Objective. We will discuss non linear as well as boundary and interior layer problems. This discussion includes also nonuniform grids.

Agenda. In today's class, we will discuss the following.

1. Announcements
2. Discuss Chapter 2, Sections 2.16 - 2.20 of the text.

Topic: Nonlinear boundary value problems. Your text gives the following nonlinear boundary value problem:

$$\theta''(t) = -\sin(\theta(t)) \quad \text{in } (0,T), \quad \theta(0) = \alpha, \quad \theta(T) = \beta.$$

Following the methods we used to solve linear problems numerically, we arrive at

$$\frac{1}{h^2}(\theta_{i-1} - 2\theta_i + \theta_{i+1}) + \sin(\theta_i) = 0, \quad i = 1, 2, \cdots, m,$$

with $h = T/(m+1)$. This is a system of nonlinear equations of the form

$$G(\theta) = 0,$$

with $G : \mathbb{R}^m \to \mathbb{R}^m$. To solve this system of nonlinear equations, we use Newton's method.

Newton's method is an iterative method for solving nonlinear equations. Let $\theta^{[k]}$ denote the approximation for θ at step k in Newton's method. Then, we expand $G(\theta^{[k+1]})$ in a Taylor series about $\theta^{[k]}$ and obtain

$$G(\theta^{[k+1]}) = G(\theta^{[k]}) + G'(\theta^{[k]})(\theta^{[k+1]} - \theta^{[k]}) + \cdots.$$

Using only the first two terms in the expansion above, we set

$$G(\theta^{[k]}) + G'(\theta^{[k]})(\theta^{[k+1]} - \theta^{[k]}) = 0.$$

Let $\delta^{[k]} = \theta^{[k+1]} - \theta^{[k]}$. Then, rearranging terms in the equation above, we obtain

$$J(\theta^{[k]})\delta^{[k]} = -G(\theta^{[k]}),$$

with $J(\theta) = G'(\theta) \in \mathbb{R}^{m\times m}$ is the Jacobian matrix whose entries are

$$J_{ij}(\theta) = \frac{\partial}{\partial \theta_j} G_i(\theta).$$

For the case in which

$$G_i(\theta) = \frac{1}{h^2}(\theta_{i-1} - 2\theta_i + \theta_{i+1}) + \sin(\theta_i),$$

we find that

$$J_{ij}(\theta) = \frac{\partial}{\partial \theta_j} G_i(\theta) = \begin{cases} \frac{1}{h^2} & j = i \pm 1 \\ -\frac{2}{h^2} + \cos(\theta_i) & j = i \\ 0 & \text{otherwise.} \end{cases}$$

Thus, we compute $\theta^{[k+1]}$ from $\theta^{[k]}$ by evaluating

$$\theta^{[k+1]} = \theta^{[k]} + \delta^{[k]},$$

where $\delta^{[k]}$ satisfies

$$\frac{1}{h^2} \begin{bmatrix} (-2 + h^2 \cos(\theta_1)) & 1 & & \\ 1 & (-2 + h^2 \cos(\theta_2)) & 1 & \\ \ddots & \ddots & \ddots & \\ & 1 & (-2 + h^2 \cos(\theta_m)) \end{bmatrix} \begin{bmatrix} \delta_1^{[k]} \\ \delta_2^{[k]} \\ \vdots \\ \delta_m^{[k]} \end{bmatrix} = - \begin{bmatrix} G_1(\theta^{[k]}) \\ G_2(\theta^{[k]}) \\ \vdots \\ G_m(\theta^{[k]}) \end{bmatrix},$$

with

$$G_1(\theta^{[k]}) = \frac{1}{h^2} \left(\alpha - 2\theta_1^{[k]} + \theta_2^{[k]} \right) + \sin(\theta_1^{[k]}),$$

and

$$G_m(\theta^{[k]}) = \frac{1}{h^2} \left(\theta_{m-1}^{[k]} - 2\theta_1^{[k]} + \beta \right) + \sin(\theta_m^{[k]}).$$

In summary, the procedure to solve the nonlinear boundary value problem

$$G(\theta) = \theta'' + \sin(\theta) = 0 \quad \text{in } (0,T), \quad \theta(0) = \alpha, \quad \theta(T) = \beta.$$

is given by the following.

