

## Objectives:

- Errors in Finite Difference Methods
- Shooting method
- Examples
- **Materials:** Gerald and Wheatley, Chapter 7; Golub and Ortega, Chapter 3; Forsythe, et al., Chapter 6

## Errors in finite difference method

Consider the errors in solving

$$\frac{d^2v(x)}{dx^2} = c(x)v(x) + d(x); \quad 0 \leq x \leq 1; \quad (1)$$

using finite differences. Define  $v_1, v_2, \dots, v_n$  as the numerical solutions at  $x_1 = h, x_2 = 2h, \dots, x_n = 1 - h$  obtained using finite differences (that is the exact solution to  $Av = d$ ); and  $v(x_1), v(x_2), \dots, v(x_n)$  as the exact solution to equation 1. Define  $\sigma_i = L(x_i, h)$  to be the *local discretization error* and  $e_i$  to be the *global discretization error* at  $x_i$ . The global discretization error for the system will be the  $\max_{1 \leq i \leq n} \text{abs}(v_i - v(x_i))$ . We will derive expressions for  $\sigma_i$  and  $e_i$ , and a bounds for the global discretization error.

The local discretization error is estimated by the difference between the discretized estimate of  $v''(x)$  and the true value of  $v''(x)$ :

$$\sigma_i = L(x_i, h) = \frac{1}{h^2} [v(x_i + h) - 2v(x_i) + v(x_i - h)] - c(x_i)v(x_i) - d(x_i). \quad (2)$$

We can evaluate equation 2 by recalling how we derived the centered difference form for  $v''(x)$  using Taylor Series expansion:

$$\begin{aligned} v(x+h) &= v(x) + hv'(x) + \frac{h^2}{2}v''(x) + \frac{h^3}{6}v^{(iii)}(x) + \frac{h^4}{24}v^{(iv)}(x) + \dots; \\ v(x-h) &= v(x) - hv'(x) + \frac{h^2}{2}v''(x) - \frac{h^3}{6}v^{(iii)}(x) + \frac{h^4}{24}v^{(iv)}(x) - \dots; \\ v(x+h) + v(x-h) &= 2v(x) + h^2v''(x) + \frac{h^4}{12}v^{(iv)}(x) + \dots \\ v''(x) &\approx \frac{v(x+h) - 2v(x) + v(x-h)}{h^2} - \frac{h^2}{12}v^{(iv)}(x) \end{aligned} \quad (3)$$

Combining equations 2 and 3 we conclude that  $\sigma_i = L(x_i, h) \sim O(h^2)$ .

Next, we relate the local error to the global error. This requires comparing the exact numerical solution ( $v$  such that  $Av = d$ ) to the exact solution ( $v(x)$ ) of equation 1. The numerical expression that we derived for  $v_i$  was

$$\frac{v_{i-1} - 2v_i + v_{i+1}}{h^2} - c_i v_i - d_i = 0; \quad i = 1, \dots, n. \quad (4)$$

The global discretization error at any grid point,  $i$ , is  $e_i = v(x_i) - v_i$ . If we subtract 4 from the expression for local error (equation 2), and use  $e_i$  defined above, we get

$$-e_{i-1} + (2 + c_i h^2) e_i - e_{i+1} = -h^2 \sigma_i; \quad i = 1, \dots, n. \quad (5)$$

Note that this has a similar form to our general matrix equation. The solution will be  $e = -h^2 A^{-1} \sigma$ . To evaluate the behavior of the global discretization error, we need to consider how  $A^{-1}$  behaves as  $h$  approaches 0. Consider a special case, where  $c(x) \geq \gamma > 0$  for all  $0 \leq x \leq 1$ . Then  $c_i > \gamma$  for  $i = 1, \dots, n$ . Let  $e = \max[abs(e_i)]$ ; and  $\sigma = \max[abs(\sigma_i)]$ . We've just shown that  $\sigma \sim O(h^2)$ . From equation 5 we see

$$\begin{aligned} (2 + \gamma h^2) abs(e_i) &\leq 2e + h^2 \sigma; \quad i = 1, \dots, n \\ (2 + \gamma h^2) e &\leq 2e + h^2 \sigma; \\ \gamma h^2 e &\leq h^2 \sigma \\ e &\leq \frac{\sigma}{\gamma} \sim O(h^2). \end{aligned} \quad (6)$$

So, as long as  $c(x)$  is positive, the error in the finite difference method will be second order. This means that doubling the grid resolution will decrease errors by a factor of 4. Also note that the error can get large as  $\gamma$  gets small.

