Lecture 34: Second Order Equations: Special Topics

5.3. Second Order Equations.

Built upon Newton's Second Law of Motion ($F = ma$), many models in science and engineering lead to second order differential equations of the generic form $x''(t) = f(t, x(t), x'(t))$. We have seen that such equations can be converted to systems of first order equations and solved using the techniques we have been studying in the preceding lectures (see below for details). However, second-order problems often posses special structure that can be exploited. In this lecture, we briefly introduce two such concepts: geometric integration and boundary value problems.

5.3.1. Geometric Integration.

Over the past two decades there has been a growing appreciation of the fact that some numerical methods capture special features of the exact solution, and thus may be preferred over fancier methods of higher order.[†] For example, gravitational systems (in the absence of dissipative forces such as atmospheric drag) conserve energy. If one applies a standard one-step or multistep method to such a problem, the numerical solution will not exhibit such energy conservation, and thus the solutions are, to some degree, not physically sensible. Such effects are minimized as the step size h is reduced, but they will still persist. If given the choice, one might like to use a numerical method that produces approximate solutions that also preserve energy.

Remarkably, such methods exist for a variety of conserved quantities (typically deriving from Hamiltonian systems). Often these methods are implicit, but it is worth mentioning one important special explicit case. For problems of the form

$$x''(t) = f(x(t)),$$

there exists a simple explicit scheme called the *Störmer–Verlet* algorithm. Let $v(t) = x'(t)$ and suppose $v_k \approx v(t_k)$ and $x_k \approx x(t_k)$. Then the algorithm takes the form

$$\begin{aligned} v_{k+1/2} &= v_k + \tfrac{1}{2} h f(x_k) \\ x_{k+1} &= x_k + h v_{k+1/2} \\ v_{k+1} &= v_{k+1/2} + \tfrac{1}{2} h f(x_{k+1}). \end{aligned}$$

Note that operations can be arranged so that only one evaluation of f is required per step. Thus, for essentially the same computational expense of the forward Euler method, one obtains an energy-preserving integrator.

5.3.2. Boundary Value Problems.

So far all the differential equations we have studied have been *initial value problems*. We are always given $x(t_0) = x_0$ (or $x(t_0) = x_0$ and $x'(t_0) = v_0$ for a second-order system), i.e., the complete state of the system at time t_0. If faced with a second order equation,

$$x''(t) = f(t, x(t), x'(t)),$$

[†] See the excellent text *Geometric Numerical Integration: Structure-Preserving Algorithms for Ordinary Differential Equations* by E. Hairer, C. Lubich, and G. Wanner, Springer, Berlin, 2002.

we can covert to a system of two first order equations. Let $v(t) = x'(t)$. Then

$$\begin{bmatrix} x(t) \\ v(t) \end{bmatrix}' = \begin{bmatrix} v(t) \\ f(t, x(t), v(t)) \end{bmatrix}.$$

An initial value problem will supply values of both $x(t_0)$ and $v(t_0)$.

In some situations we have may have, for example, $x(t_0)$ and $x(t_{\rm final})$, rather than $x(t_0)$ and $v(t_0)$. This is an example of a *two-point boundary value problem.* Such problems require an entirely different approach. For one thing, solutions need not even exist for some pairs of $x(t_0)$ and $x(t_{\rm final})$. When the solution does exist, here are several approaches for finding it that readily generalize to higher order problems.

Shooting Method.

Suppose we are given

$$x''(t) = f(t, x(t), x'(t)),$$

with $x(t_0) = x_0$ and $x(t_{\rm final}) = \omega$.

The shooting method begins with a *guess* of a condition for $x'(t_0) = v(t_0)$, say

$$x'(t_0) = \widehat{v},$$

resulting in an initial value problem

$$\widehat{x}''(t) = f(t, \widehat{x}(t), \widehat{x}'(t)), \qquad \widehat{x}(t_0) = x_0, \quad \widehat{x}'(t_0) = \widehat{v}$$

that can be integrated using any of the techniques we previously studied. Since the guess for $\widehat{v}$ was probably not the slope of the true solution, $x'(t_0)$, the solution of the initial value problem will not in general satisfy the condition at the right boundary, i.e.,

$$\widehat{x}(t_{\rm final}) \neq x(t_{\rm final}).$$

The shooting method thus adjusts the value of $\widehat{v}$ and tries again. This procedure resembles the action of adjusting angle of a cannon barrel (hence the initial slope of a shell shot out of that barrel) to zero-in on some distant target, hence the name. Techniques for solving nonlinear equations, such as Newton's method or the secant method, can be used to find the value of $\widehat{v}$ that is a zero of the function

$$g(\widehat{v}) = \widehat{x}(t_{\rm final}; \widehat{v}) - \omega.$$

Finite Differences.

We next present an alternative to the shooting method for the linear boundary value problem

$$x''(t) + p(t)x'(t) + q(t)x(t) = f(t), \qquad \text{given values for } x(t_0) \text{ and } x(t_{\rm final}),$$

that leads ultimately to a linear algebra problem. Construct a grid $t_0, t_1, \ldots, t_n = t_{\rm final}$, where $t_j = t_0 + hj$ for $h = (t_{\rm final} - t_0)/n$. Then expanding in Taylor series, we see that for $1 \leq j \leq n-1$

$$x''(t_j) \approx \frac{x(t_{j+1}) - 2x(t_j) + x(t_{j-1})}{h^2} + O(h^2)$$

and

$$x'(t_j) \approx \frac{x(t_{j+1}) - x(t_{j-1})}{2h} + O(h^2).$$

We do not know $x(t_{j+1})$, $x(t_j)$, and $x(t_{j-1})$ exactly, so we will replace them by the approximations

$$x''(t_j) \approx \frac{x_{j+1} - 2x_j + x_{j-1}}{h^2}$$

and

$$x'(t_j) \approx \frac{x_{j+1} - x_{j-1}}{2h},$$

where $x_0 = x(t_0)$ and $x_n = x(t_{\text{final}})$ are exact. The goal now is to find $x_1, \ldots, x_{n-1}$. We obtain a linear system of the form

$$\left[\begin{array}{ccccc} \alpha_1 & \gamma_1 & & & \\ \beta_2 & \alpha_2 & \gamma_2 & & \\ & \ddots & \ddots & \ddots & \\ & & \beta_{n-2} & \alpha_{n-2} & \gamma_{n-2} \\ & & & \beta_{n-1} & \alpha_{n-1} \end{array}\right] \left[\begin{array}{c} x_1 \\ x_2 \\ \vdots \\ x_{n-2} \\ x_{n-1} \end{array}\right] = \left[\begin{array}{c} f(t_1) - (1/h^2 - p(t_0)/2h)x_0 \\ f(t_2) \\ \vdots \\ f(t_{n-2}) \\ f(t_{n-1}) - (1/h^2 + p(t_n)/2h)x_n \end{array}\right],$$

where

$$\alpha_j = -\frac{2}{h^2} + q(t_j) \qquad \beta_j = \frac{1}{h^2} - \frac{p(t_j)}{2h} \qquad \gamma_j = \frac{1}{h^2} + \frac{p(t_j)}{2h}$$

for $j = 1, \ldots n-1$. To solve the differential equation, we simply have to solve the linear algebraic system $\mathbf{Ax} = \mathbf{f}$, which we can do using the QR factorization discussed at the beginning of the semester, or the LU factorization we shall begin discussing in the next lecture. Nonlinear boundary value problems result in a nonlinear system of equations, which you can tackle using techniques that will be taught in CAAM 454/554 in the Spring.