1. Define the grid $t_i = ih$ with $i = 1, \cdots, m$ and $h = T/(m+1)$.
2. Make an initial guess corresponding to $\theta_i^{[0]}$ for $i = 1, 2, \cdots, m$.
3. Set $k = 0$.
4. Compute the $m \times 1$ vector $G(\theta^{[k]})$ using $\theta_0^{[k]} = \alpha$ and $\theta_{m+1}^{[k]} = \beta$.
5. Compute the $m \times m$ matrix $J(\theta^{[k]})$.
6. Solve the tridiagonal linear system $J(\theta^{[k]})\delta^{[k]} = -G(\theta^{[k]})$.
7. Check to see if $\|\delta^{[k]}\| < \varepsilon$ with ε denoting a user-defined termination parameter. If not, go back to Step 4 with $k \leftarrow k+1$ and $\theta^{[k+1]} \leftarrow \theta^{[k]} + \delta^{[k]}$

Notice that we need to provide an initial guess for the solution. The solution to which we converge depends on our initial guess. We can see this by experimenting with different initial guesses. For this problem, we say that solutions are locally unique meaning that there are no other solutions nearby to it. Thus, different initial guesses near this locally unique solution converges to it. Depending on our problem, we may have to think very carefully about how to choose an initial guess appropriately.

Now because Newton's method converges to a solution does not imply necessarily that this numerical solution is the exact solution of the boundary value problem. In fact, Newton's method converges to the solution of the discrete system with h fixed. To study the convergence of the numerical method, we still need to go through consistency and stability calculations.

The local truncation error τ_i is given by

$$\begin{aligned}\tau_i &= \frac{1}{h^2}\left[\theta(t_{i-1}) - 2\theta(t_i) + \theta(t_{i+1})\right] + \sin(\theta(t_i)) \\ &= \theta''(t_i) + \frac{1}{12}h^2\theta^{(iv)}(t_i) + \sin(\theta(t_i)) + O(h^4) \\ &= \frac{1}{12}h^2\theta^{(iv)}(t_i) + O(h^4).\end{aligned}$$

The local truncation error is $O(h^2)$ and is the same as the linear problem we studied previously. Notice that the vector τ has entries $\tau_i = G(\theta(t_i))$. Let $\hat{\theta}$ denote the vector whose entries are $\hat{\theta}_i = \theta(t_i)$. That is, the entries of $\hat{\theta}$ are the values of $\theta(t)$ evaluated at $t = t_i$. Then, we have

$$\begin{aligned}G(\theta) &= 0 \\ G(\hat{\theta}) &= \tau.\end{aligned}$$

Thus,

$$G(\theta) - G(\hat{\theta}) = -\tau.$$

By Taylor expanding $G(\theta)$ about $\theta = \hat{\theta}$, we find that

$$G(\theta) = G(\hat{\theta}) + J(\hat{\theta})(\theta - \hat{\theta}) + O(\|\theta - \hat{\theta}\|^2).$$

Let $E = \theta - \hat{\theta}$ denote the vector of errors. Then, we find that

$$J(\hat{\theta})E = -\tau + O(\|E\|^2).$$

If we ignore the higher order terms, we have a linear relation between the local and global errors. This motivates the following definition of stability for $\hat{J}^h$, the Jacobian matrix of the difference formulas evaluated at the true solution on a grid with mesh width h.

Definition 2.2 *The nonlinear difference method $G(\theta) = 0$ is stable in some norm $\|\cdot\|$ if the matrices $(\hat{J}^h)^{-1}$ are uniformly bounded in this norm as $h \to 0$, i.e. there exist constants C and h_0 such that*

$$\|(\hat{J}^h)^{-1}\| \leq C \quad \textit{for all } h < h_0.$$

It is not obvious that if we show that the Jacobian matrix is stable in the sense given in Definition 2.2 and $\|\tau^h\| \to 0$ that the method converges and $\|E^h\| \to 0$ as $h \to 0$. However, it is true. It is not obvious because we are trying to show that $\|E\|$ is small, so we cannot assume that terms of $O(\|E\|^2)$ are small without taking careful steps.

Notice again that convergence of the numerical method does not imply convergence of Newton's method to solve the nonlinear equations. The best that we can do is to show that for a convergence method, Newton's method will converge from a sufficiently good guess.

