

1. (10 points) We'll have much to say about *boundary-value problems* in the next few weeks, mostly in the context of PDEs in more than one space dimension. As a starting point, we'll consider here *two-point boundary-value problems* (BVPs). Such a BVP consists of an ODE together with conditions on the solution imposed at two distinct values of the independent variable. Note the contrast with the *initial-value problems* (IVPs) we've been considering, in which a value of the solution is specified at a single value of the independent variable. Under mild assumptions, an IVP has a unique solution, at least locally in time. BVPs, on the other hand, may have no solutions, infinitely many solutions, or other "interesting" properties.¹ Notwithstanding these "interesting" possibilities, BVPs are of interest in many important applications, and MATLAB has very good codes for solving them (type "`doc boundary-value problems`" in the command window for information).

Here we'll consider a simple method not implemented in the MATLAB BVP codes called the *method of shooting*. To illustrate this, suppose we have a BVP $y'' + g(t, y) = 0$, $y(0) = a$, $y(T) = b$. If we specify $y'(0) = s$ for some s , then we expect the IVP $y'' + g(t, y) = 0$, $y(0) = a$, $y'(0) = s$ to have a unique solution; denote this by $y(t, s)$. To solve the BVP, we need to find s such that $y(T, s) = b$. The idea of shooting is to try a value of s , observe the value of $y(T, s)$ relative to b , then correct s according to some procedure, then try again, and so on. A more refined view is to define a *residual function* by $r(s) \equiv y(T, s) - b$ and then apply a zero-finding procedure to solve $r(s) = 0$. There are many procedures that one might consider for this; we'll talk more about these in class soon.

Consider the pendulum ODE from Homework 4:

$$\theta'' + \sin(\theta) = 0, \tag{1}$$

¹The ODE $y'' + y = 0$ provides an instructive example. This has general solution $y(t) = \alpha \cos(t) + \beta \sin(t)$. Suppose we impose boundary conditions $y(0) = a$ and $y(T) = b$ for some $T > 0$. From the first BC, we have $\alpha = a$, and so $y(t) = a \cos(t) + \beta \sin(t)$. The second BC then requires $b = a \cos(T) + \beta \sin(T)$, or $\beta \sin(T) = b - a \cos(T)$. If $T \neq k\pi$ for any positive integer k , then $\beta = (b - a \cos(T)) / \sin(T)$, and the BVP has a unique solution. If $T = k\pi$ for some positive integer k , then there is *no* solution if $(b - a \cos(T)) \neq 0$; however, if $(b - a \cos(T)) = 0$, then β can be arbitrary, and there are infinitely many solutions (an entire one-parameter family).

Another instructive example is the BVP $y'' + \lambda y = 0$, $y(0) = y(\pi) = 0$, which may be familiar, e.g., from a first course in PDEs. This has no non-trivial solutions unless $\lambda = k^2$ for a positive integer k , in which case any scalar multiple of $\sin(kt)$ is a solution.

where θ is the angle of the pendulum from the vertical. Suppose we impose the initial condition $\theta(0) = -\pi/2$ (horizontal to the left). What should the initial angular velocity $\theta'(0)$ be so that $\theta(1) = \pi/2$ (horizontal to the right)?

Suggestion: Form the residual function $r(s) \equiv \theta(1, s) - \pi/2$, where $\theta(t, s)$ is the solution with initial angular velocity s , and apply a zero-finding procedure to solve $r(s) = 0$. You may use any procedure you'd like, but MATLAB's `fzero` is perfectly suited to a simple one-variable problem like this.

2. (10 points) We've seen a number of IVPs that depend on parameters, for example the clarinet-reed problem (Homework 1), the predator-prey problem (Homework 3), the Lorenz equation (Homework 4), and the damped-oscillator problem (in many assignments). In these examples, the parameters are in the ODEs, but in other problems the initial conditions may also depend on parameters.

It is often useful to determine how the solution of a parameter-dependent IVP changes as the parameters change, in particular how sensitive the solution is to changes in the parameters. For this, it would clearly be useful to know the derivatives of the solution with respect to the parameters, if these can be obtained.² Can they?

Let's consider an IVP that depends on a parameter α , as follows:

$$y' = f(t, y, \alpha), \quad y(0) = y_0(\alpha). \quad (2)$$

In general, α may be a vector of parameters, but let's assume it's a scalar for simplicity. It can be shown without much difficulty that if f is continuously differentiable in α , then y is indeed differentiable with respect to α , and the derivative of y with respect to α (denoted y_α) satisfies the IVP

$$y_\alpha' = f_y(t, y, \alpha)y_\alpha + f_\alpha(t, y, \alpha), \quad y_\alpha(0) = y_0'(\alpha), \quad (3)$$

where $y_0'(\alpha) = \frac{d}{d\alpha}y_0(\alpha)$ and f_y and f_α are partial derivatives of f with respect to y and α , respectively. (In the system case, f_y is the Jacobian matrix and f_α is a vector.) Note that (3) is obtained just by differentiating (2) with respect to α .

²These derivatives are often referred to as *sensitivities* and are often of interest in applications such as chemical reaction simulations for guidance on how accurately parameters need to be estimated.

Since the solution y of (2) appears in (3), solving (3) numerically must be done in conjunction with solving (2). To illustrate, for a particular value of α , we might define

$$Y = \begin{pmatrix} y \\ y_\alpha \end{pmatrix}, \quad F(t, Y) = \begin{pmatrix} f(t, y, \alpha) \\ f_y(t, y, \alpha)y_\alpha + f_\alpha(t, y, \alpha) \end{pmatrix}, \quad Y_0 = \begin{pmatrix} y_0(\alpha) \\ y_0'(\alpha) \end{pmatrix}, \quad (4)$$

and then solve the IVP

$$Y' = F(t, Y), \quad Y(0) = Y_0. \quad (5)$$

Consider again the pendulum ODE (1). For a given s , again denote by $\theta(t, s)$ the solution satisfying the initial conditions $\theta(0) = -\pi/2$ and $\theta'(0) = s$. What is $\theta_s(1, s)$ when s is the value determined in the previous problem such that $\theta(1, s) = \pi/2$?

Guidance: In this case, the initial angular velocity s is the parameter of interest. The usual way of solving the IVP for the pendulum ODE is to set $y_1 = \theta$, $y_2 = \theta'$ and solve

$$y' = f(t, y) \equiv \begin{pmatrix} y_2 \\ -\sin(y_1) \end{pmatrix}, \quad y(0) = \begin{pmatrix} -\pi/2 \\ s \end{pmatrix}.$$

Note that in this case, s appears explicitly only in the initial conditions and not in f . To obtain the IVP (5), we can define $y_3 = \theta_s$, $y_4 = \theta_s'$ and set

$$Y = \begin{pmatrix} y_1 \\ y_2 \\ y_3 \\ y_4 \end{pmatrix}, \quad F(t, Y) = \begin{pmatrix} y_2 \\ -\sin(y_1) \\ y_4 \\ -\cos(y_1)y_3 \end{pmatrix}, \quad Y_0 = \begin{pmatrix} -\pi/2 \\ s \\ 0 \\ 1 \end{pmatrix}.$$

Taking s to be the value such that $\theta(1, s) = \pi/2$, you can integrate this ODE to obtain the desired value $y_3(1) = \theta_s(1, s)$.