question helps us define the system, then select the system boundary and the relevant system variables.

For this first step of model formation, we can use some very simple tools. We draw our system as a box diagram. The boundary of the box corresponds to the system boundary. Inside the box we draw the system variables $\mathcal{V}_i$. From outside the box, the external relations $\mathcal{R}_i$ influence the system. In many cases, these external relations consist of mass flows from the environment into the system. Therefore, the external relations are also called input variables or mass input. But there could also be other kinds of external relations, for instance, solar radiation, atmospheric temperature, or a bank's interest rate. We connect the system variables with arrows that indicate the relations between them. These are the internal relations of the system. They could, for instance, be mass flows between the system variables.

One natural system that we will use as an example throughout this book is a lake. Figure 2.1 shows a first simple model to describe a chemical substance in a lake.

Fig. 2.1: A lake as a box diagram with three variables



The dimension of a model equals the number of system variables.

Example 2.1: A lake as a black box

The model has three variables: the amount or mass of a chemical substance in the lake water M_{aq} , in the lake's sediment M_{sed} and in its living organisms M_{bio} (for instance in fish). The substance to be modeled reaches the lake by a tributary river. This mass input represents the system's external relation. The loss of substance through the lake's outflow is symbolized by an arrow pointing out from the box. The exchange of substance between lake water, sediment and biomass is also symbolized by arrows connecting the three variables. These are the internal relations.

The number of system variables is called the *dimension* of a model. The example above represents a *three-dimensional* model with the three system variables M_{aq} , M_{sed} and M_{bio} . In order to formulate the model mathematically, we must describe the internal relations (the mass flows between the three system variables) and the external relations. By doing so, we arrive at the system or model equations. They usually contain additional quantities: the model parameters. In the next section, we will illustrate the method to create the system equations step by step with an example.

2.2 Static Models

We will begin with a simple example: a static model of a lake. It might allow us to answer questions about the correlation between the influx of a substance through the lake's inlet and its average concentration in the lake. The substance we are interested in is phosphorus, which often enters surface waters from sewage and agricultural fertilisers.

Let's first think about how the system looks schematically (Fig. 2.2). Our model is one-dimensional, it has *one* system variable: the phosphorus concentration in the lake C_{aq} (unit: mg m^{-3}). The external relation of the system (the phosphorus input) is the influx of dissolved phosphorus into the lake J_{in} (unit: kg year^{-1}). It could either be constant or it could

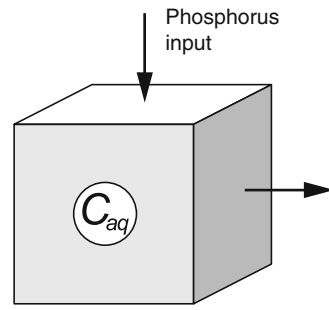


Fig. 2.2: *Static lake model: Average phosphorus concentration in the lake as a function of the current phosphorus input*

fluctuate with time. In a first attempt, we assume that there is an *immediate* relation between the phosphorus input at time t and the average phosphorus concentration in the lake measured at the same time. Mathematically, this can be formulated as follows¹:

Is there a correlation between $J_{in}(t)$ and $C_{aq}(t)$?

$$C_{aq}(t) = \text{Function of } J_{in} = f[J_{in}(t)] \quad (2.1)$$

We assume that the lake in question has been under surveillance for several years and that a data set exists from which we can calculate $C_{aq}(t)$ and $J_{in}(t)$ for different times. To find the unknown function in Eq. (2.1), we can sketch the values of $C_{aq}(t)$ and $J_{in}(t)$ in a two-dimensional diagram. Let's look at a numerical example:

Example 2.2: Phosphorus in a lake — static model

In a lake, the nutrient load constantly increases over a period of many years. This so-called eutrophication of the lake is established through the following measurements. They demonstrate a correlation between the yearly phosphorus input $J_{in}(t)$ via inlets and wastewater treatment plants, and the average total phosphorus concentration in the lake that year $C_{aq}(t)$. The following data were measured in four not necessarily consecutive years.

$J_{in}(t)$ [kg year ⁻¹]	1,500	2,100	2,800	4,200
$C_{aq}(t)$ [mg m ⁻³]	20	30	36	56

¹ With this example, we by no means suggest that this model is reasonable. It is merely a first attempt, the general validity of which we will later discuss in detail.