Topic: Singular perturbations and boundary layers. Consider the linear, Dirichlet boundary value problem

$$\varepsilon u'' - u' = f \quad \text{in } (0,1), \quad u(0) = \alpha, \quad u(1) = \beta, \quad 0 < \varepsilon \ll 1.$$

The new twist on this problem is the presence of the small parameter ε. If we consider the limit as $\varepsilon \to 0$, we find that the differential equation reduces to

$$-u' = f.$$

We lose the highest derivative in the differential equation and have only a first-order differential equation. That means that there is only one integration constant. Therefore, we cannot impose two boundary conditions. We can impose only one. Since this problem is solvable analytically, we find that for $f(x) = -1$

$$u(x) = \alpha + x + (\beta - \alpha - 1)\left(\frac{\mathrm{e}^{x/\varepsilon} - 1}{\mathrm{e}^{1/\varepsilon} - 1}\right).$$

The solution looks like a simple linear function except near the boundary $x = 1$ at which the solution changes rapidly to reach the value β. We call this region of rapid change the "boundary layer."

We call this differential equation a singularly perturbed equation. Using matched asymptotics, we learn how to add a so-called boundary layer solution. Here, we examine the ramifications of this boundary layer on the numerical solution of this boundary value problem. Figure 1 shows results from our "standard" numerical method to solve Dirichlet two-point boundary value problems on the grid $x_i = ih$ for $i = 1, 2, \cdots, m$ with

$h = 1/(m+1)$:

$$\begin{aligned} \frac{\varepsilon}{h^2}(-2U_1+U_2) - \frac{1}{2h}U_2 &= -1 - \frac{\varepsilon}{h^2}\alpha - \frac{1}{2h}\alpha, \quad i=1 \\ \frac{\varepsilon}{h^2}(U_{i-1}-2U_i+U_{i+1}) - \frac{1}{2h}(-U_{i-1}+U_{i+1}) &= -1, \quad i=2,\cdots,m-1 \\ \frac{\varepsilon}{h^2}(U_{m-1}-2U_m) + \frac{1}{2h}U_{m-1} &= -1 - \frac{\varepsilon}{h^2}\beta + \frac{1}{2h}\beta, \quad i=m. \end{aligned}$$

We observe in Fig. 1 that the numerical solution undergoes oscillatory errors near the boundary layer. As we increase the resolution of the grid, we see that the numerical solution begins to capture the correct solution behavior.

