

Introduction to Mathematical Modeling and Computer Simulations

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Chapter 1

Principles of Mathematical Modeling

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Chapter 1

Principles of Mathematical Modeling

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Mathematical Modeling describes a process and an object by use of the mathematical language. A process or an object is presented in a “pure form” in Mathematical Modeling when external perturbations disturbing the study are absent. Computer simulation is a natural continuation of the Mathematical Modeling. *Computer simulation* can be considered as a computer experiment which corresponds to an experiment in the real world. Such a treatment is rather related to numerical simulations. Symbolic simulations yield more than just an experiment. They can be considered as a transformation of a mathematical model by computer, since symbolic simulations keep parameters of the model in symbolic form that corresponds to a set of actual experiments. One can obtain numerical results as in actual experiments only after substitutions of the symbolic parameters with the numerical data. Therefore, symbolic simulations complete the mathematical model and embrace actual experiments.

Mathematical Modeling of stochastic processes is based on the probability theory, in particular, that leads to using of random walks, Monte Carlo methods and the standard statistics tools.

Symbolic simulations are usually realized in the form of solution to equations in one unknown, to a system of linear algebraic equations, both ordinary and partial differential equations (ODE and PDE). Discrete methods such as Finite Element Methods or Finite-Difference Methods for finding approximate solutions of ODE and PDE are usually used in the form of numerical simulations.

1.1 How to develop a mathematical model

1.1.1 A simple mathematical model

Consider a simple example of the free falling object from a height h using Mathematical Modeling. How to describe the trajectory of the object? The first questions which should be posed are the questions “where” and “when”, i.e., we have to describe the space where the free fall is taking place and the time when it happens. Let gravity be the only force acting upon the falling object. In this case, only one axis is needed to describe the space. Let it be the axis OY shown in Fig.1.1. It is necessary to fix a unit segment on the axis which shows the direction and the line unit. In Fig.1.1, the axis OY is chosen to point in the downward direction. Meters can be chosen as the length unit on OY . However, dimensionless units are frequently used in Mathematical Modeling, which enables the result to be obtained in the easiest way. Dimensionless results are transformed into dimension form at the last stage. We will discuss this question later in Sec.1.4. Now, we are going to fix a dimensionless line unit. The time unit t is also fixed as a dimensionless unit. It is assumed that the object begins to fall at the initial time $t = 0$.

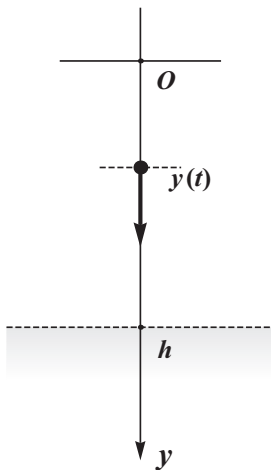


FIGURE 1.1: Falling of material object (point)

After answering the questions “where” and “when” we should analyse conditions of the fall. If the object is a stone, the air resistance can be ignored. However, it may not be done for a leaf. Let us study a stone now. Then one can consider the stone as a material point, i.e., as a point on the OY axis for each time t .

Next, one should use a physical law of the falling material point. It follows from the gravitational law that an object near the surface of the Earth falls with the constant acceleration g (equal to $9.81 \frac{m}{sek^2}$ in the SI units). *Projectile motion* is a motion in which a material point moves along a trajectory under the action of gravity only. Such a material point is called *projectile*.

Mathematics, “hard artillery”, arises at the following step to formally describe reality. We are interested in representing the motion of the point in time as a function $y(t)$ which shows the coordinate of the material point in time t . The function $y(t)$ is called the trajectory in mechanics. The velocity of the point is the derivative with respect to time $v(t) = y'(t)$, acceleration is the second derivative $a(t) = y''(t)$. Now, one can write the law in

the mathematical form

$$\text{“point falls with constant acceleration } g\text{”} \Leftrightarrow a(t) = g \Leftrightarrow y''(t) = g \quad (1.1)$$

We have got the ordinary differential equation (1.1). Its general solution has the form

$$y(t) = \frac{gt^2}{2} + C_1t + C_2, \quad (1.2)$$

where C_1 i C_2 are arbitrary constants. The solution (1.2) of equation (1.1) is obtained by double integration of (1.1), where C_1 and C_2 are constants of integrations. The trajectory of the material point has to be uniquely determined and could not depend on the arbitrary constants C_1 and C_2 . How to fix them? First, the law (1.1) does not take into account the information about when and how the stone is thrown. In our case, the material point is located at the point $y = 0$ of the axis OY at the time $t = 0$. Hence,

$$y(0) = 0. \quad (1.3)$$

Moreover, the object can be thrown with any initial velocity v_0 . If one just drops the stone, the initial velocity is equal to zero. If one applies a force and throws the stone down or up the initial velocity v_0 does not vanish. Hence, we have the second condition

$$y'(0) = v_0. \quad (1.4)$$

The conditions (1.3)–(1.4) are called initial in the theory of ordinary differential equations and the problem (1.3)–(1.4) is called Cauchy's problem. This problem is properly posed and has a unique solution. It is necessary to substitute $C_1 = v_0$ i $C_2 = 0$ in the general formula (1.2) in order to fulfil the initial conditions (1.3)–(1.4). As a result we obtain the required particular solution

$$y(t) = \frac{gt^2}{2} + v_0t. \quad (1.5)$$

The mathematical problem has been solved. The height h has to be taken into account to find the time T when the projectile reaches the earth. The following equation with respect to T is obtained by substitution of $t = T$ and $y = h$ into (1.5)

$$h = \frac{gT^2}{2} + v_0T. \quad (1.6)$$

Out of two solutions

$$T_1 = \frac{-v_0 + \sqrt{2gh + v_0^2}}{g}, \quad T_2 = \frac{-v_0 - \sqrt{2gh + v_0^2}}{g}$$

we must take the first one, since the second solution is always negative which contradicts the physical treatment of the problem ($T > 0$).

Remark 1.1. It is a common practice to precisely describe “operating conditions” in pure mathematics. For instance, in order to work with a function mathematicians must define a domain of the function. If a derivative is used, a mathematician must say “let a function $y(t)$ be differentiable in a set A ”. If a mathematician writes $\frac{a}{m}$, before this he/she must write $m \neq 0$. However, in applied mathematics the mass m is always non-negative. Thus, $\frac{a}{m}$ for $m = 0$ has no any sense. For instance, an applied mathematician writes $y'(t)$ assuming that this derivative exists. So, usually in applied mathematics if something is written, it is tacitly assumed that it exists.