Figure 2.3 shows the pairs of data in a two-dimensional diagram. All data points lie roughly on a straight line. From that, we can conclude that the function in question is a linear relation of the form $f(x) = p \cdot x$. Now, we can mathematically formulate the linear relation between phosphorus input $J(t)$ and average phosphorus concentration $C_{aq}(t)$:

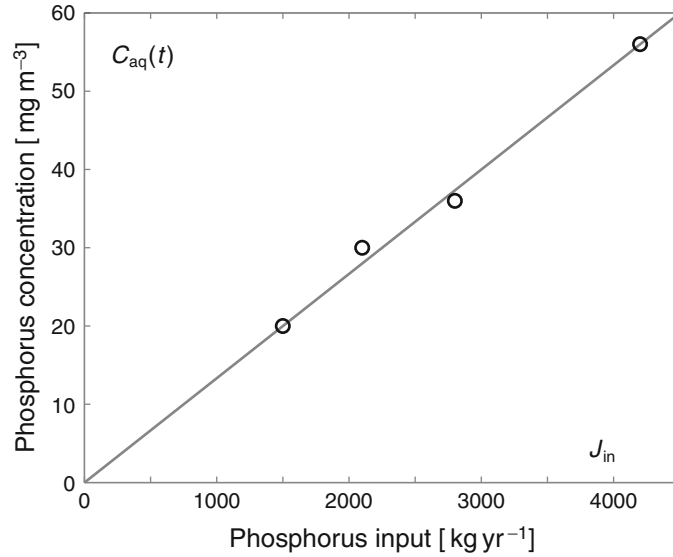
$$C_{aq}(t) = p \cdot J_{in}(t) \quad (2.2)$$

The coefficient p is the model parameter. It can be calculated as the ratio between the pairs of data. The resulting average value is:

$$p = \overline{\left(\frac{C_{aq}(t)}{J_{in}(t)} \right)} = 1.33 \times 10^{-2} \frac{\text{mg m}^{-3}}{\text{kg year}^{-1}} \quad (2.3)$$

where the bar atop the quotient signifies the average of the data pairs.

Fig. 2.3: The data pairs $J_{in}(t)$ and $C_{aq}(t)$ in a two-dimensional space. The data points lie approximately on a straight line



The above phosphorus model is called *static*, because for every value of the external relation $\mathcal{R}$ (in this example, the input $J_{in}(t)$) there is a precisely defined value of the system variable $\mathcal{V}$. Mathematically speaking, a static model with one system variable has the following form²:

$$\mathcal{V} = \text{Function of } \{\mathcal{R}\} = f(\mathcal{R}) \quad (2.4)$$

² Not in all cases can we explicitly describe the system variable $\mathcal{V}$ (as we did in Eq. 2.4). It can also be given through an implicit equation, such as $e^{a\mathcal{V}} = b\mathcal{V}$.

Equation (2.4) is called the system equation of the model. The function $f(\mathcal{R})$ can have an arbitrarily complicated form and can be defined by one or several model parameters p . If the function $f(\mathcal{R})$ is linear, as is the case in Eq. (2.2), the model is called linear.

We have described the system “phosphorus in a lake” with a linear, static model. By using Eq. (2.2), we can predict how the lake’s phosphorus concentration changes in response to a changed phosphorus input. We cannot, however, make any statement about how long it takes until the phosphorus concentration reaches its new value after the input variable has been changed. In a static model, the change takes place instantaneously. A dynamic model is needed in order to describe the transition from one state to another.

A static model cannot adequately describe changes through time.

Before we delve deeper into dynamic models in Sect. 2.3, we will briefly discuss the importance of units and dimensions.

2.2.1 Handling Dimensions and Units

Mathematical models link model variables by mathematical relations. Model variables generally have a dimension (see Appendix B). In most cases, the combination of the three basic dimensions mass (M), time (T) and length (L) is sufficient to express the dimension of every variable. Units are formed by explicitly choosing a system of measurement for the dimensions; therefore, units are a specific representation of dimensions and should not be confused with them. As long as we only work with algebraical expressions, the choice of units is irrelevant. Only the dimensions have to match on both sides of an equation. Yet, as soon we give specific values to variables in an equation, a consistent set of units is needed.

Let’s take another look at Eq. (2.3) in the example above. The unit of mass in the numerator (mg) is different from the one in the denominator (kg). It can be adjusted through the conversion $1 \text{ mg} = 10^{-6} \text{ kg}$. Then, the following holds:

$$\begin{aligned} p &= 1.33 \times 10^{-2} \frac{\text{mg m}^{-3}}{\text{kg year}^{-1}} \\ &= 1.33 \times 10^{-8} \frac{\text{mg m}^{-3}}{\text{mg year}^{-1}} \\ &= 1.33 \times 10^{-8} \text{ year m}^{-3} \end{aligned}$$

The parameter p therefore has the dimension of an *inverse volume flow rate* (T L^{-3}). We will get to know the physical significance of this parameter in Sect. 4.2. For now, let’s look at another example:

Example 2.3: Dimensions and units

A wastewater treatment plant with a water volume of $1,000 \text{ m}^3$ is accidentally contaminated with 10 kg of a toxic substance. How high is the concentration of that substance in the treatment plant after the accident?