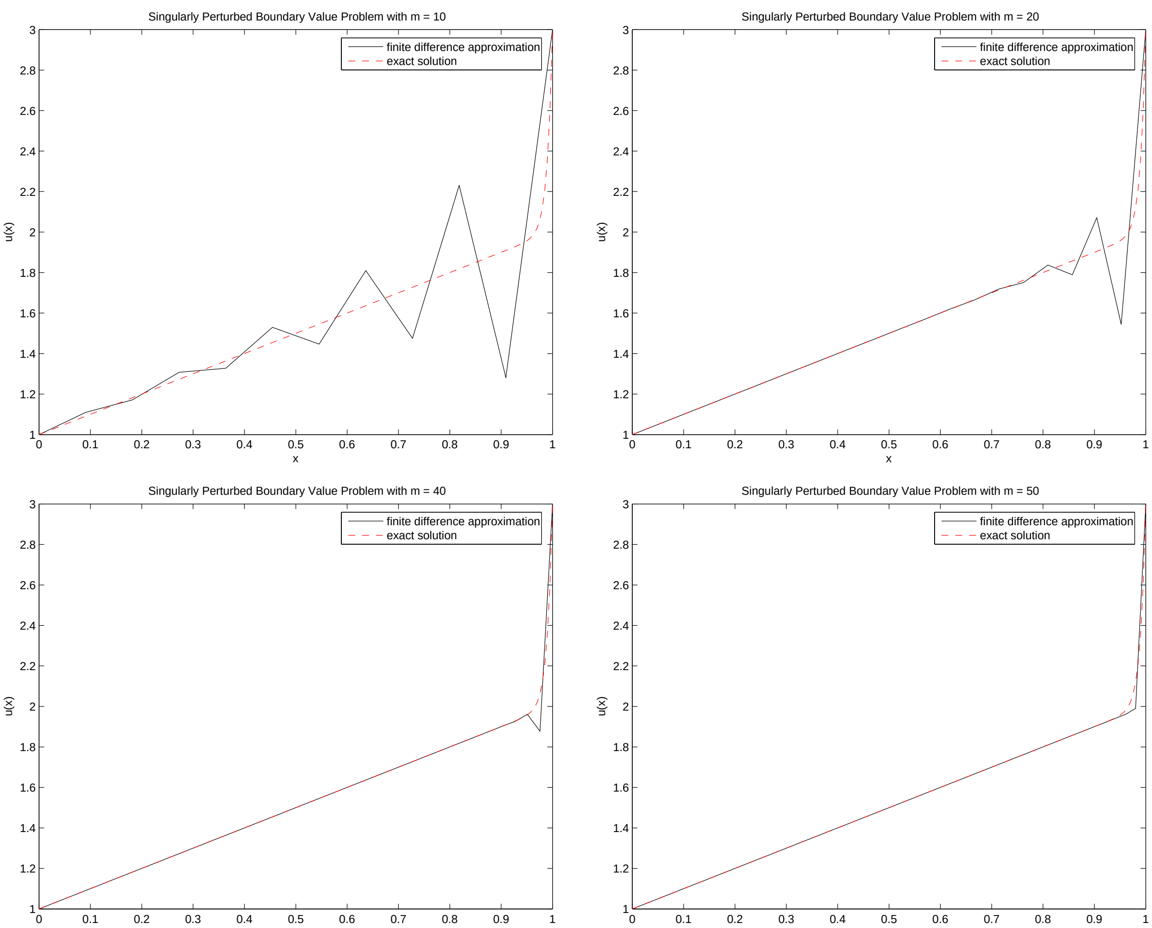

Figure 1: Solution to the singularly perturbed boundary value problem $\varepsilon u'' - u' = -1$ on $(0,1)$ with $u(0) = 1$, $u(1) = 3$ and $\varepsilon = 0.01$. The upper left plot corresponds to $m = 10$, the upper right plot corresponds to $m = 20$, the lower left plot corresponds to $m = 40$ and the lower right plot corresponds to $m = 50$.

Topic: Interior Layers. For singularly perturbed problems, sometimes we find that there is a region within the interior where the solution undergoes rapid change. Consider the problem

$$\varepsilon u'' + u(u' - 1) = 0 \quad \text{in } (a,b), \quad u(a) = \alpha, \quad u(b) = \beta.$$

This problem has an "interior layer" in which the solution undergoes a rapid change somewhere in the interior of the domain. The added difficulty here is that we need to determine where this interior layer is. Through experimentation with the numerical method, we find that we must have the right combination of mesh resolution and initial guess to obtain the correct numerical solution. Figure 2 shows some example results.

