`average[dataset, 10000]`, modeled after the C program, takes three to four times longer to yield, of course, the same result. In each case, the workstation calculates these results about ten times faster than the PC.

The C program, however, is compiled first, for example by the command `gcc -o sum sum.c -lm`, and then called by its name `sum`. Now it takes only 8.5 seconds on the PC and 0.56 seconds on the HP to obtain the result, even though the number of steps has been increased by a factor of 100. This demonstrates a significant disadvantage of *Mathematica*: for numerical calculations, it is extremely slow compared to C or similar languages.

Literature

Kernighan B.W., Ritchie D.M. (1988) The C Programming Language. Prentice Hall, Englewood Cliffs, NJ

Wolfram S. (1996) The Mathematica Book, 3rd ed. Wolfram Media, Champaign, IL, and Cambridge University Press, Cambridge

1.2 The Nonlinear Pendulum

The mathematical pendulum is a standard example in any physics course on classical mechanics. The linear approximation of this problem is suitable for a high school physics course. The exact solution is expressed by an elliptic integral, but only a computer affords us the opportunity to visualize and thoroughly analyze these nonelementary functions. Therefore, we want to place this standard example of theoretical physics at the beginning of our textbook.

Physics

Let us start with the physical model: a pointlike mass m suspended from a massless, rigid string of length l swings in the earth's gravitational field. Let $\varphi(t)$ be the angle of displacement from the pendulum's equilibrium position at time t; friction is neglected. According to the laws of mechanics, the energy E of the pendulum is constant, so

$$E = \frac{m}{2}\, l^2\, \dot{\varphi}^2 - m\, g\, l\, \cos\varphi = -m\, g\, l\, \cos\varphi_0 \,, \tag{1.1}$$

where φ_0 denotes the maximum displacement angle with $\dot{\varphi}_0 = 0$, and $\dot{\varphi} = \mathrm{d}\varphi/\mathrm{d}t$ is the angular velocity. From this equation, one can obtain $\varphi(t)$ by using a little trick: one separates t and φ by solving (1.1) first for $(\mathrm{d}\varphi/\mathrm{d}t)^2$ and then for the differential $\mathrm{d}t$. For the half period in which φ increases with t, one obtains

$$\mathrm{d}t = \sqrt{\frac{l}{2g}}\, \frac{\mathrm{d}\varphi}{\sqrt{\cos\varphi - \cos\varphi_0}} \,. \tag{1.2}$$

For a suitable choice of $t = 0$ ($\varphi(0) = 0$, $\dot{\varphi}(0) > 0$), integration of this equation yields

$$t(\varphi) = \sqrt{\frac{l}{2g}} \int_0^{\varphi} \frac{d\varphi'}{\sqrt{\cos\varphi' - \cos\varphi_0}} \, . \tag{1.3}$$

Obviously, the period T is four times the time the pendulum needs to reach its maximum angle φ_0:

$$T = 4\, t(\varphi_0) \, . \tag{1.4}$$

Since the integrand of (1.3) diverges as $\varphi' \to \varphi_0$, it makes sense to use the substitution

$$\sin\psi = \frac{\sin(\varphi/2)}{\sin(\varphi_0/2)} \, , \tag{1.5}$$

which results in the following integral:

$$t(\varphi) = \sqrt{\frac{l}{g}} \int_0^{\psi} \frac{d\psi'}{\sqrt{1 - \sin^2(\varphi_0/2)\sin^2\psi'}} = \sqrt{\frac{l}{g}}\, F\left(\psi, \sin\frac{\varphi_0}{2}\right) \, . \tag{1.6}$$

Now, the integrand diverges only for an amplitude $\varphi_0 = \pi$. The function F is called an elliptic integral of the first kind. According to (1.5), $\psi = \pi/2$ for $\varphi = \varphi_0$; therefore, the period T is

$$T = 4\sqrt{\frac{l}{g}}\, F\left(\frac{\pi}{2}, \sin\frac{\varphi_0}{2}\right) = 4\sqrt{\frac{l}{g}}\, K\left(\sin\frac{\varphi_0}{2}\right) \, . \tag{1.7}$$

The function K is called a complete elliptic integral of the first kind. Both F and K are available in *Mathematica.*

For small values of the displacement φ, the potential energy is approximately quadratic. As is well known, the force is a linear function of φ in this case, and the solution of the equation of motion is a sinusoidal oscillation with a period $T = 2\pi\sqrt{l/g}$. For larger amplitudes φ_0, the force becomes a nonlinear function of φ, and T depends on φ_0.