1.1.2 Use of a computer

The above example has been solved “by hand” without any computer, since the calculations are simple. It is in accordance with the principle:

Principle of hand calculations. *If you can calculate something without any computer, try to do it “by hand”. If you cannot or you are not sure in your calculations, try to use a computer.*

For instance, let somebody not be sure in equations (1.5)–(1.6) based on derivatives and integrals. Let us solve the problem by use of the operator **DSolve** in *Mathematica*¹

```
In[1]:= DSolve[{x'[t] == g, x[0] == 0, x'[0] == v0},
             x[t], t]
```

```
Out[1]= {{x[t] -> 1/2 (g t^2 + 2 t v0)}}
```

One can copy the resulting function and further paste it into the definition of the function $y(t)$. However, it is easier to extract $y(t)$ from the expression `Out[1]` as follows

```
In[2]:= y[t_] = %[[1, 1, 2]]
```

```
Out[2]= 1/2 (g t^2 + 2 t v0)
```

Here, `%` means that the latest result is taken, i.e., `Out[1]`, the triple `1, 1, 2` denotes the coordinates, so `1, 1` yields the expression² `Rule[x[t], 1/2(g t^2 + 2 t v0)]`. Then, `2` means the second element out of this expression.

Solve the equation (1.6) and take the proper solution:

¹In *Mathematica*, v_0 means the value of the function v at the point 0. We write the symbol $v0$ instead of v_0 in *Mathematica*’s code in order to use $v0$ as a separate independent variable.

²You can investigate full form the expressions with the **FullForm** operator.

```
In[3]:= Solve[h == y[t], t]
```

$$\text{Out[3]} = \left\{ \left\{ t \rightarrow \frac{-v_0 - \sqrt{2gh + v_0^2}}{g} \right\}, \left\{ t \rightarrow \frac{-v_0 + \sqrt{2gh + v_0^2}}{g} \right\} \right\}$$

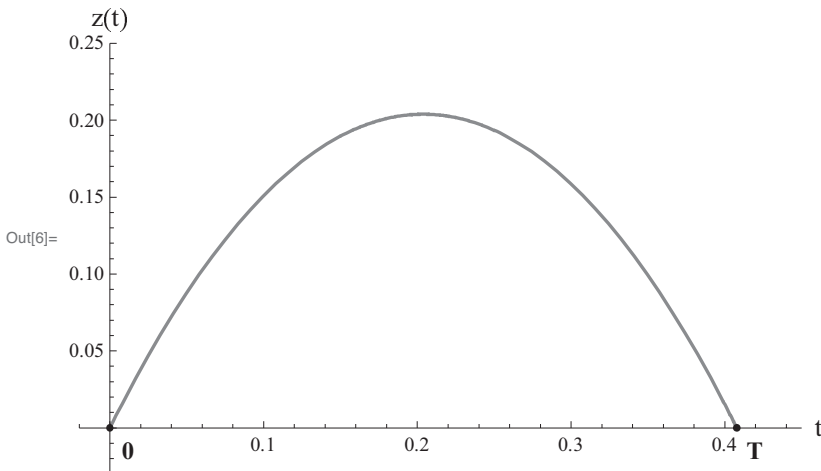
```
In[4]:= T = %[[2, 1, 2]]
```

$$\text{Out[4]} = \frac{-v_0 + \sqrt{2gh + v_0^2}}{g}$$

Fix the values of the parameters g, h, v_0 and prepare a graph to demonstrate the location of the material point in time. It can be done by use of the operator **Plot** as **Plot[h-y[t], {t, 0, T}]**. To get a better visualisation one can do it in a more complicated way:

```
In[5]:= {g = 9.81, h = 0, v0 = -2};
```

```
In[6]:= Show[Plot[h - y[t], {t, 0, T}, AxesLabel -> {"t", "z(t)"},
  LabelStyle -> 16, PlotRange -> {{-0.02, 0.45}, {-0.03, 0.25}},
  PlotStyle -> Directive[Darker[Gray, 0.1], Thick],
  AspectRatio -> Automatic, TicksStyle -> 12],
  Graphics[{Text[Style["T", FontSize -> 15, Bold], {1.03 T, -0.015}],
  Text[Style["0", FontSize -> 15, Bold], {0.03 T, -0.015}],
  {PointSize[Medium], Point /@ {{T, 0}, {0, 0}}}],
  ImageSize -> 450]
```



MATLAB Example Box 1.1

When computations are performed with the MATLAB package, one can use *Command Window* to enter commands at the command line (indicated by the prompt `»`). Let us define variable g

```
>> g = 9.80665;
```

Now, we transform the considered equation (1.1) into a system of ODEs. Using $y'_k = y^{(k-1)}$ ($k = 1, 2, 3$) we obtain

$$\begin{aligned}y'_1(t) &= y_2(t), \\ y'_2(t) &= y_3(t) = g,\end{aligned}$$

with the corresponding initial values

$$\begin{aligned}y_1(0) &= h, \\ y_2(0) &= v_0.\end{aligned}$$

Let us define the initial values and place them into a single array

```
>> h = -1;
>> v0 = -3;
>> init_vals = [h, v0]
```

Define the function representing right sides of the above system

$$\mathbf{f}(t, y_1, y_2) = (y_2(t), g) \quad (1.7)$$

using *anonymous function* as follows

```
>> f = @(t, y) [y(2); g];
```

We are going to solve the equation numerically, hence we have to provide the range of the integration

```
>> t_interval = [0 1];
```

Now we are ready to use the built-in solver function `ode45`

```
>> [T, Y] = ode45(f, t_interval, init_vals);
```

Here, the solver returns two arrays: the array `T` contains time points corresponding to rows of the solution array `Y`. One can combine both arrays and plot the solution

```
>> plot(T, -Y(:,1))
```

