Dynamics

This chapter discusses the numerical computation of solu8tions of ordinary differential equations ma'odeling dynamics systems. Differential equations are equations involving derivatives that were used to determine a function, which is the solution. Here, we discuss ordinary differential equations, equations involving derivatives with respect to a single variable, which we call t. In general discussions, we seek a function, x(t), and the differential equation is written in the form

$$\dot{x} = \frac{dx}{dt} = f(x) \ . \tag{1}$$

Here, both x and f have n components: $x(t) = (x_1(t), \dots, x_n(t)) \in \mathbb{R}^n$, and $f(t) = (f_1(t), \dots, f_n(t)) \in \mathbb{R}^n$. The components of x(t) determine the state of the system at time t, and f(x) represents the dynamics. In most real problems, f will depend on a number of problem parameters also.

For example, here is a model of a simple oscillator (such as a mass connected to a spring sliding on a table) subject to friction. The friction coefficient, γ also might change with time if friction causes the mass or the table to heat up. This is modeled through the equations

$$\gamma(t) = \gamma_0 + \gamma_1 \theta(t) , \qquad (2)$$

where $\theta(t)$ is the temperature (say, in degrees centigrade) at time t and γ_0 and γ_1 are fixed coefficients. When $\gamma_1 > 0$, the friction coefficient increases when the temperature increases. An oscillator with mass m, spring constant k, position q(t), and momentum p(t) is governed by the equations

$$m\dot{q} = p \,, \tag{3}$$

$$\dot{p} = -kq - \gamma \dot{q} , \qquad (4)$$

The $-\gamma \dot{q}$ term in the p equation represents the force of friction. The rate of work done by this friction force is force $\times \dot{q} = \gamma \dot{q}^2$. We suppose the rate of heating is proportional to this rate of work and that heat dissipates with rate r, bringing the temperature back to the ambient temperature, θ_0 . With this, the temperature evolution equation is

$$\dot{\theta} = -r(\theta - \theta_0) + \mu \gamma \dot{q}^2 \ . \tag{5}$$

We want to put this formulation into the generic form (1). The state of the system is determined by the three variables q, p, and θ . Although the friction coefficient, $\gamma(t)$, is time dependent, it is determined by the other variables. For this reason, $x(t) = (q(t), p(t), \theta(t))$. We identify f by writing explicit formulas for the components of x in terms of x and parameters. We find $f_1(x) = \dot{x}_1$ by solving (3) for \dot{q} :

$$\dot{q} = \frac{1}{m}p. \tag{6}$$

We find $f_2 = \dot{p}$ in terms of x, (i.e., in terms of q, p, and θ) by using (6) to put p instead of \dot{q} on the right, and by using (2) to eliminate γ in favor of components of x. This gives

$$\dot{p} = -kq - \frac{\gamma_0 + \gamma_1 \theta}{m} p \,. \tag{7}$$

In the same way we can eliminate \dot{q} and γ from the right side of (??) to get

$$\dot{\theta} = -r(theta - \theta_0) + \frac{\mu(\gamma_0 - \gamma_1 \theta)}{m^2} p^2 . \tag{8}$$

This puts the equations (3), (2), (4), (5) in the form (1), with

$$f(x) = \begin{pmatrix} \frac{1}{m}p \\ -kq - \frac{\gamma_0 + \gamma_1 \theta}{m}p \\ -r(\theta - \theta_0) + \frac{\mu(\gamma_0 - \gamma_1 \theta)}{m^2}p^2 \end{pmatrix} = \begin{pmatrix} \frac{1}{m}x_2 \\ -kx_1 - \frac{\gamma_0 + \gamma_1 \theta}{m}x_2 \\ -r(x_3 - \theta_0) + \frac{\mu(\gamma_0 - \gamma_1 x_3)}{m^2}x_2^2 \end{pmatrix}$$

Note that f depends on x and also on a large number of time independent parameters, m, k, γ_0 , γ_1 , r, and μ . This is typical.

We write the dynamics in the form (??) for the purpose of general mathematical discussion. In software it is fine to have something closer to the original formulation, such as:

int fEval(double x[3], double f[3]) { // Evaluate f for given x

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double qDot, pDot, gamma, thetaDot;
double q, p, theta;
q = x[0]; // Vector components start with 0 in C, as always.
p = x[1];
theta = x[2];

qdot = (1/m)*p;
gamma = gamma0 + gamma1*theta;
pDot = -k*q - gamma*qdot;
thetaDot = -r*( theta - thetaO ) + mu*gamma*qDotqDot;

f[0] = qDot;
f[1] = pDot;
f[2] = thetaDot;
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return 0; // Nothing can possibly go wrong.

The advantage of this point of view is that we can write a general program that solves any problem of the form (1).

We focus on the *initial value problem*. For this, in addition to the dynamics (1), we also specify *initial conditions*, $x(t_0) = x_0$. It is traditional to write x_0

for the initial conditions without intending it to mean the zeroth component of x. In the initial value problem, x(t) represents the state of the system at time t. We presume to know the state at some specific time, t_0 , and seek to compute the state at later times, $t > t_0$. The task, then, is to find x(t) for $t > t_0$ given $x(t_0)$.

Because of Newton's law: F = ma, it is common in physical applications for problems to be formulated using second order differential equations. Suppose we have l particle coordinates $q = (q_1, \ldots, q_l)$ and corresponding force components $F = (F_1(q), \ldots, F_l(q))$. Then Newton's law is

$$m_i \ddot{q}_i = F_i(q)$$
.

We put this into the standard format (1) using the extra variables $p_j = m_j q_j$ (not the only possible choice). Then we have

$$\dot{q}_j = \frac{1}{m_j} p_j ,$$

$$\dot{p}_j = F_j(q) .$$

This gives n = 2l, $x = (q_1, \ldots, q_l, p_1, \ldots, p_l)$, and $f_j = \dot{q}_j = \frac{1}{m_j} p_j$, and $f_j + l = \dot{p}_j = F_j(q)$, for $j = 1, \ldots, l$. In this process, we have replaced a system of l second order equations with an equivalent system of n = 2l first order equations.

We could reduce higher order differential equations as well. Consider, for example, the single third order equation $\frac{d^3q}{dt^3} = q^2$. For this, take $x_1 = q$, $x_2 = \dot{q}$, and $x_2 = \ddot{q}$. Then we have $f_1 = x_2$, $f_2 = x_3$, and $f_3 = x_1^2$. A single third order equation has become a system of three first order equations.