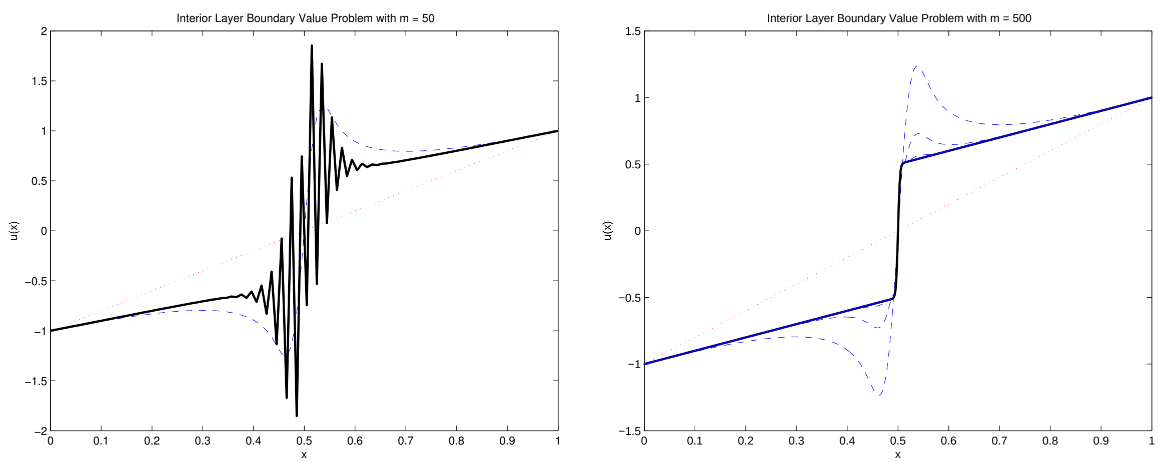

Figure 2: Solution to the singularly perturbed, nonlinear boundary value problem $\varepsilon u'' + u(u' - 1) = 0$ on $(0,1)$ with $u(0) = -1$, $u(1) = 1$ and $\varepsilon = 0.001$. The left plot shows the first three iterations of Newton's method with $m = 50$. The initial guess is plotted as a dotted red curve. The third iteration is plotted as the solid black curve. The right plot shows seven iterations of Newton's method with $m = 500$ which converged below the tolerance value set at 10^{-12}. The initial guess is plotted as a dotted red curve. The solid black curve shows the solution to which Newton's method converged.

The key point in both boundary layer and interior layer problems is that we need to resolve highly a region in which the solution undergoes a rapid change. However, outside of the boundary/interior layer, the solution is very smooth and does not require such a high resolution. In other words, the boundary/interior layer dictates the resolution needed to compute a good solution.

Topic: Nonuniform Grids. For boundary/interior layer problems when we use a uniform grid, we must choose a mesh width h small enough to resolve the rapid change of the solution within the boundary/interior layer. However, this fine mesh is unnecessary to resolve the solution away from the boundary/interior layer. Far fewer points are needed in those regions. Because of this observation, we might consider computing numerical solutions on nonuniform grids to develop a more efficient numerical method.

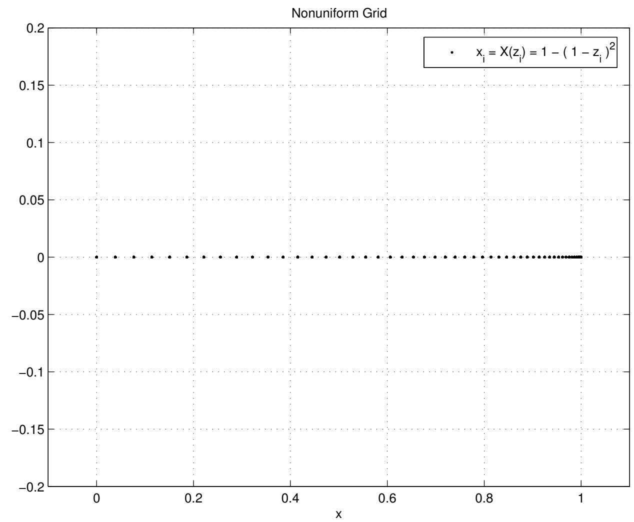

Figure 3: The result from mapping a uniform grid $z_i = ih$ with $h = 1/(m+1)$ to the nonuniform grid $x_i = X(z_i) = 1-(1-z_i)^2$. Notice that the nonuniform grid is finer near the end point $x = 1$.

Consider the boundary layer problem:

$$\varepsilon u'' - u' = -1 \quad \text{in } (0,1), \quad u(0) = \alpha, \quad u(1) = \beta, \quad 0 < \varepsilon \ll 1.$$

We have established that there is a boundary layer at $x = 1$. Thus, we can consider a nonuniform grid in which the mesh is very fine near $x = 1$ and much coarser away from $x = 1$. To construct this nonuniform grid, consider first the uniform grid $z_i = ih$ for $i = 0, 1, \cdots, m+1$ with $h = 1/(m+1)$. Now, consider the grid mapping function $x = X(z)$ that maps the uniform grid to a nonuniform grid. We want to design this grid mapping function $X(z)$ to "cluster" points near $x = 1$ and to space points nearly uniform away from that region. One choice is

$$x = X(z) = 1-(1-z)^2.$$

A plot of this nonuniform grid appears in Fig. 3. Notice that this mesh becomes finer and finer near $x = 1$.

We can compute a numerical solution using finite differences on nonuniform grids. We could determine the analytical form for the finite difference approximations, but in Matlab, it is easier just to use the Vandermonde matrix formulation to determine the coefficients of the finite difference approximation. In doing so, we obtain results shown in Fig. 5.