The dimension of a concentration is (ML^{-3}) , or mass (M) per volume (L^3). Therefore, we can calculate the average concentration C in the plant with the data we have. To do so, we insert the mass of the substance (in kg) and the plant's volume (in m^3). We then get the concentration in kg m^{-3} :

$$C = \frac{10 \text{ kg}}{1,000 \text{ m}^3} = 0.01 \text{ kg m}^{-3} \quad (2.5)$$

The units kg and m are so-called metric or SI units.^a If possible, SI units should be used in scientific work. Often, however, it makes sense to convert the units into others that can more easily be visualized. The units of the average concentration in the sewage treatment plant, for instance, could be converted as follows:

$$0.01 \text{ kg m}^{-3} = 0.01 \times \frac{10^3 \text{ g}}{10^3 \text{ L}} = 0.01 \text{ g L}^{-1} = 10 \text{ mg L}^{-1} \quad (2.6)$$

Thus 10 mg of the toxic substance are dissolved in 1 L of water.

^a SI units were defined as the “système international d’unités” at a conference in Paris in 1960. They form the international standard units.

Most common spreadsheet and statistics software allows the user to graphically display the empirical relation between data pairs (like in Fig. 2.3) and to estimate the function by a regression. If we relate data pairs of two or more measured variables by a linear or nonlinear regression, a static model is produced where the regression equation becomes the model equation.

Since setting up model equations by regression analysis is very easy, one will often forget to verify whether the equation makes any physical sense. Even in literature, one occasionally finds model equations that have different dimensions on both sides. Furthermore, equations are often set up in a way that makes them valid only for a specific set of units.

In order to demonstrate this point, let's look at experimental data on the growth of an algae population under varying nitrate concentrations in water. The measurements were analyzed by a nonlinear equation.

Example 2.4: Nonlinear regression and the pitfall of units

A scientist determines the specific growth rate^a G of an algae population at different nitrate concentrations C in water. A nonlinear fit of the data yields:

$$G = 0.1 C^{0.6} \quad (2.7)$$

G Specific growth (per hour)
 C Nitrate concentration

Unfortunately, the author of the model forgot to specify in which units the nitrate concentration should be inserted in Eq. (2.7). One user of the model may express nitrate concentration in mol m^{-3} and receives a value that is smaller by a factor of 4.9 than the result of another user who fills in the concentration C in mgN L^{-1} . To make the formula compatible for both users, they would both have to use the same units. But which ones are the correct ones?

^a Specific growth rate (G) is the *relative* increase in biomass per unit of time. Independently of the dimension and unit in which biomass is given, the dimension of G is always (T^{-1}) .

For a serious modeler there are three ways to prevent this kind of confusion:

- (1) The easiest, but not always the best way: We simply write the correct units in square brackets behind each variable:

$$G (\text{h}^{-1}) = 0.1 (C (\text{mgN L}^{-1}))^{0.6} \quad (2.8)$$

This notation makes the equation confusing and difficult to read.

- (2) A better way is to replace the numerical factor by the symbol p and to separately give the value of p together with the correct unit:

$$G = p C^{0.6}, \quad \text{with } p = 0.1 \text{ h}^{-1}(\text{mgN L}^{-1})^{-0.6} \quad (2.9)$$

G (h^{-1}) Specific growth rate
 C (mgN L^{-1}) Nitrate concentration

If we would now like to insert the concentration in mol m^{-3} , we have to keep in mind that $1 \text{ mgN L}^{-1} = 1 \text{ gN m}^{-3} = \frac{1}{14} \text{ mol m}^{-3}$. Thus, the parameter can be converted as follows:

$$\begin{aligned} p &= 0.1 \text{ h}^{-1}(\text{mgN L}^{-1})^{-0.6} \\ &= 0.1 \text{ h}^{-1}\left(\frac{1}{14} \text{ mol m}^{-3}\right)^{-0.6} \\ &= 0.1 \text{ h}^{-1}(14)^{0.6}(\text{mol m}^{-3})^{-0.6} \\ &= 0.49 \text{ h}^{-1}(\text{mol m}^{-3})^{-0.6} \end{aligned}$$

Since this procedure is rather complicated, it may be better to transform the concentration values into the proper units and then apply Eq. (2.7).

- (3) The safest way, however, is to use non-dimensional variables wherever fractional exponents could appear. Applied to Eq. (2.7), we should use the following expression:

$$G = G^0 \left(\frac{C}{C^0} \right)^{0.6} \quad (2.10)$$

G	(h^{-1})	Specific growth rate
C	(mgNL^{-1})	Nitrate concentration

where G^0 is the “reference growth rate” at the “reference concentration” C^0 . The pair of reference values can be chosen arbitrarily, preferentially somewhere in the middle of the range of available data. We can satisfy ourselves that for $C^0 = 1 \text{ mgNL}^{-1}$, G^0 must be 0.1 h^{-1} for Eqs. (2.7) and (2.10) to be equivalent. Now, changing the units of concentration is much easier. One only has to adjust the units of the reference concentration accordingly.

■ Tabloid units

Editor: “You want a front page headline because of a laughable 10 Curies in RadonCorp’s waste?”—Journalist: “How about 400 billion Becquerel?”^a—“Much better. You’ve got journalism in your blood after all!”