We want to study the effect of the nonlinearity. To be able to compare different curves for $\varphi(t)$, we normalize φ with φ_0 and t with T. In addition, we look at the phase-space diagram $\dot{\varphi}$ versus φ for various energies E. The generation of higher harmonics with increasing nonlinearity is visualized by a Fourier transformation. Finally we want to expand T in terms of the quantity $\sin^2(\varphi_0/2)$, which is a measure of the nonlinearity.

Algorithm

The functions $K(k)$ and $F(\psi, k)$ are available in *Mathematica* and are called by the commands

```
EllipticK[k^2]
```

and

```
EllipticF[psi, k^2]
```

One has to be careful about the arguments since, unfortunately, there are various conventions for using them. Thus, we have $K(k)$ =`EllipticK[k^2]` and correspondingly for the other elliptic integrals. According to (1.7), the period is simply obtained by

```
T[phi0_] = 4 EllipticK[Sin[phi0/2]^2]
```

where we have set $\sqrt{l/g} = 1$. The command `Plot` draws the period as a function of φ_0:

```
Plot[ T[phi0], {phi0, 0, Pi}, PlotRange -> {0,30} ]
```

Since T diverges as $\varphi_0 \to \pi$, one should use `PlotRange` and ignore *Mathematica*'s warning about $T(\pi)$.

The function $t(\varphi)$ is obtained from `EllipticF` according to (1.6). We, however, want to calculate the inverse, $\varphi(t)$. These functions are available as well; we have (using again $\sqrt{l/g} = 1$)

```
psi[t_,phi0_]=JacobiAmplitude[t, Sin[phi0/2]^2]
```

and

```
sinepsi[t_,phi0_]=JacobiSN[t, Sin[phi0/2]^2]
```

Now we replace the variable ψ with φ according to (1.5), normalize φ with φ_0 and t with T (defining $x = t/T$), and finally obtain the normalized function

```
phinorm[x_,phi0_]:=
  2 ArcSin[Sin[phi0/2] sinepsi[x T[phi0], phi0]]/phi0
```

Moreover, the function `JacobiSN[t, Sin[phi0/2]^2]` has the correct symmetry, so it provides the solution not only for $0 \leq x \leq 1/4$, but for all x. We want to have a look at the function $\varphi_{\mathrm{norm}}(x) = \varphi(x)/\varphi_0$ for various values of the amplitude φ_0. To this end, we generate an array of five φ_0 values, `phi0[1] = N[0.1 Pi]`, ..., `phi0[5] = N[0.999 Pi]` and form a list of functions

```
flist = Table[phinorm[x,phi0[i]],{i,5}]
```

We can now draw this list using `Plot`, after first applying the command `Evaluate` to it.

In order to study the generation of higher harmonics with increasing nonlinearity φ_0, we expand $\varphi(t)$ into a Fourier series. This is most easily accomplished by using the built-in command `Fourier`; to do this, however, one has to generate a list of discrete values $\varphi(t_i), i = 1, \ldots, N$ (see next section). Then one obtains the absolute values of the complex Fourier coefficients as a list:

```
foulist = Abs[Fourier[list]]
```

If, in (1.1), the energy E is kept constant, one obtains curves in the $(\dot{\varphi}, \varphi)$ plane, the so-called phase space. Plotting these curves is surprisingly simple in *Mathematica*, by calling `ContourPlot` for the function $E(\dot{\varphi}, \varphi)$. The option `Contours->{E1, E2, ..., En}` can be used to have n contours plotted for various values of `E`.

Finally, a remark concerning the series expansion of $T(\varphi_0)$. The new version (3.0) of *Mathematica* allows for a direct Taylor expansion of (1.7) by using the command `Series`, whereas older versions will output only formal derivatives of of `EllipticK`.