The other way of computing in MATLAB, adapted in this book, is running scripts written in the MATLAB Editor (files with code organized by functions saved with `.m` extension). Below the source code of file `script01.m` is presented. Note that the very first function, which is called the *primary function*, should have the same name as the name of the file.

```
% primary function
function script01()

% initial values
```

```

v0 = -2;
h = -3;
t_interval = [0 1];

% solution of the ODE
[T, Y] = ode45(@f, t_interval, [h v0]);

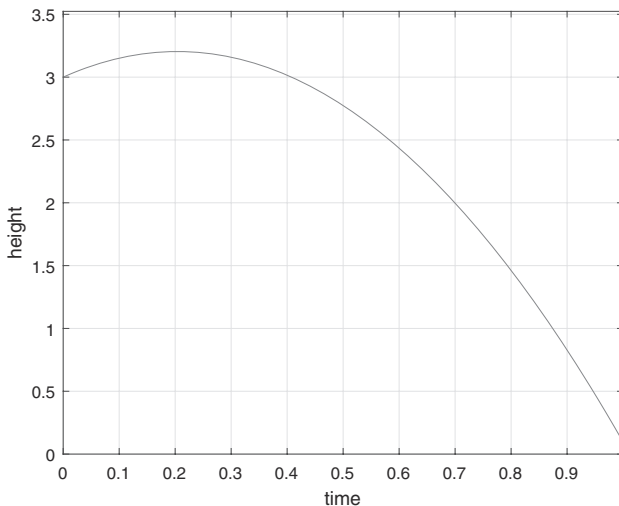
% plot
H = -Y(:,1); % height of the body
plot(T, H)
xlabel('time')
ylabel('height')
grid on
ylim([0 max(1.1*H)])

% subfunction
function dy = f(t, y)
    g = 9.80665;
    dy = zeros(2,1); % a column vector
    % yk denotes (k-1)st derivative of y
    dy(1) = y(2); % y1'(t) = y2(t)
    dy(2) = g; % y2'(t) = y3(t) = g

```

The script can be run simply by pressing the Run button from the Editor as well as by typing its name into the command window

```
>> script01
```



The graph of the function $z(t) = h - y(t)$ is drawn with all the numerically given parameters. After such a success one can think that an ordinary differential equation can be solved by means of computer without any course of calculus. It is enough just to write **DSolve** or something else in another package, to press a button and everything is displayed. But the question is, which buttons should be pressed? A computer is a continuation of our knowledge.

In order to perform simple computations and to solve simple problems a user need not know calculus. But a step aside from a standard way could lead to trouble. A poorly prepared user could rather repeat manipulations but could not solve a new simple problem. It is possible to give many examples when incorrect or superficial use of computer by engineers yields incorrect results. Below, we present such an example.

Calculate 10 partial sums of the series beginning with the partial sum 1160 for series

$$\sum_{k=1}^{\infty} \frac{1}{k} \quad (1.8)$$

We have³

$$\text{In}[1]:= \mathbf{s}_n := \sum_{k=1}^n \frac{1}{k}$$

In[2]:= **Table**[\mathbf{s}_n , {n, 1660, 1670}]

Out[2]:= {7.99209, 7.99269, 7.99329, 7.99389, 7.9945,
7.9951, 7.9957, 7.9963, 7.9969, 7.9975, 7.99809}

Direct observations of the results could yield the conclusion that this series converges to 8. However, this series (1.8), which is known as the *harmonic series* diverges⁴. In order to avoid such mistakes one should use the following:

Principle of the stupid computer. *Do not trust the computer. If you do not know what are you computing, use the weaker principle of hand calculations. If it is possible to check the computer result “by hand”, do it.*

However, the customer is not always right. A computer gives the correct answer to a question, but the user does not understand it and blames the computer on the basis of the above principle. Here, the following principle has to be taken into account:

Presumption principle of innocence of the computer. *The answer you get depends on the question you ask.*

Presumption principle of innocence of the computer completes the principle of the stupid computer. The computer answers the question and the computer does not care that the question is stupid. Its task is to answer the question in general, without comment, as in the army. It is worth mentioning that *Mathematica* sometimes warns us. Below, *Mathematica* warns about the divergent series

³The symbol $\mathbf{n}_$ means for all n ($\forall n$) in *Mathematica*'s codes; $\mathbf{n}_$ or $\mathbf{x}_$ must be used for any argument in definitions of functions.

⁴it is possible to say in wider sense that it converges to $+\infty$

$$\ln[3]:= \sum_{k=1}^{\infty} \frac{1}{k};$$

Sum::div : Sum does not converge. >>

and division by zero

$$\ln[4]:= \frac{17}{0}$$

Power::infy : Infinite expression $\frac{1}{0}$ encountered. >>

MATLAB Example Box 1.2

The following script plots partial sums of another divergent series

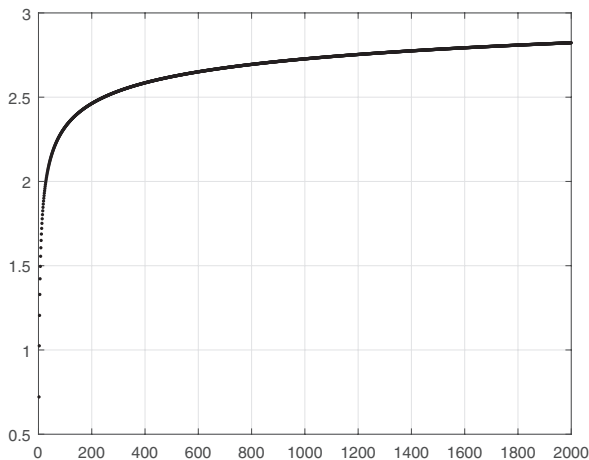
$$\sum_{k=2}^{\infty} \frac{1}{k \log(k)}. \quad (1.9)$$

```
function script02()

% array of indexes {2,3,...,2000}
k = [2:2000];

% corresponding sequence and partial sums
sequence = 1.0 ./ (k .* log(k));
partial_sums = cumsum(sequence);

% plot
plot(k, partial_sums, 'k')
grid on
```



As we can see, such visual observation may also suggest convergence of the series. Note that the operators $\cdot /$ and $\cdot *$ are examples of generalized arithmetic operations. Here, division and multiplications are performed element by element resulting in a new array. Here, the `cumsum` operator computes the cumulative sum (a vector of partial sums of a given vector).

1.1.3 Development of mathematical models

In [Sec.1.1.1](#), steps of the development of a mathematical model are demonstrated in a simple example. These steps can be applied to general models.

Steps taken to create a mathematical model:

- i) to introduce spatial variables (description of geometry) and time;
- ii) to think about dimensional units; to introduce the units perhaps during solution of the mathematical problem;
- iii) to introduce assumptions and conditions, first, as simple as possible;
- iv) to formulate the law (physical, economical, biological, empirical etc.);
- v) to develop a mathematical description, first, as simple as possible;
- vi) to try to solve the mathematical problem “by hand”; if that does not work, to try a numerical method; to compare the results if different methods are applied;
- vii) verification of the model; if the results are suspect to get back to the previous steps;

The following comment on the above steps is important.