^a Curie and Becquerel are both units for the radioactivity of a radiation source. 1 Becquerel corresponds to one decay per second. 1 Curie = 37 billion Becquerel.

Summing up, verifying the dimensions and units when we set up and solve system equations is one of the easiest and most efficient ways to prevent mistakes. The following rules may help:

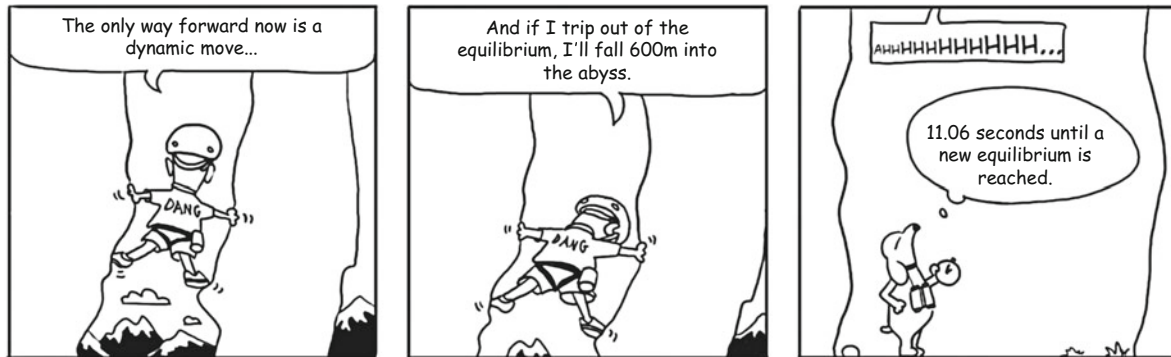
- The algebraic expressions to the left and right of the equals sign must always have the same dimension.
- Addition and subtraction are only possible if all algebraic terms have the same dimension.
- When inserting concrete numbers into an algebraic equation, their units have to be compatible. In other words, they have to be chosen so that the same combination of units results on both sides of the equals sign.
- Exponents in equations are non-dimensional (and therefore also without units). The same holds for arguments in transcendental functions

such as $\sin(\cdot)$, $\cos(\cdot)$ or $\exp(\cdot)$. Ensure that you only have fractional powers or transcendental functions of *non-dimensional* variables in your equations.

Appendix B gives an overview of dimensions and units.

2.3 Dynamic Models

Equilibrium



In Sect. 2.2 we have described the system “phosphorus in a lake” with a static model. As we discovered, with such a model we can calculate the average concentration of phosphorus in the lake water as a function of the input concentration. However, the model neglects the fact that it takes some time for the system to adjust to the new input value. With a static model, we can make no statement about how rapidly the phosphorus concentration in the lake changes if there is a sudden change in the input concentration. If we want to describe a system’s dynamics in time, static models are no longer sufficient: we need a dynamic model.

Often, adjustment processes to a change in the external relation are particularly important to understand natural systems, as is the case in the following example:

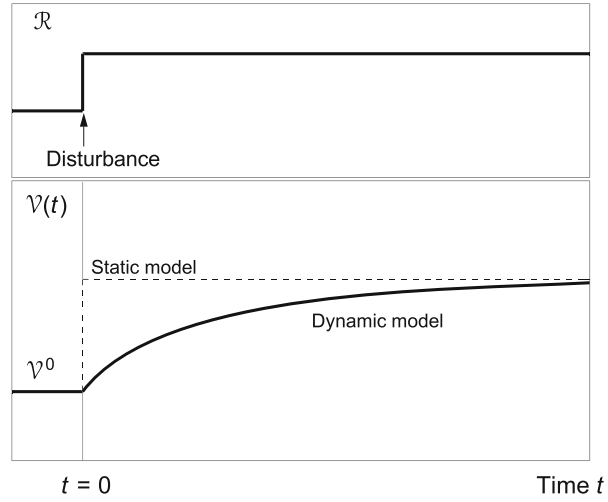
Example 2.5: Carbon dioxide in the atmosphere

Burning fossil fuels releases carbon dioxide into the atmosphere. The *current* atmospheric concentration of carbon dioxide (CO_2) does not directly depend on the *current* rate of fossil fuel consumption. Rather, the gradual increase of CO_2 mirrors the slow adjustment process of the global carbon cycle to the increased input of CO_2 into the atmosphere. The CO_2 concentration in the atmosphere will continue to rise even if the growth of fossil fuel consumption were to be reduced or halted completely. In Chap. 5, we will examine a dynamic model for the global carbon cycle (in Example 5.12).

A dynamic model describes the system's time-dependent answer to an external change.

In general terms, a dynamic model can describe how rapidly the system variable $\mathcal{V}$ changes when the external relation $\mathcal{R}$ varies. The dynamic model describes the time-dependent answer to the external change. Figure 2.4 shows the adjustment of a linear system to a disturbance that occurs suddenly at time $t = 0$. The solid line represents the simulation with a dynamic model. The system variable $\mathcal{V}(t)$ does not react immediately to the disturbance, but adjusts gradually to a new system state in equilibrium with the changed external relation $\mathcal{R}$. The static model, depicted as a dashed line, disregards this adjustment behaviour; the system variable immediately changes to the new system state.