A possible way to handle this problem is to start with the integral (1.6) for $\psi = \pi/2$. The integrand is

```
f = 1/Sqrt[1 - m Sin[psi]^2]
```

with $m = \sin^2(\varphi_0/2)$. `f` can be expanded in terms of `m`, e.g., up to 10th order in `m` about 0,

```
g = Series [f, {m,0,10}]
```

Then, every single term can be integrated over ψ by using `Integrate`. Finally, the value $\sin^2(\varphi_0/2)$ is substituted back for `m` via `/. m -> Sin[phi0/2]^2`.

Results

We have investigated the effect of the amplitude φ_0, which is a measure of the nonlinearity, on the motion of the pendulum. Figure 1.1 shows the period T as a function of the amplitude φ_0. It takes the pendulum an infinite amount of time to come to rest at the highest apex ($\varphi_0 = \pi$). We can see that at first, with increasing φ_0, T does not deviate greatly from the value for the harmonic pendulum, $T = 2\pi$. Only for amplitudes above $90° = \pi/2$ is T significantly larger. The influence of φ_0 on the curve $\varphi(t)$ is evident in Fig. 1.2, where the ratio φ/φ_0 is plotted as a function of t/T in order to compare different

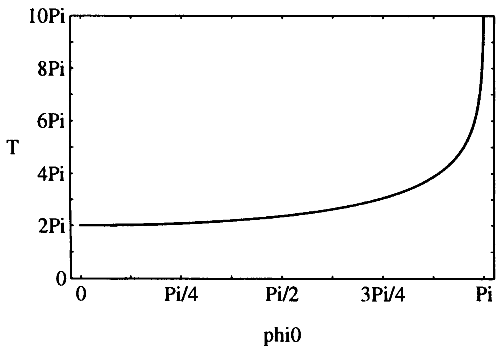

Fig. 1.1. The period T as a function of the amplitude φ_0

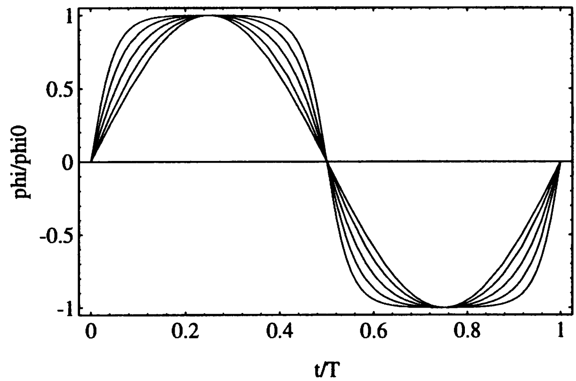

Fig. 1.2. Normalized displacement $\varphi_{\mathrm{norm}}(t/T)$ of the pendulum for various amplitudes $\varphi_0 = \pi/10$, $4\pi/5$, $19\pi/20$, $99\pi/100$, and $999\pi/1000$ (from the inside out)

curves (note: T diverges as $\varphi_0 \to \pi$). For small φ_0, we have a sinusoidal oscillation. For increasing φ_0, the time the pendulum spends near the apex $\pm\varphi_0$ becomes larger and larger; consequently, $\varphi(t)$ becomes flatter and flatter and turns into a step function for $\varphi_0 = \pi$.

If one decomposes $\varphi(t)$ into harmonic oscillations $b_s \exp(-\mathrm{i}\omega_s t)$, then, because of the periodicity $\varphi(t) = \varphi(t+T)$, the frequencies ω_s are integer multiples of $2\pi/T$. The discrete Fourier transformation available in *Mathematica* takes the frequencies $\{\omega_s = (2\pi/T)(s-1),\ s = 1,\ldots,N\}$ at N data points $\{\varphi(t_r),\ r = 1,\ldots,N\}$ and calculates the coefficients according to

$$b_s = \frac{1}{\sqrt{N}} \sum_{r=1}^{N} \varphi(t_r) \exp\left(2\pi\mathrm{i}\frac{(s-1)(r-1)}{N}\right) .$$

The symmetry $\varphi(T/2+t) = -\varphi(t)$ means that the coefficients b_s vanish for all odd s. The first nonvanishing coefficient, b_2, is the amplitude of the fundamental harmonic $\omega_2 = 2\pi/T$. The other coefficients $b_4, b_6, b_8, \ldots$ yield the amplitudes of the higher harmonics $3\,\omega_2, 5\,\omega_2, 7\,\omega_2, \ldots$. For $\varphi_0 = 0.999\pi$, the expression `foulist` contains the absolute values of the coefficients b_s, which are displayed via the command `ListPlot` in Fig. 1.3.

