Two-point Boundary Value Problems: Numerical Approaches

Math 615, Spring 2010

Two-point Boundary Value Problems: Numerical Approaches Bueler

classical IVPs and BVPs

serious example

finite difference

shooting

serious example: solved

exercises

Ed Bueler Dept of Mathematics and Statistics University of Alaska, Fairbanks elbueler@alaska.edu

abbreviations

- ODE = ordinary differential equation
- PDE = partial differential equation
- IVP = initial value problem
- BVP = boundary value problem
- MOP = MATLAB or OCTAVE or PYLAB

Value Problems: Numerical Approaches Bueler

classical IVPs and BVPs

Two-point Boundary

serious example

finite difference

shooting

serious example: solved

Outline

1 classical IVPs and BVPs with by-hand solutions

- 2 a more serious example: a BVP for equilibrium heat
- Inite difference solution of two-point BVPs
- A shooting to solve two-point BVPs
- 5 a more serious example: solutions



wo-point Boundary
Value Problems:
Numerical
Approaches
Buolor

classical IVPs and BVPs serious example finite difference

shooting

serious example: solved

classical ODE problems: IVP vs BVP

Example 1: ODE IVP. find y(x) if

$$y'' + 2y' - 8y = 0,$$
 $y(0) = 1,$ $y'(0) = 0$

Example 2: ODE BVP. find y(x) if

$$y'' + 2y' - 8y = 0,$$
 $y(0) = 1,$ $y(1) = 0$

Two-point Boundary Value Problems: Numerical Approaches Bueler

classical IVPs and BVPs

serious example

finite difference

shooting

serious example: solved

classical ODE problems: IVP vs BVP

Example 1: ODE IVP. find y(x) if

$$y'' + 2y' - 8y = 0,$$
 $y(0) = 1,$ $y'(0) = 0$

Example 2: ODE BVP. find y(x) if

$$y'' + 2y' - 8y = 0,$$
 $y(0) = 1,$ $y(1) = 0$

- both problems can be solved by hand
- in fact, the ODE has constant coefficients so we can find characteristic polynomial and general solution ... like this:
 if y(x) = e^{rx} then r² + 2r 8 = (r + 4)(r 2) = 0 so

$$y(x) = c_1 e^{-4x} + c_2 e^{2x}$$

- *Example 1* gives system $c_1 + c_2 = 1$, $-4c_1 + 2c_2 = 0$ for coefficients; get solution $y(x) = (1/3)e^{-4x} + (2/3)e^{2x}$
- *Example 2* gives system $c_1 + c_2 = 1$, $e^{-4}c_1 + e^2c_2 = 0$ for coefficients; get solution $y(x) = (1 e^{-6})^{-1}e^{-4x} + (1 e^{6})^{-1}e^{2x}$

Two-point Boundary Value Problems: Numerical Approaches Bueler

lassical IVPs and 3VPs

serious example

finite difference

shooting

serious example: solved

just for practice: viewing solns with MATLAB/OCTAVE

```
x = 0:.001:1;
y1 = exp(-4*x); y2 = exp(2*x);
yIVP = (1/3)*y1 + (2/3)*y2;
yBVP = (1/(1-exp(-6)))*y1 + (1/(1-exp(6)))*y2;
plot(x,yIVP,x,yBVP), grid on
legend('IVP soln','BVP soln')
```



Two-point Boundary Value Problems: Numerical Approaches Bueler

lassical IVPs and BVPs

serious example

finite difference

shooting

serious example: solved

obvious name: "two-point BVP"

again:

Example 2: ODE BVP. find y(x) if

$$y'' + 2y' - 8y = 0,$$
 $y(0) = 1,$ $y(1) = 0$

- *Example 2* is called a "two-point BVP" because the solution is known at two points (duh!)
- a two-point BVP includes an ODE and the value of the solution at two different locations
- the ODE can be of any order, as long as it is at least *two*, because first-order ODEs cannot satisfy two conditions (generally)
- *but* there is no guarantee that a two-point BVP can be solved (see below), even though that is the usual case
- we will also be considering boundary value problems for PDEs in this course (i.e. problems including no initial values); these are "∞-point BVPs" I suppose

Two-point Boundary Value Problems: Numerical Approaches Bueler

lassical IVPs and VPs

serious example

finite difference

shooting

serious example: solved

recall: a standard manipulation of a 2nd order ODE Consider the general linear 2nd-order ODE:

$$y'' + p(x)y' + q(x)y = r(x)$$
 (1)

Also consider the (almost-completely) general 2nd-order ODE:

$$y'' = f(x, y, y')$$
 (2)

- these can be written as systems of coupled 1st-order ODEs
- in fact, equation (1) is equivalent to

$$\begin{pmatrix} y' \\ v' \end{pmatrix} = \begin{pmatrix} v \\ -p(x)v - q(x)y + r(x) \end{pmatrix}$$

• and equation (2) is equivalent to

$$\begin{pmatrix} \mathbf{y}'\\ \mathbf{v}' \end{pmatrix} = \begin{pmatrix} \mathbf{v}\\ f(\mathbf{x},\mathbf{y},\mathbf{v}) \end{pmatrix}$$

- first order systems are the form in which we can apply a numerical ODE solver to solve both IVPs and BVPs
- ... but BVPs generally require additional iteration

Two-point Boundary Value Problems: Numerical Approaches Bueler

classical IVPs and BVPs

serious example

finite difference

shooting

serious example: solved

why IVP are better problems than BVPs

- IVPs with well-behaved parts do have unique solutions
- we say they are "well-posed"; specifically:
- Theorem. Consider the system of ODEs

$$\mathbf{y} = \mathbf{f}(t, \mathbf{y}), \tag{3}$$

where $\mathbf{y}(t) = (y_1(t), \dots, y_d(t))$ and $\mathbf{f} = (f_1, \dots, f_d)$ are vector-valued functions. If \mathbf{f} is continuous for t in an interval around t_0 and for \mathbf{y} in some region around \mathbf{y}_0 , and if $\partial f_i / \partial y_j$ is continuous for the same inputs and for all i and j, then the IVP consisting of (3) and $\mathbf{y}(t_0) = \mathbf{y}_0$ has a unique solution $\mathbf{y}(t)$ for at least some small interval $t_0 - \epsilon < t < t_0 + \epsilon$ for some $\epsilon > 0$.