## Shooting method

For a  $2^{nd}$  order b.v.p. (boundary value problem), the **shooting method** uses one of the two boundary values specified. A guess is made at a second boundary condition (usually a combination of  $v(x)$  and  $v'(x)$  are used for  $x$  located at one of the boundaries, and the problem is solved using a method for ordinary differential equations. Often, a Runge-Kutta method would be used at this step. The value obtained for the second (as yet unused) boundary condition is compared to the value specified, and the error is used to guess another value of the unspecified boundary condition. The third guess can be a linear combination of the first two; weighted so as to give the exact value for the second boundary value that was specified. For linear boundary value problems, the third guess will be exact, so that only three iterations are required.

## Examples

### Using Shooting Method

Shooting methods can be used for the general problem  $v''(x) = f(x, v(x), v'(x))$ ; whether  $f(x, v(x), v'(x))$  is linear or not. If  $f(x, v(x), v'(x))$  is linear, the shooting method will converge in three iterations. Assume that you need to solving the general equation

$$\begin{aligned} A \frac{d^2v}{dx^2} + B \frac{dv}{dx} + Cv &= D; \quad x_0 \leq x \leq x_L; \\ BC's : v(x_0) &= \alpha; \quad v(x_L) = \beta. \end{aligned} \quad (7)$$

In this example, assume that we are solving a linear equation  $(v'' - (1 - x/5)v = x, 1 \leq x \leq 3, v(x = 1) = 2; v(x = 3) = -1$ . To start the shooting method; assume a value for  $v'(1)$ . A good guess might be  $g_1 = v'(1) = \frac{v(3) - v(1)}{3 - 1} = -1.5$ . You now can solve the second order initial value problem;  $(v_1'' - (1 - x/5)v_1 = x, 1 \leq x \leq 3, v_1(x = 1) = 2; v_1'(x = 1) = -1.5$ . Gerald and Wheatley complete this calculation using the Runge - Kutta - Fehlberg routine (see handout). This solution results in an (incorrect) estimate of  $v_1(3) = 4.79 > v(3)$ .

The next step is to adjust the estimate of the slope  $v'(1)$ . Because the first guess overshoot the desired value of  $v(3)$ ; try a smaller slope, like  $v_2'(1) = -3.0$ . The second iteration then involves solving a new second order initial value problem;  $(v_2'' - (1 - x/5)v_2 = x, 1 \leq x \leq 3, v_2(x = 1) = 2; v_2'(x = 1) = -3.0$ . Again using the R-K-F solution results in an incorrect guess for  $v_2(3) = 0.4360$ . (See Gerald and Wheatley for solutions.)

Next, the shooting method uses a "smarter" way to choose the next estimate of the slope,  $v_3(1)$ . Because the problem is linear, the estimates of  $v_i(3)$  are linearly related to the estimates of the slopes,  $v_i'(1)$ . This can be used to choose the third and final guess of  $v_i'(1)$ :

$$v_3'(x = 1) = g_3 = g_1 + (g_2 - g_1) \frac{v(x_L) - v_1(x_L)}{v_2(x_L) - v_1(x_L)}. \quad (8)$$

The solution to the third initial value problem;  $(v_3'' - (1 - x/5)v_3 = x, 1 \leq x \leq 3, v_3(x = 1) = 2; v_3'(x = 1) = g_3$  will be the exact solution of the boundary value problem. Gerald and Wheatley work through this example.

The error within the solution will depend on the method used to solve the initial value problems. If higher-order methods (like the R-K-F) are used, then the shooting method will be more accurate than a second-order finite difference method.

### Using Finite Differences

The same problem can be solved using finite differences. Split the range  $1 \leq x \leq 3$  into sub-intervals of width  $h$ , so that  $x_0 = 1; x_1 = 1 + h, \dots, x_i = 1 + ih, \dots, x_n = 3 - h, x_{n+1} = 3$ . This implies that  $h = 2/(n + 1)$ . Estimate

$v''$  using centered differences to obtain the general difference equation;  $-v_{i-1} + [2 + h^2(1 - x_i/5)]v_i - v_{i+1} = -h^2x_i$ . Next; apply the boundary conditions for the general equations for  $i = 1; i = n$  to get  $[2 + h^2(1 - x_1/5)]v_1 - v_2 = 2 - h^2x_1$ ;  $-v_{n-1} + [2 + h^2(1 - x_n/5)]v_n = -1 - h^2x_n$ . The matrix equation,  $Av = d$  can be solved using Gaussian Elimination for tri-diagonal matrices. Gerald and Wheatley complete solutions for different values of  $h$ .