Fig. 2.4: A dynamic model can describe the adjustment of the system variable $\mathcal{V}(t)$ to a changed external relation $\mathcal{R}$ (disturbance). The state $\mathcal{V}^0$ corresponds to the equilibrium of the system variable $\mathcal{V}$ with the external relation $\mathcal{R}$ before the disturbance occurred ($t < 0$)



The system equation of a dynamic model is significantly different from Eq. (2.4). On the left-hand side of the equation we write the system variable's change with time:

$$\text{Temporal change of } \mathcal{V} = f(\mathcal{R}, \mathcal{V}) \quad (2.11)$$

If the temporal change of the system variable $\mathcal{V}$ is smooth, i.e. not made up by sudden jumps,³ it can be described by the first derivative of the system variable with respect to time. The mathematical model is therefore

³ Mathematicians call such a function *differentiable*.

a first order differential equation⁴ with respect to time:

$$\frac{d\mathcal{V}}{dt} = f(\mathcal{R}, \mathcal{V}) \quad (2.12)$$

The function $f(\mathcal{R}, \mathcal{V})$ is called the change or velocity function of the system variable.

In order to calculate the adjustment of the model to a changed input variable, we have to integrate the differential equation (2.12). To do so, we need an initial value $\mathcal{V}^0$, that is, the value of the system variable at an arbitrary time t_0 . The model calculation begins at time t_0 . Usually, we set $t_0 = 0$. It is important to note that the solution of the differential equation (2.12) depends on the initial value $\mathcal{V}^0$. This is a crucial difference to the static model (Eq. 2.4), where there is no such dependency.

In many cases a dynamic model is developed to draw up a balance of a specific quantity, such as the mass of a chemical substance, the number of individuals of a specific species, or even just a quantity of money. In the resulting system equations we can characterize the temporal change of that quantity in the system as the difference between input and output. Let's look at an example:

Example 2.6: Phosphorus in a lake — dynamic model

The dynamic phosphorus model of a lake can be described as the mass balance of phosphorus in the lake water. First, let's describe the mass balance in words:

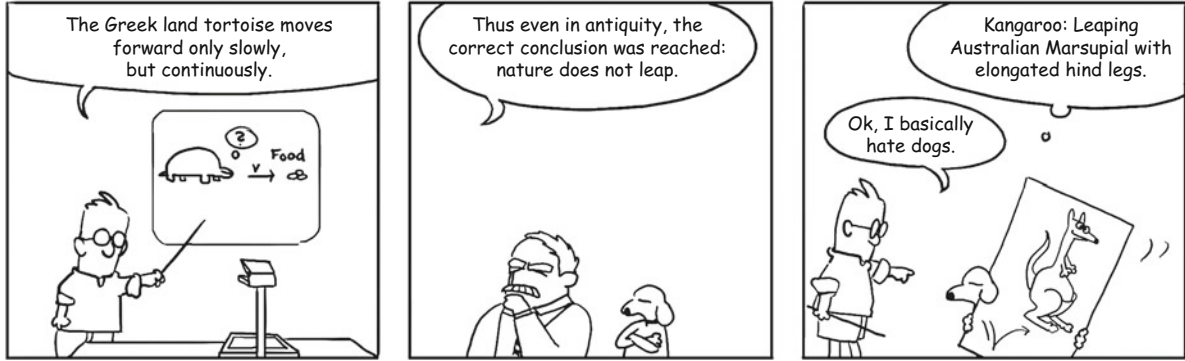
$$\begin{aligned} & \left\{ \begin{array}{l} \text{Temporal change of the} \\ \text{phosphorus mass in the lake} \end{array} \right\} = \\ & \left\{ \begin{array}{l} \text{Inflow via inlet} \\ \text{per unit of time} \end{array} \right\} - \left\{ \begin{array}{l} \text{Outflow via outlet} \\ \text{per unit of time} \end{array} \right\} \\ & - \left\{ \begin{array}{l} \text{Net uptake through} \\ \text{biota per unit of time} \end{array} \right\} - \left\{ \begin{array}{l} \text{Net uptake through} \\ \text{sediment per unit of time} \end{array} \right\} \end{aligned}$$

To integrate this equation, we need to specify the terms on the right-hand side of the equals sign. We can either use explicit numerical values or algebraic expressions that create a link to the system variable. In addition, we need an initial value for the phosphorus mass in the lake. We will discuss this in more detail in Chap. 4.

⁴ In a first order (n -th order) differential equation, the function that constitutes its solution is no higher than in its first (n -th) derivative. The models we deal with here are usually first order with respect to time. In physics, particularly in classical mechanics, they are often second order with respect to time. For the solution of these differential equations this distinction is only marginally relevant, because one can convert an n -order differential equation into n first order equations.