Principle of the simplest model. *At the beginning do it in the simplest way, even it does not yield acceptable results.*⁵

In the step vi), it is worth doing most of the work “by hand” in order to simplify computations. We can say even more. For instance, instead of the computation of the series $S = \sum_{n=1}^{\infty} \frac{1}{n^2}$ it is worth looking up in the handbook (for example, implemented in *Mathematica*) and rewriting the result $S = \frac{\pi^2}{6}$.

Thus, it is not necessary to perform calculations “by hand”⁶. For instance, the best method to calculate an integral is to find the answer in the handbook⁷. Hence, the most important is to know where to find the answer. This requires good mathematical education. To know where to look is also a type of knowledge. In this case, another type of memory is required, not the one

⁵c.f. Albert Einstein: “Everything should be made as simple as possible, but not simpler.”

⁶if only it is useful as an exercise

⁷Information as a part of knowledge becomes very important in the modern world. An apt example is *Google Search* used by students and researchers more often than printed textbooks

that is frequently required to pass exams. In particular, development of mathematical models means the proper selection of existing models scattered in textbooks, internet etc.

During development of the model one should mind that the model has to correspond to the real phenomena both qualitatively and quantitatively. This contradicts the principle of the simplest model. Anyway, we recommend following this principle gradually tending to be in correspondence with reality.⁸

After verification of the simple model, this model can be improved by advanced study. For instance, if instead of the stone (see [Sec.1.1.1](#)) a leaf is falling, it is better first to discuss the falling of the leaf in vacuum. Then, it is possible to complete the model taking into account air resistance. Following this approach we pass from the stone to the leaf below. The equation of the force equilibrium is similar to (1.1):

$$m y''(t) = m g, \quad (1.10)$$

where the exterior force $ma(t) = my''(t)$ presented in the left part in accordance with Newton's law. The gravitational force mg is in the right part. The corrected model for the leaf has the form

$$m y''(t) = m g - k v(t), \quad (1.11)$$

where $F = -kv(t)$ with $k \geq 0$ is the air resistance. It is assumed here that the air resistance is proportional to the velocity of the fall $v(t)$. It is an empirical law, sometimes it has the form $F = -kv^2(t)$ or may be more complicated. Then equation (1.11) becomes

$$y''(t) + \frac{k}{m} y'(t) = g. \quad (1.12)$$

The differential equation (1.12) with the initial conditions (1.3)–(1.4) has a unique solution.

$$\text{In[1]:= DSolve}\left[\left\{y''[t] == g - \frac{k}{m} y'[t], y[0] == 0, y'[0] == v_0\right\}, y[t], t\right]$$

$$\text{Out[1]:= } \left\{ \left\{ y[t] \rightarrow \frac{e^{-\frac{kt}{m}} m \left(g m - e^{\frac{kt}{m}} g m + e^{\frac{kt}{m}} g k t - k v_0 + e^{-\frac{kt}{m}} k v_0 \right)}{k^2} \right\} \right\}$$

$$\text{In[2]:= } \%[[1, 1, 2]] // \text{Expand}$$

$$\text{Out[2]:= } -\frac{g m^2}{k^2} + \frac{e^{-\frac{kt}{m}} g m^2}{k^2} + \frac{g m t}{k} + \frac{m v_0}{k} - \frac{e^{-\frac{kt}{m}} m v_0}{k}$$

The trajectory $y(t)$ has been constructed. Further investigation and computations can be performed by the scheme presented in the previous [Secs 1.1.1-1.1.2](#).

⁸Zvi Artstein [9]: "Nature is a very good approximation of Mathematics".

MATLAB Example Box 1.3

One can simulate the considered model numerically as well and observe how the acceleration decreases due to the air resistance. Consider the following MATLAB script.

```
function script03()
    % parameters
    g = 9.80665;
    v0 = 0;
    m = 1;
    k = 1;
    h = 100;
    t_interval = [0 10];

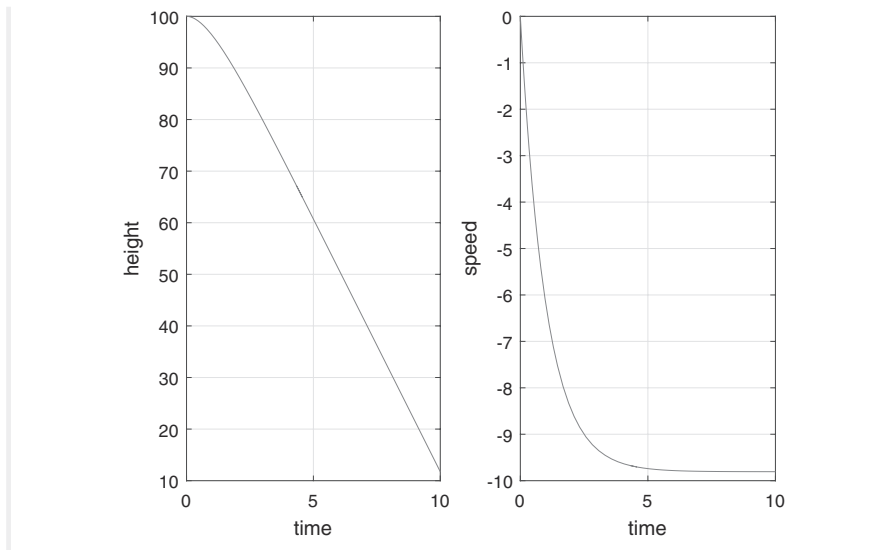
    % solution of the equation
    f = @(t, y) f(t, y, v0, m, k, g);
    [T, X] = ode45(f, t_interval, [0 v0]);

    % plots of height and velocity in time
    H = h - X(:,1);      % height
    V = -X(:,2);        % speed

    subplot(1,2,1); % left subplot
    plot(T, H)
    xlabel('time')
    ylabel('height')
    grid on

    subplot(1,2,2); % right subplot
    plot(T,V)
    xlabel('time')
    ylabel('speed')
    grid on

function dy = f(t, y, v0, m, k, g)
    dy = zeros(2,1);
    dy(1) = y(2);
    dy(2) = g - k/m * y(2);
```



The final solution should not be given by exact formulae. Consider the example of the cooling coffee described in the excellent book by Amelkin [5].

Example 1.1. Anatol and Vladimir ordered two cups of coffee with cream in a bar. Two cups of hot coffee with the same temperature are simultaneously prepared. Anatol and Vladimir take the following steps. Anatol adds cream to coffee and covers the cup by a napkin. Vladimir covers the cup by a napkin and adds cream to his coffee 10 min later when they simultaneously begin to drink their coffee. Who drinks hotter coffee?