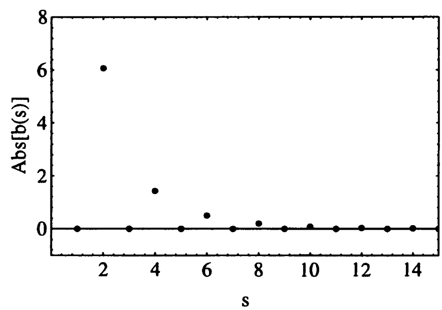

Fig. 1.3. Absolute values of the Fourier coefficients of the anharmonic oscillation $\varphi(t)$ for an amplitude $\varphi_0 = 0.999\pi$

The alternation between displacement φ and angular velocity $\dot{\varphi}$ can be illustrated in $(\varphi, \dot{\varphi})$ phase space; this eliminates the time t. Figure 1.4 shows such phase-space curves for different energies E. For small φ_0, one obtains a circle that becomes deformed as the energy increases. For $E > m\,g\,l$, the pendulum overshoots its apex; it moves in only one direction and has an angular velocity $\dot{\varphi} \neq 0$ even at the apex.

By using the command

```
tseries = 4 Integrate[g, {psi, 0, Pi/2}] /. m -> Sin[phi0/2]^2
```

one obtains the symbolic expansion of T in terms of $\sin^2(\varphi_0/2)$. *Mathematica* produces the following somewhat unwieldy output on the monitor:

```
                 phi0 2             phi0 4             phi0 6
         Pi Sin[----]     9 Pi Sin[----]     25 Pi Sin[----]
                  2                  2                  2
  2 Pi + ------------ + -------------- + ---------------- +
               2              32                 128

                phi0 8                phi0 10                phi0 12
  1225 Pi Sin[----]    3969 Pi Sin[----]     53361 Pi Sin[----]
                2                     2                       2
> ---------------- + ------------------ + ------------------- +
        8192                 32768                  524288

                 phi0 14                  phi0 16
  184041 Pi Sin[----]    41409225 Pi Sin[----]
                  2                        2
> ------------------- + --------------------- +
        2097152                536870912

                   phi0 18                    phi0 20
  147744025 Pi Sin[----]    2133423721 Pi Sin[----]
                     2                          2
> ---------------------- + ----------------------- +
        2147483648                34359738368
```

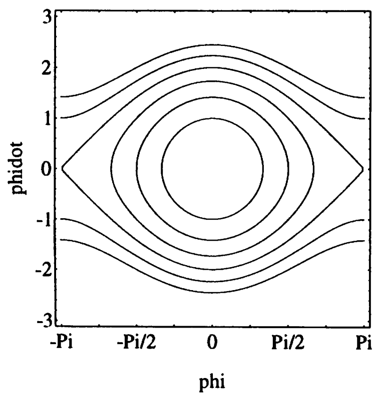

Fig. 1.4. Phase-space plot of $\dot{\varphi}$ versus φ for different energies $E/(m\,g\,l) = -1/2$, 0, 1/2, 1, 3/2, and 2 (from the inside out)

```
             phi0 2 11
> O[Sin[----] ]
              2
```

Therefore, in the future, we will give the corresponding TEX form for results of this kind. This form can, by the way, be obtained in *Mathematica* with the command `TeXForm` and can be translated by using TEX or LATEX:

$$2\,\pi + \frac{\pi\sin^2\frac{\varphi_0}{2}}{2} + \frac{9\,\pi\sin^4\frac{\varphi_0}{2}}{32} + \frac{25\,\pi\sin^6\frac{\varphi_0}{2}}{128} + \frac{1225\,\pi\sin^8\frac{\varphi_0}{2}}{8192}$$

$$+ \frac{3969\,\pi\sin^{10}\frac{\varphi_0}{2}}{32768} + \frac{53361\,\pi\sin^{12}\frac{\varphi_0}{2}}{524288} + \frac{184041\,\pi\sin^{14}\frac{\varphi_0}{2}}{2097152}$$

$$+ \frac{41409225\,\pi\sin^{16}\frac{\varphi_0}{2}}{536870912} + \frac{147744025\,\pi\sin^{18}\frac{\varphi_0}{2}}{2147483648}$$

$$+ \frac{2133423721\,\pi\sin^{20}\frac{\varphi_0}{2}}{34359738368} + \mathcal{O}(\sin^2\frac{\varphi_0}{2})^{11} \; .$$

A comparison with the exact function $T(\varphi_0)$ reveals that the error of this approximation is of the order of at most a few percent as long as φ_0 is less than 120°; beyond that, it increases significantly.