2.4 Discrete Time Models

Leaps of nature



Before the discovery of quantum mechanics scientists were convinced that system variables such as temperature, velocity or concentration change continuously. It was postulated that *nature does not leap*. But at closer examination, this is also incorrect for many systems that have nothing to do with quantum mechanics. For instance, let's model an elephant herd in a national park in Africa. The herd's size changes with every birth and every death by a whole number—that is, the variable “number of individuals” leaps. There are also systems that only change at specific times. A typical example is a savings account that does not have its interest added continuously, but only once per year or once every quarter.

Not every variable changes continuously with time.

If a system variable doesn't change continuously, but—as shown in Fig. 2.5—only at discrete points in time $t_0, t_1, t_2, \dots$, we can simulate the system with a *discrete time model* of the form

$$\mathcal{V}^{(k+1)} = f(\mathcal{R}^{(k)}, \mathcal{V}^{(k)}) \quad (2.13)$$

This means that the state $\mathcal{V}^{(k+1)}$ is calculated from $\mathcal{V}^{(k)}$ according to a specific “recipe”. The superscript index k in parentheses indicates the system state at time t_k . Unlike in a differential equation Eq. (2.12), the system variable's change in time is not described infinitesimally by the first derivative, but by the change occurring during the time step $(t_{k+1} - t_k)$.⁵ A more detailed description of these models follows in Chap. 7.

⁵ In order to show the connection of Eq. (2.13) to the differential equation (2.12) of the continuous model, the left-hand side of the former is often written as the difference between two consecutive time steps, $\mathcal{V}^{(k+1)} - \mathcal{V}^{(k)}$. In this way the differential equation (2.12) becomes a so-called difference equation. See Chap. 7 for details.

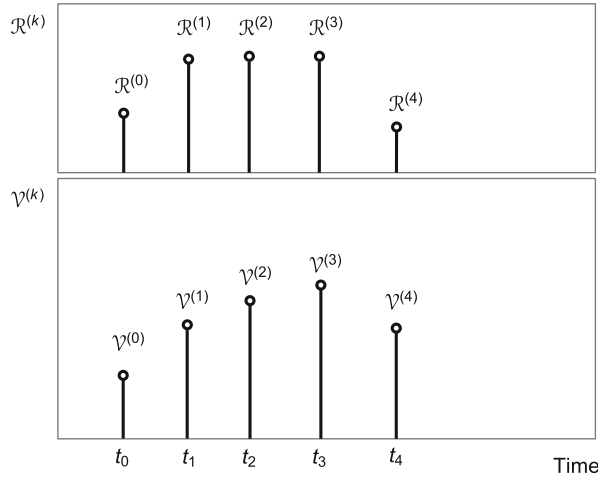


Fig. 2.5: With a discrete model, the system variable $\mathcal{V}^{(k)}$ changes in “jumps” or discrete time steps t_k . It may be driven by an external relation $\mathcal{R}$ that changes with time

2.5 Spatially Continuous Models

So far, we assumed that the system variable only depends on time. Yet, natural systems also have a spatial dimension. As long as we are only interested in the average phosphorus concentration and assume that it is distributed homogeneously in the lake, we do not need to consider any spatial variation of the system variable. Instead, we can think of the entire lake volume as one large box. We call such a spatially homogeneous model a *box model*.

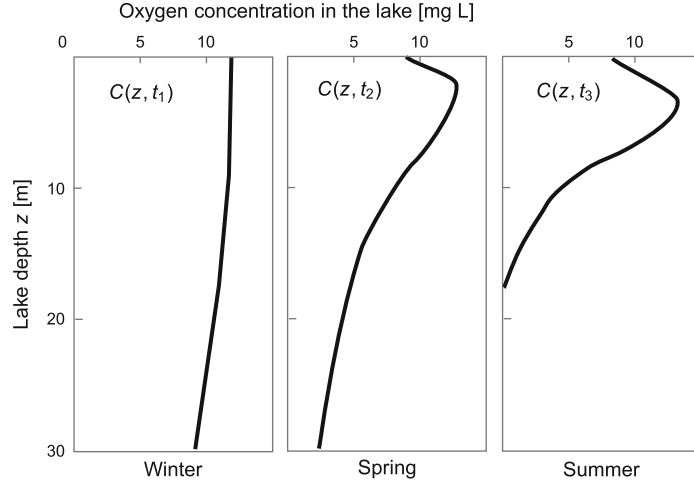
Often, however, the spatial distribution of a substance in the system is particularly important. For instance, we are interested in the oxygen distribution in different depths z of a lake. Figure 2.6 shows the oxygen profile in a lake at different times. To describe such a spatial distribution, we have to treat the lake as a spatial continuum in one or all three spatial dimensions. The oxygen distribution then appears in the system equation as a function of both time t and depth z , which we write as $C(z, t)$. The model equation thus becomes a *partial* differential equation. We call these models *spatially continuous* and distinguish them from box models. The analytic solution of partial differential equations is usually difficult—they are solved computationally. We will look at some simple examples in Chap. 8.