In order to solve this problem in accordance with the book [5] one can develop a mathematical model of the cooling coffee based on the theory of heat conduction, solve the stated problems and calculate the temperature of Anatol's and Vladimir's coffees 10 min later.

However, in this case we are interested only in the question, in which cup the coffee is hotter. We are not interested in the values of the temperature. The stated problem can be formulated in another way. When does coffee lose less heat in 10 min? Does it happen when Anatol decreases its temperature by adding cream at the time $t = 0$ min or when coffee is cooled at the time $t = 10$ min? In order to answer this question we need only one law of the heat conduction: *dissipation (loss) of heat is proportional to the difference of temperatures of the object (coffee) and environment*. Hence, hotter coffee loses more heat. Therefore, Anatol drinks hotter coffee than Vladimir.

Similar questions arise in other regimes of heating and cooling, for instance in buildings. In order to reach a given temperature at a fixed time with minimal dissipation one has to heat the object at that fixed time, not earlier.

The above problem is based on the estimations of energy. We do not take

into account the daily change of prices of energy⁹.

Principle of the energy estimations. *Estimate energy before you make a deal.*

This principle helps us to answer the following questions. Is the force of the artillery gun sufficient to overcome the gravitational force to go into space? (the answer is negative) Can the Moon cause an earthquake? “Does the flap of a butterfly’s wings in Brazil set off a tornado in Texas?”¹⁰ Edward N. Lorenz asked this question and illustrated it by an example of dynamical system which describes the *butterfly effect* when a small change in one state of a deterministic system can result in large differences in a later state. Such a question is closely related to stability discussed in [Sec.1.3](#).

1.2 Types of models

Types of the mathematical models can be the following:

- a) deterministic and stochastic (random);
- b) discrete and continuous;
- c) linear and non-linear.

a) An example of the deterministic model is given in [Sec.1.1.1](#), see for instance equation (1.12). Let one check the model by means of experiments and see that a light wind impacts the result. But how to introduce this wind into the model? How to estimate the random influence of the wind? Equation (1.12) was useful but should be revised. Let us consider the question from another point of view. Introduce the wind into equation (1.12) by force, namely, add a random value $\xi(t)$:

$$my''(t) = mg - ky(t) + m\xi(t). \quad (1.13)$$

If the vertical component of the wind force $m\xi(t)$ is known, the differential equation (1.13) can be solved. However, $\xi(t)$ is just a symbol which does not solve the problem and hides it in a new symbol. This term $\xi(t)$ will be useful if it is described by the rules used in the probability theory. Below, we outline a simple scheme based on the standard course of probability.

Following the description of the normal distribution we can describe

⁹The cost of electric energy at night is usually lower than during day. Moreover, the cost at night can be negative. Hence, the economic problem to minimize costs complicates the energy problem.

¹⁰http://eaps4.mit.edu/research/Lorenz/Butterfly_1972.pdf

the random function $\xi(t)$ by two constants, the mathematical expectation $a = E[\xi(t)]$ and the standard deviation $\sigma = \sqrt{E[\xi^2(t)] - E^2[\xi(t)]}$. In the considered case, a expresses the expected averaged wind force acting on the body at time t . Let it be equal to zero that corresponds to the symmetrically expected gusts in the y direction. Application of the expectation operator to (1.13) yields

$$mY''(t) = mg - kY'(t), \quad (1.14)$$

where $Y(t) = E[y(t)]$ denotes the expected trajectory. Next, equation (1.14) can be solved similarly to equation (1.12).

In order to estimate the deviation of the random function $y(t)$, first, we estimate the term $m\xi(t)$ in (1.13) by the bounds $-C\sigma \leq m\xi(t) \leq C\sigma$ where the positive constant C is determined by the chosen confidence interval estimate. Next, we substitute $\pm C\sigma$ in (1.13) instead of $m\xi(t)$ and obtain two ODE

$$mY''_{\pm}(t) = mg - kY'_{\pm}(t) \pm C\sigma. \quad (1.15)$$

Ultimately, we can estimate the expected trajectory and its bounds within the chosen confidence interval as displayed in [Fig.1.2](#).

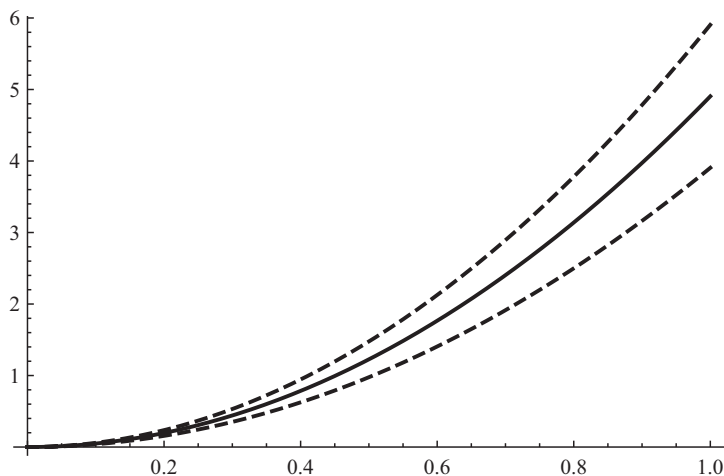


FIGURE 1.2: The expected trajectory (solid line) and its bounds (dashed line).

b) Calculate the mass of the cylinder having various circular sections expressed by the shape function $S = S(x)$ for $x \in [a, b]$ (see [Fig.1.3](#)). It is assumed that the cylinder consists of the homogeneous material of the density ρ . Let us divide the cylinder into small cylinders with the heights Δx_i ($i = 1, 2, \dots, n$). The mass of the i -th cylinder is equal to $\Delta m_i = \rho \pi S^2(\xi_i) \Delta x_i$, where the point ξ_i is arbitrarily chosen in (x_i, x_{i+1}) . If the latter interval is sufficiently small, its mass Δm_i is calculated quite accurately. The total mass

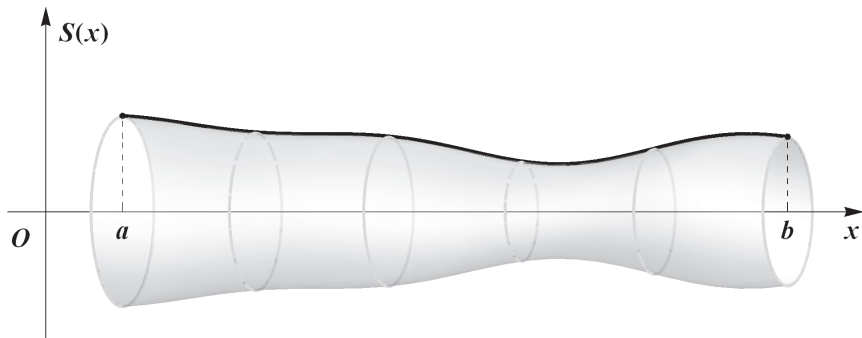


FIGURE 1.3: Radius $S(x)$ of the circular section at the point x .

of the cylinder is approximately equal to

$$M_n = \sum_{i=1}^n \Delta m_i = \rho\pi \sum_{i=1}^n S^2(\xi_i) \Delta x_i. \quad (1.16)$$

Thus, the mass of the cylinder is calculated by the *discrete model*.