Exercises

1. Calculate the period T as a function of φ_0, once using `EllipticK` and then with `NIntegrate`. Compare the processing times and the precision of the results.
2. What is the contribution of the higher harmonics to $\varphi(t)$ as a function of the amplitude φ_0 ($\widehat{=}$ increasing nonlinearity)? Calculate the Fourier coefficients $|b_s|/|b_2|$ as functions of φ_0.
3. Program the following algorithm for evaluating the complete elliptic integral $K(\sin\alpha)$ and compare the result with `EllipticK`[$\sin^2\alpha$]:

Start:	$a_0 = 1\,,$	$b_0 = \cos\alpha\,,$
Iteration:	$a_{i+1} = (a_i + b_i)/2\,,$	$b_{i+1} = \sqrt{a_i b_i}\,,$
Stop:	$\mid a_n - b_n \mid < \varepsilon\,,$	
Verify:	`EllipticK`[$\sin^2\alpha$] $\simeq \dfrac{\pi}{2a_n}\,.$	

Literature

Baumann G. (1996) Mathematica in Theoretical Physics: Selected Examples from Classical Mechanics to Fractals. TELOS, Santa Clara, CA

Crandall R.E. (1991) Mathematica for the Sciences. Addison-Wesley, Redwood City, CA
Zimmerman R.L., Olness F.I., Wolpert D. (1995) Mathematica for Physics. Addison-Wesley, Reading, MA

1.3 Fourier Transformations

Surprisingly often, physics problems can be described to a good approximation by linear equations. In such cases, the researcher has a powerful tool at his or her disposal: the decomposition of the signal into a sum of harmonic oscillations. This tool, which has been thoroughly investigated mathematically, is the *Fourier transformation.* The transformation can be formulated in a particularly compact way with the help of complex-valued functions. Almost any signal, even a discontinuous one, can be represented as the limit of a sum of continuous oscillations. An important application of Fourier transformations is the solution of linear differential equations. The expansion of a function in terms of simple oscillations plays a big role not only in physics, but also in image processing, signal transmission, electronics, and many other areas.

Frequently, data are only available at discrete points in time or space. In this case, the numerical algorithms for the Fourier transformation are particularly fast. Because of this advantage, we want to investigate the Fourier transformation of discrete data here. In the following sections we will use it to smooth data, to calculate electrical circuits, and to analyze lattice vibrations.

Mathematics

Let a_r, $r = 1, \ldots, N$ be a sequence of complex numbers. Its Fourier transform is the sequence b_s, $s = 1, \ldots, N$, with

$$b_s = \frac{1}{\sqrt{N}} \sum_{r=1}^{N} a_r \, \exp\left[2\pi \mathrm{i} \frac{(r-1)\,(s-1)}{N}\right] . \tag{1.8}$$

This formula has the advantage of being almost symmetric in a_r and b_s, since the inverse transformation is

$$a_r = \frac{1}{\sqrt{N}} \sum_{s=1}^{N} b_s \, \exp\left[-2\pi \mathrm{i} \frac{(r-1)\,(s-1)}{N}\right] . \tag{1.9}$$

Thus, the signal $\{a_1, \ldots, a_N\}$ has been decomposed into a sum of oscillations

$$c_s\,(r) = \frac{b_s}{\sqrt{N}} \, \exp\left[-\mathrm{i}\omega_s\,(r-1)\right] \tag{1.10}$$

with frequencies $\omega_s = 2\pi(s-1)/N$. The coefficient $b_s = |b_s| \exp\,(\mathrm{i}\varphi_s)$ consists of an amplitude and a phase. Both (1.8) and (1.9) can be extended to all