2.6 Stochastic Models

Solutions of differential equations have the property of being completely determined once the initial conditions are given. In other words: A system always develops in exactly the same way if it starts from the same initial state. Such behavior is called deterministic.

Our experience with a multitude of natural systems teaches us something different: many phenomena, from the weather to the dynamics of

Fig. 2.6: The oxygen distribution in a lake can be described as a function of time t and depth z . The figure shows the vertical oxygen profile in a lake with a maximum depth of 30 m at three different times t_1, t_2 and t_3



the stock exchange, appear to lie outside the possibility of deterministic analysis and prediction. In most cases—except in the case of very simple systems—we can at best predict the future within certain time limits. For instance, we may be able to predict that the system will develop into the state S_1 with a probability of p_1 , into the state S_2 with the probability p_2 , and so forth. This behavior is called stochastic.

There are many different reasons for the occurrence of stochastic processes. The most obvious reason is connected to quantum mechanics, which in several respects replaced our physical thinking over the course of the twentieth century. In quantum mechanics, the deterministic equations of classical mechanics are replaced with probability relations. For instance, we cannot predict when exactly a specific radioactive isotope will decay, that is, we cannot describe the isotope's behavior with a classical (deterministic) equation.

In many cases (but not in all), this kind of random process can be eliminated by assuming a macroscopical perspective. For instance, if we analyze a large number of identical isotopes, we can describe the behavior of the overall system relatively accurately through the half-life of the isotope. We can thus predict the time when half of the original isotopes will have decayed. The stochastic events at the microscopic scale can (at least approximately) be brought back to the deterministic scale by summing up many individual processes. We find similar examples in thermodynamics: The macroscopic variables *pressure* or *temperature* combine a large number of microscopic (stochastic) molecular processes. Example 2.7 illustrates by analogy the movement of atoms in an ideal gas: the movement is stochastic on the level of the single molecules (balls), but their overall behavior results in the macroscopic phenomenon of molecular diffusion (see Chap. 8).

Example 2.7: The bed of nails, a stochastic system

Figure 2.7 depicts schematically a classic toy made of nails fixed on an inclined wooden board—a bed of nails. A ball, starting from a fixed position $x = 0$, rolls down the slope and periodically hits a nail such that the ball's path either continues to the left or right with the same probability. The nails are depicted as squares, the numbers in the squares give the probability that an individual ball arrives at this nail. After n collisions (in the figure, $n = 6$) the ball lands with a specific probability in one of the final positions (seven in our example). The path of a specific ball cannot be predicted. But if a large number of balls is sent through the system, and if the entire setup is built perfectly symmetrically, we will find a characteristic distribution of balls in the final boxes. These probabilities are called Bernoulli numbers.

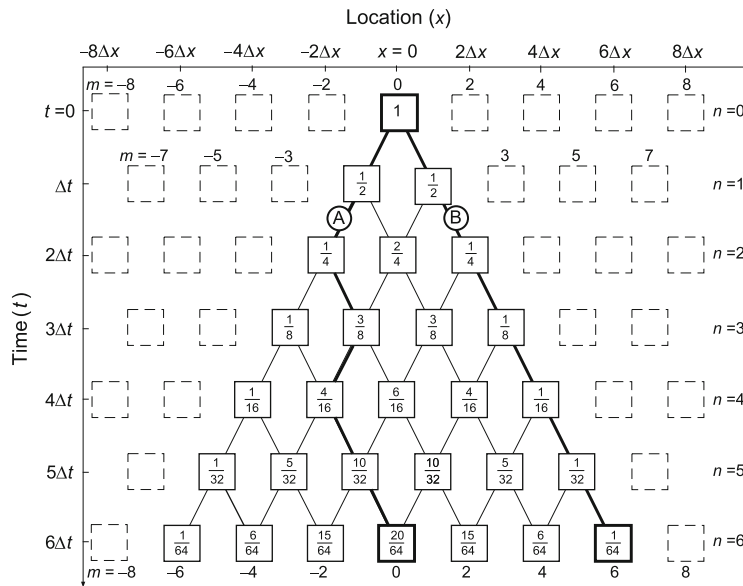


Fig. 2.7: A schematic representation of the path of a ball through the bed of nails. The path of an individual ball cannot be predicted. If a large number of balls are successively sent through the system, we find a characteristic probability distribution in the final boxes. These probabilities are called Bernoulli numbers. Drawn in bold are two individual paths A and B. Path B leads to the right six times, it has a probability of $2^{-6} = 1/64$. The meaning of the variables labeled location (x) and time (t) will be discussed in Sect. 8.4

In fact, we don't need to go all the way to quantum mechanics to explain the stochastic behavior of some natural systems. Even the classical equations of physics, using regular differential equations, contain the seed of randomness. As we will see in Chap. 6, three coupled differential equations are sufficient to introduce stochastics into models. Such systems of equations may have the special property that after a finite time, and starting from almost identical initial states, they develop states which are very different from each other. This happens even though the model equations themselves are entirely deterministic. Since every observation is subjected to some error, we are not able to determine the *absolute* equality of states.