Determining the order of accuracy of a method for a nonuniform grid is understandibly more complicated than for a uniform grid. In general, we lose second order accuracy, but we retain it for sufficiently smooth solutions. Please read Section 2.18 in your text for more details.

This method for resolving boundary/interior layers works well, but we must prescribe the grid mapping

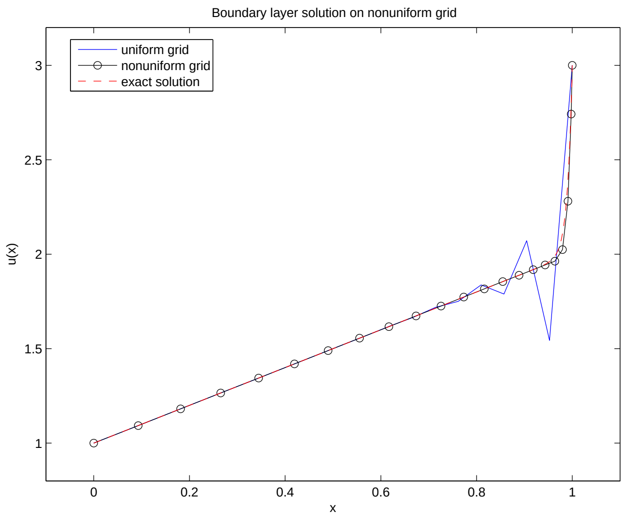

Figure 4: Comparison of the boundary layer problem using a uniform grid, a nonuniform grid and the exact solution. For the numerical calculations, we used only $m = 20$ with $\varepsilon = 0.01$.

function $x = X(z)$. What if we do not know where we need to resolve our grid? There are methods that perform adaptive mesh selection automatically, but those topics are beyond the scope of this course. In fact, they are very much a current research topic.

Another approach that is useful for these problems are called continuation or homotopy methods. To explain this approach, suppose we wish to solve the interior layer problem above for $\varepsilon = 10^{-5}$. Rather than try to solve this problem immediately, we first consider a "smoother" problem using $\varepsilon = 0.1$. We use that solution to inform us on how to solve the problem with $\varepsilon = 0.01$ from which we learn to study $\varepsilon = 0.005$ and so on. Figure 5 shows numerical results of applying this continuation method. In this way, we discover how to prescribe the grid mapping function, for example. For nonlinear problems, these smoother solutions give us good initial guesses to apply Newton's method.

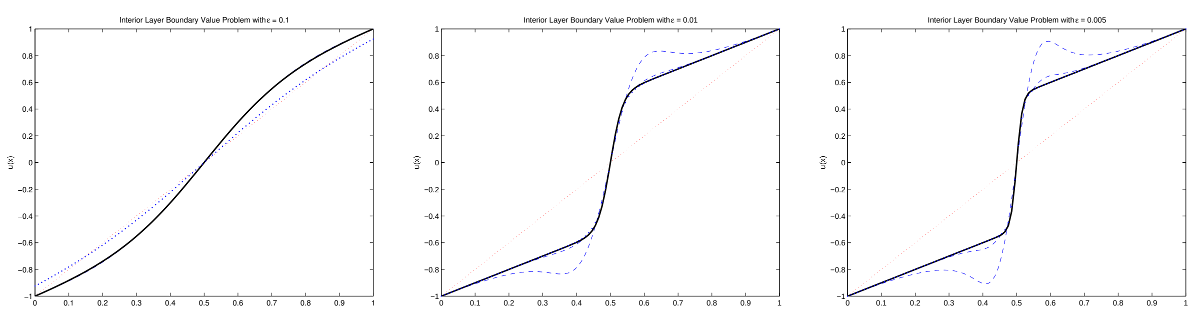

Figure 5: Solution to the singularly perturbed, nonlinear boundary value problem $\varepsilon u'' + u(u' - 1) = 0$ on $(0,1)$ with $u(0) = -1$, $u(1) = 1$. Here, we have used $m = 100$ for all three cases corresponding to $\varepsilon = 0.1$ (left plot), $\varepsilon = 0.01$ (center plot) and $\varepsilon = 0.005$ (right plot).