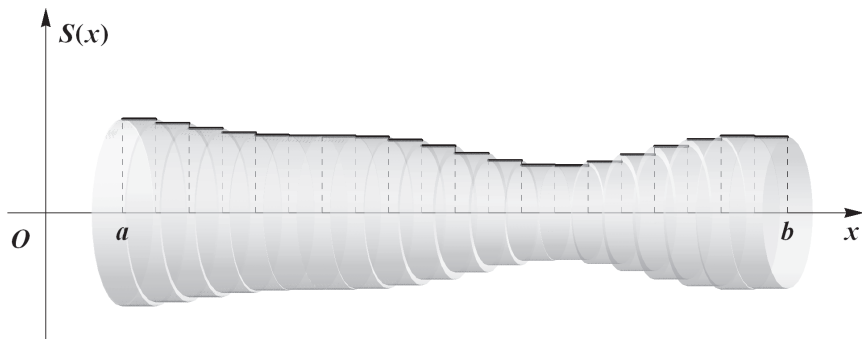


FIGURE 1.4: Partition of the cylinder. The total mass of the cylinder is approximated by the sum of the masses of small cylinders.

Let the value $\delta = \max_i \Delta x_i$ tend to zero, i.e., $[a, b]$ is divided into small intervals whose lengths become smaller and smaller. Then the sum (1.16) tends to a value M , which can be considered as the exact total mass of the cylinder. The sum M_n is called the *Riemann sum* in calculus. The limit M is called the *definite integral* of the function $\rho\pi S^2(x)$ on the interval (a, b) :

$$M = \int_a^b \rho\pi S^2(x) \, dx. \quad (1.17)$$

This integral presents the *continuous model* to calculate the mass.

Application of these two models yields a method to calculate a value (mass) of the complicated objects via small simple ones.

Principle of transition: *continuous* \leftrightarrow *discrete*. *To divide a continuous object into small parts, to apply a simple formula to every part, to calculate the sum for all the parts and get back to the continuous object through the limit operation.*

One can divide an object under the study into parts in space and in time. Partition by the mass $m = \rho x$, where ρ denotes the linear density, is equivalent to partition in space on x .

In mathematics, the principle of transition is the benchmark of the Riemann integral theory including multidimensional, curvilinear and surface integrals. In continuum mechanics this principle is used in the framework of calculus and theory of partial differential equations. Real medium is discrete on the molecular level. Hence, the real mass of the cylinders is rather given by formula (1.16). However, summation over all molecules is practically impossible and integration is more simple than summation in this case. This does not concern nanotechnology when few molecules are taken in consideration.

Remark 1.2. The above example can help to delineate the difference between pure mathematical and practical approaches. Assume that the radius of the body sections presented in Fig.1.3 is described by the Dirichlet function

$$D(x) = \begin{cases} 1, & \text{if } x \text{ is irrational,} \\ 0, & \text{if } x \text{ is rational.} \end{cases} \quad (1.18)$$

There are rational and irrational numbers in every interval of the real axis. If all the points ξ_i are irrational in the sum (1.16), then $D(\xi_i) = 1$ and the total mass of the cylinder is equal to $\rho \sum_{i=1}^n \Delta x_i = \rho(b - a)$. On the other hand, if the points ξ_i are rational, then $D(\xi_i) = 0$. Thus, the total mass of the cylinder vanishes. This means that the cylinder is so porous that it does not possess a mass; it is between 0 and $\rho(b - a)$. In this book, we take the side of applied mathematicians. Therefore, we do not consider such strange objects without any mass. However, such examples are very interesting in pure mathematics since they yield new mathematical topics for investigations¹¹.

c) Linear models are frequently used in practice since they are simple and properly describe real phenomena. The definition of the linear model can be given in terms of the linear operator (function):

Definition 1.1. Operator $L : X \rightarrow Y$ is called linear if for any $x, x_1, x_2 \in X$ and an arbitrary real (complex) number λ

- i) $L(x_1 + x_2) = L(x_1) + L(x_2)$;
- ii) $L(\lambda x) = \lambda L(x)$.

¹¹Frequently, an independently developed pure abstract theory has serious applications many years later after its creation.

Example 1.2. The function $y = ax$ is a linear operator $L : \mathbb{R} \rightarrow \mathbb{R}$.

Example 1.3. The differentiation operator $\frac{d}{dt} : f \mapsto f'$ is a linear operator. This is true due to the rules $\frac{d}{dt}(f_1 + f_2) = \frac{df_1}{dt} + \frac{df_2}{dt}$ and $\frac{d}{dt}(\lambda f) = \lambda \frac{df}{dt}$.

Example 1.4. If you conduct a uniaxial tensile test on an elastic material you can observe that the force σ per surface of unit area acting on the material is proportional to its deformation $\epsilon = \frac{\Delta\ell}{\ell}$ where $\Delta\ell$ denote displacement of the specimen and ℓ its length. This is Hooke's law which can be written in the form $\sigma = k\epsilon$ where the constant k depends on the material. Linear Hooke's law is valid for small deformation ϵ . Plastic transformations can occur for a large displacement when the coefficient k depends on ϵ . This yields the nonlinear law $\sigma = k(\epsilon)\epsilon$ under simple loading. It is interesting to note that rubber and a metal are elastic materials but with different values of k .

Cybernetics is a multidisciplinary science based on the *black box* when one considers an object which transforms inputs $x \in X$ to outputs $y \in Y$ and is not interested in the interior of the transformation box (Fig.1.5).



FIGURE 1.5: Illustration of the black box. A set of inputs and outputs determines the object without any study of the interior structure.