With nonlinear differential equations, almost identical initial conditions can later lead to completely different system states.

Thus, apparently identical systems may develop differently. This is called deterministic chaos. The weather is a typical example for chaotic behavior. We are capable of predicting the weather over a period of a few days relatively well. But our limited knowledge of the atmosphere's state and other relevant factors means that a prognosis over 2 months will likely remain impossible.

When modeling, we can use various techniques to give essentially deterministic equations a whiff of stochastics. The simplest possibility is to introduce a randomly varying external relation. In this book, however, we will focus primarily on deterministic systems.

In this chapter, we got a general idea of some different model types and thereby encountered some properties with which we can characterize models. These properties include the pairs *static-dynamic*, *discrete-continuous* (either in space or in time) and *deterministic-stochastic*. In the following chapters, we will discuss the different model types in more detail.

Deterministic Chaos



2.7 Questions and Problems

Question 2.1: Explain the difference between internal and external relations.

Question 2.2: Most dynamic models implicitly contain a static model. The opposite is not true, however. Why?

Question 2.3: What is the difference between a dimension and a unit? Which of the two is unambiguously defined for every variable?

Question 2.4: What does the dimension of a model mean? (Note: Comparing questions 2.3 and 2.4 will make clear that *dimension* has a different meaning in mathematics than it does in physics.)

Question 2.5: Which of the following statements is correct?

- A box model is spatially discrete.
- A box model is always continuous in time.

Question 2.6: Look for some examples of systems that contain a stochastic component.

Question 2.7: Grubs live in the ground for 3 years and hatch as May beetles in spring of the fourth year. Sketch a simple regional model for May beetles. In particular, you should think about the following issues: choice of the system variables, type of model (dynamic or static, in space or in time, discrete or continuous).

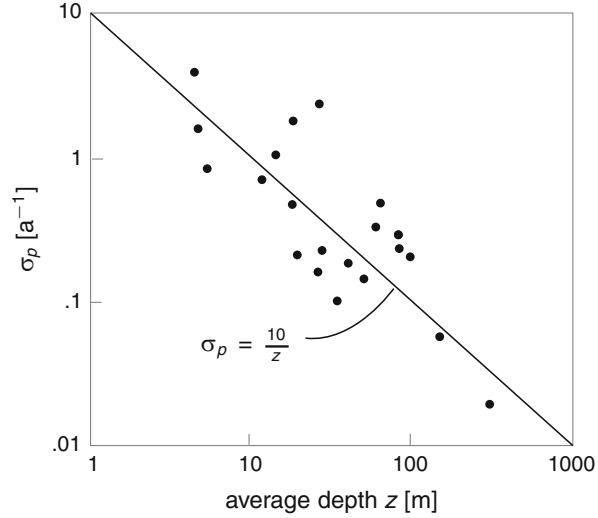
Problem 2.1: Mass balance

A small lake has an inlet and an outlet. Establish the mass balance of a soluble substance in the lake, for the following two cases:

- (a) A factory is built on the lake shore. From time t_0 onwards, it continuously discharges a substance into the lake. This substance is volatile, i.e. it can evaporate into the atmosphere, but is not degraded in the lake. It doesn't deposit in the sediment.
- (b) Through an accident, a large amount of a toxic substance enters the lake at time t_0 . This substance is degraded in the lake water and deposited in the sediment. After the accident, no more of the substance is added to the lake.

In both cases, you can assume that the substance's concentration in the inlet is zero.

Fig. 2.8: *Phosphorus sedimentation, according to Vollenweider (1976)*



Problem 2.2: Determining the dimension of parameters

The following differential equation describes the progression through time of a substance's concentration profile in a vertical well shaft:

$$\frac{\partial C(z, t)}{\partial t} = -k_1 + k_2 \frac{\partial^2 C}{\partial z^2} + k_3 \frac{\partial C}{\partial z} + k_4 C(C^* - C)$$

Determine the dimensions (expressed by (M,L,T)) of the parameters k_1 , k_2 , k_3 , k_4 and C^* . C is the concentration of a substance, z a length and t the time. Hint: How is the dimension of a first or second derivative of a variable determined?

Problem 2.3: Phosphorus sedimentation

Empirically established correlations should also be correct in terms of their dimensions. Figure 2.8 shows the relation between average lake depth z in meters and the specific phosphorus sedimentation rate $\sigma_p = \frac{10}{z}$ in year^{-1} for several lakes. What unit must the factor 10 have? What is the physical meaning of that factor?

Problem 2.4: Bed of nails

If we extend the bed of nails shown in Fig. 2.7 by two steps (to $n = 8$), the final boxes span from $m = -8, -6, \dots, +6, +8$. What is the probability that a ball hits the box in the center ($m = 0$)? Calculate the Bernoulli numbers at level $n = 8$.



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