The rule of the transformation $K : x \rightarrow y$ is interesting in cybernetics (roughly speaking, software structure of K , not its hardware). That is why this object is called the black box. Such an approach is frequently used in the theory of signals. A signal $x(t)$ depending on time t is transformed into $y(t)$ by the integral operator:

$$(Kx)(t) := y(t) = \int_0^T k(\tau, t)x(\tau) \, d\tau. \tag{1.19}$$

One can check that the operator (1.19) is linear. Let the kernel have the special structure $k(\tau, t) = k(\tau - t)$. Then, the operator

$$(Kx)(t) := y(t) = \int_0^T k(\tau - t)x(\tau) \, d\tau \tag{1.20}$$

is called *the convolution* of $k(\tau)$ and $x(\tau)$. The transformation $K : x \rightarrow y$ can be non-linear [23]

$$(Kx)(t) := y(t) = \int_0^T k(\tau, t, x(\tau)) \, d\tau, \tag{1.21}$$

where $k(\tau, t, x)$ is a function of three variables.

1.3 Stability of models

One of the most important characteristic of the model is its stability. Mechanical illustration of stability is displayed in Fig.1.6. Stability can be discussed on a parameter and in time.



FIGURE 1.6: Stable (a) and not stable (b) locations of a ball

Consider the function (1.5) which is continuously dependent on the initial velocity v (parameter of the model) in the closed interval $[0, T]$. This means that for any $t \in [0, T]$ and for sufficiently small changes of v_0 the function (1.5) has small increments. More precisely, let v_1 and v_2 be two such values of the initial velocity that $|v_1 - v_2| < \varepsilon$ for any fixed positive number ε . Let $y_1(t)$ and $y_2(t)$ be functions of the form (1.5) with the velocities v_1 and v_2 , respectively. Then

$$\max_{[0, T]} |y_1(t) - y_2(t)| = \max_{[0, T]} |v_1 t - v_2 t| = T|v_1 - v_2| < T\varepsilon.$$

This inequality implies that for sufficiently small $\varepsilon > 0$, the maximal value of the difference $|y_1(t) - y_2(t)|$ for $t \in [0, T]$ is also small, i.e., the discussed problem is stable for v_0 .

On the other hand, the time T can be a large number, it can even be equal to $+\infty$. Then $\max_{t \in [0, +\infty]} |y_1(t) - y_2(t)| = +\infty$ for $|v_1 - v_2| < 0.000001$. This means that the problem is unstable in v .

A similar situation takes place for weather prediction (see the footnote on page 16 with the reference to Lorenz's paper and the advanced book [6]). Equations of the air flow on the Earth scale can be stable. Let us say for simplicity that a function $y(t)$ describing the air flow satisfies inequality

$$\max_{[0, T]} |y_1(t) - y_2(t)| < c(T)\varepsilon.$$

Here, the constant $c(T)$ depends on the prediction time T . The value $c(T)$ can be bounded for T which lasts for about a week, what yields well estimations for $y(t)$. However, $c(T)$ abruptly increases for greater T in such a way that $c(T)\varepsilon$ also increases. The stable process becomes unpredictable.

In main, stability is treated as T tends to infinity. Linear homogeneous ODE with constant coefficients have solutions presented as a sum of modes. Each mode has the form $y(t) = P(t) \exp(\lambda t)$ where $P(t)$ is a polynomial, $\lambda = \alpha + i\beta$ is a complex constant and i denotes the imaginary unit. A mode is called stable if it is bounded as $t \rightarrow +\infty$. Euler's formula $\exp(\lambda t) = e^{\alpha t}(\cos \beta t + i \sin \beta t)$ yields

Theorem 1.1. *Let $P(t)$ be a non-constant polynomial. A mode $y(t) = P(t) \exp(\lambda t)$ is stable if and only if $\operatorname{Re} \lambda = \alpha < 0$.*

Formally, one can divide models into stable and unstable ones. But a physicist will not permit us to do it referring to the principle of stability:

Principle of stability. *A mathematical model must be stable.*

The study of the unstable problem should not give reasonable results since small exterior changes or small changes in the initial data can yield large deviation in the obtained results. But at the beginning of the study no one knows whether the model is stable. Therefore, one should first develop a model, investigate it and only after its verification it is possible to claim its stability. It follows from the above examples that the same model can be stable and unstable. It is worth investigating the conditions under which the problem is stable.

Concluding remarks and further reading concerning this section.

Not everyone accepts the principle of stability in such a form and investigates unstable processes following the principle by Dirac stated on page 126. This can be reasonable, for instance, in biological and chemical pattern formations [22, 33]. In the theory of turbulence, the amplitude of the average velocity can be considered when the local velocity is unpredictable [2].

Various mathematical approaches to stability are discussed in courses of ODE and PDE (see Sec.4.3, Sec.4.8 and [5], [41], [33], [22]). The numerical stability is discussed in Sec.8.6.1 ([35], [52]).

1.4 Dimension, units, and scaling

1.4.1 Dimensional analysis

Mathematical models contain measurable values. One cannot say that a dimension value is large or small because it depends on the units in which

it is expressed. For example, the length L can be measured in meters (m), centimeters (cm), miles etc. The length L will be called an abstract dimension and the length m a special one. One can treat L as a variable which takes special values m , cm , etc., which can be written as $L = m$. Everybody may introduce his/her own dimension unit. It is only necessary to relate it to the accepted units. The following three dimensions of units are accepted in physics and technology: SI, CGS and English units. Besides the length L we introduce the abstract units of mass M and time T . The velocity has the abstract unit $\frac{L}{T}$ and the special one with $L = m$ and $T = sec$ where sec denotes second. It is convenient to introduce brackets for the units. For instance, $[\rho] = ML^{-3}$ means that the density ρ is considered in dimension units and measured in mass per volume. Similarly, $[5\frac{kg}{m^3}] = kg\ m^{-3}$ means that the density is measured in kilo per spatial meter and is equal to 5 in these units. The expression $[\rho'] = 1$ denotes that ρ' is measured in dimensionless units.

Consider the example from [Sec.1.1.1](#) in the abstract units $[m] = M$, $[t] = T$, $[y] = L$, $v_0 = LT^{-1}$, $[g] = LT^{-2}$. We are interested in the units which appear in equation (1.5). The first term $\frac{gt^2}{2}$ on the right-hand side has the dimension $[\frac{gt^2}{2}] = [g][t]^2 = LT^{-2}T^2 = L$. The second term v_0t on the right-hand side has the dimension $[v_0t] = [v_0][t] = LT^{-1}T = L$. Hence, the right-hand side contains the sum of two values of the same dimension L , that confirms the proper dimensional usage of the expression $\frac{gt^2}{2} + v_0t$. The left-hand side of the equation also has the dimension L . Everything is alright. Checking the dimensions yields a simple way to check an equation. For instance, if one develops a model and gets equations $L = L + M$ or $T = LT^2$, this gives a signal that something is wrong because a meter cannot be compared to a kilo.

Principle of units. *It is forbidden to add camels to tractors. But it is possible to multiply them.*

The units of derivatives can be obtained from the definition of the derivative through the limit of the difference quotients. For instance, $[y] = L$ implies $[y'] = LT^{-1}$ and $[y''] = LT^{-2}$. We now proceed with considering the units of equation (1.12)

$$\begin{aligned} [my''] &= [mg] + [kv] \Leftrightarrow [m][y''] = [m][g] + [k][v] \\ &\Leftrightarrow MLLT^{-2} = MLLT^{-2} + [k]LT^{-1}. \end{aligned}$$

The principle of units holds if and only if $[k]LT^{-1} = MLLT^{-2}$. This implies that the unit of the air resistance, the coefficient k , must be equal to MT^{-1} . The coefficient k can be estimated in experiments. Let $M = kg$ and $T = sec$. In order to determine k one has to present the experimental results in such a way that k will be measured in kilo per second.

Dimensional analysis is applied not only to check a dimensional equation

but can suggest a type of such an equation. The main fundamental theorem of dimensional analysis is the Pi theorem [41]. We formulate it in the following reduced form

Theorem 1.2. *Let an equation (E) relate N dimensional quantities. There exists such an equation (e) which contains n dimensionless quantities and*

- i) equations (e) and (E) are equivalent;*
- ii) $n \leq N$.*

The full form of the Pi theorem is based on the dimension matrix. We explain this notation on the equation (1.5) written in the form

$$f(y, t, g, v_0) \equiv y - \frac{gt^2}{2} - v_0t = 0. \quad (1.22)$$

The dimensions are given by $[y] = L$, $[t] = T$, $[v_0] = LT^{-1}$ and $[g] = LT^{-2}$. The dimension matrix A is defined by the powers occurred at these equations. It is convenient to write A in the form of the table

	y	t	v_0	g
L	1	0	1	1
T	0	1	-1	-2

Two dimensionless values can be introduced

$$\pi_1 = t^2 \frac{g}{y}, \quad \pi_2 = t \frac{v_0}{y}. \quad (1.23)$$

The value g and v_0 are expressed through other values by equations

$$g = \pi_1 \frac{y}{t^2}, \quad v_0 = \pi_2 \frac{y}{t}. \quad (1.24)$$

Substitution of (1.24) into (1.22) yields

$$1 - \frac{\pi_1}{2} - \pi_2 = 0. \quad (1.25)$$

An experimental verification of (1.22) can be done by measurement of y , t , v_0 and g in arbitrary units. Further, π_1 and π_2 are calculated with (1.23). At the end, the value $1 - \frac{\pi_1}{2} - \pi_2$ has to be compared with zero, i.e., equation (1.25) has to be checked.

1.4.2 Scaling

Each dimensional parameter has its domain of values. Estimations of this domain are useful in the introduction of the dimensionless units by scaling.

The parameters of equation (1.12) can be made dimensionless in the following way

$$y = \ell \tilde{y}, \quad t = \tau \tilde{t}, \quad m = m_0 \tilde{m}, \quad (1.26)$$

where ℓ , τ , m_0 are characteristic values of the length, time and mass, respectively. For instance, if a book falls from a table, one can assume $\ell = 1\text{cm}$, $\tau = 1\text{sek}$, $m_0 = 0.1\text{kg}$. If a parachutist falls from an plane, one can take $\ell = 700\text{m}$, $\tau = 1\text{min}$, $m_0 = 10\text{kg}$. The choice of the scale can be arbitrary. However, it is better to take reasonable values in order to work with “usual” numbers, to avoid divisions into small numbers following the principle of the balanced computations.

The derivatives y' and y'' after the substitutions (1.26) are transformed as follows

$$\frac{dy}{dt} = \frac{\ell}{\tau} \frac{d\tilde{y}}{d\tilde{t}}, \quad \frac{d^2y}{dt^2} = \frac{\ell}{\tau^2} \frac{d^2\tilde{y}}{d\tilde{t}^2}. \quad (1.27)$$

Then equation (1.12) becomes

$$\tilde{y}'' + \tilde{k}\tilde{y}' = \tilde{g}, \quad (1.28)$$

where $\tilde{k} = \frac{k\tau}{m}$ denotes a dimensionless coefficient. This can be proved in the following way

$$[\tilde{k}] = [k]TM^{-1} = MT^{-1}TM^{-1} = 1.$$

Concluding remarks and further reading concerning this section.

A short introduction to the unit theory and scaling is presented above. Further extensions and applications can be found in [41].

Exercises

1. Describe the trajectory of the falling object thrown in a horizontal direction.
2. Describe the trajectory of the falling object thrown in a horizontal direction when the land is determined by a surface, for instance by a linear function $y = a_1x_1 + a_2x_2 + b$.
3. [Fig.1.1](#) presents a film frame of the falling object. Prepare an animation of the whole process. Calculate online the velocity and the acceleration of the point. Take into account the air resistance.

Useful *Mathematica* operators: **Animate**, **Manipulate**, **Slider**, **TrackedSymbols**, **DynamicModule**. For creating animation in MATLAB refer to Example [Box 8.1](#) on page 175.

As an advanced exercise, you can create slider manipulator in MATLAB. Refer to the documentation and investigate the `uicontrol` operator.

4. Calculate numerically the sums $\sum_{n=1}^{\infty} \frac{1}{n^m}$ for $m = 1, 2, 3, 4, \dots$
Think about the outputs **Zeta[3]** and **Zeta[3.]** in *Mathematica* for $m = 3$.
5. Let hot coffees and cold cream in Example 1.1 be replaced by cold water with ice and juice at room temperature, respectively. Who drinks colder water?
6. Calculate the mass of the circular cone of height h and radius r with constant density ρ .
7. Are the following operators linear?
A linear function $y = ax + b$ from \mathbb{R} on \mathbb{R} ;
function $Y = AX$ from \mathbb{R}^n in \mathbb{R}^n , where A is a $n \times n$ matrix;
integral operator $\int_0^{\infty} k(\tau, t)x(t) \, d\tau$.
8. Present a graphical interpretation of the stability of the process (1.5) in time when the initial velocity v_0 is measured with an error of 5%.