• given comments on last slide, the theorem covers IVPs for 2nd-order scalar ODEs

Two-point Boundary Value Problems: Numerical Approaches Bueler

lassical IVPs and 3VPs

serious example

finite difference

shooting

serious example: solved

warning about apparently-easy BVPs

Example 3: ODE BVP. find y(x) if

$$y'' + \pi^2 y = 0,$$
 $y(0) = 1,$ $y(1) = 0$

- this turns out to be impossible ... there is no such y(x)
- in fact, the general solution to the ODE is

$$y(x) = c_1 \cos(\pi x) + c_2 \sin(\pi x)$$

so the first boundary condition implies $c_1 = 1$ (because sin(0) = 0)

• ... but then the second condition says

"

$$0 = y(1) = -1 + c_2 \sin(\pi)$$
 "

and this has no solution because $sin(\pi) = 0$

 this is a constant-coefficient problem for which all the "parts" are "well-behaved"; we can even easily write down the general solution! Two-point Boundary Value Problems: Numerical Approaches Bueler

classical IVPs and BVPs

serious example

finite difference

shooting

serious example: solved

two-point BVPs related to eigenvalue problems

homogeneous linear two-point BVPs like

$$y'' + p(x)y' + q(x)y = \lambda y,$$
 $y(a) = 0, y(b) = 0$ (4)

are called Sturm-Liouville problems

- they are analogous to eigenvalue problems "Ax = λx" where the λ values and the vectors x are unknown
 - λ is an *eigenvalue*; there are finitely-many
 - $\mathbf{x} \neq \mathbf{0}$ is an *eigenvector* associated to λ
- in the Sturm-Liouville problem (4), the "matrix" is the operator

$$A = \frac{d}{dx} + p(x)\frac{d}{dx} + q(x)$$

(though the operator *A* must somehow also include the homogeneous boundary conditions)

- in (4) we seek eigenvalues $\lambda = \lambda_n$, which come in an infinite-but-countable list, and their associated eigen*functions* $y = y_n(x)$
- Sturm-Liouville theory "explains" the impossible case on the previous slide ... but this Sturm-Liouville thread will not be pursued further here ...

Two-point Boundary Value Problems: Numerical Approaches Bueler

lassical IVPs and 3VPs

serious example

finite difference

shooting

serious example: solved

Outline

1 classical IVPs and BVPs with by-hand solutions

- 2 a more serious example: a BVP for equilibrium heat
- Inite difference solution of two-point BVPs
- A shooting to solve two-point BVPs
- 5 a more serious example: solutions



wo-point Boundar
Value Problems:
Numerical
Approaches
Bueler

classical IVPs and BVPs serious example finite difference shooting serious example: solved

an equilibrium heat example

 as noted in lecture and by Morton & Mayers, a PDE like this is a general description of heat flow in a rod:

$$\rho c \frac{\partial u}{\partial t} = \frac{\partial}{\partial x} \left(k(x) \frac{\partial u}{\partial x} \right) + r(x)u + s(x)$$
(5)

recall that, roughly speaking, *ρ* is a density, *c* a specific heat, *k* a conductivity, *r*(*x*) a reaction coefficient (because *r*(*x*)*u* is the heat produced by a temperature-dependent chemical reaction, for example), and *s*(*x*) is an external (*u* independent) source of heat

Two-point Boundary Value Problems: Numerical Approaches Bueler

classical IVPs and BVPs

serious example

finite difference

shooting

serious example: solved

an equilibrium heat example, cont

• *equilibrium* means no change in time; the equilibrium version of (5) is this:

$$0 = \frac{\partial}{\partial x} \left(k(x) \frac{\partial u}{\partial x} \right) + r(x)u + s(x)$$

 because we can use ordinary derivative notation, and slightly-rearrange, the equilibrium eqaution is an ODE:

$$(k(x)u')' + r(x)u = -s(x)$$
 (6)

- let's suppose the rod has length *L*, and $0 \le x \le L$
- example boundary values are *(i)* insulation at the left end and *(ii)* pre-determined temperature at the right end:

$$u'(0) = 0, \qquad u(L) = 0$$
 (7)

Two-point Boundary Value Problems: Numerical Approaches Bueler

classical IVPs and BVPs

serious example

finite difference

shooting

serious example: solved

an equilibrium heat example, cont, cont

• some concrete, generally-non-constant choices in my example include *L* = 3 and:

$$k(x) = \frac{1}{2} \arctan(20(x-1)) + 1,$$

$$r(x) = r_0 = \frac{1}{2}, \qquad s(x) = e^{-(x-2)^2}$$





example, as code

code used to produce the previous picture

```
L = 3;

k = @(x) 0.5 * atan((x-1.0) * 20.0) + 1.0;

r0 = 0.5;

s = @(x) exp(-(x-2.0).^2);

J = 300;

dx = L / J;

x = 0:dx:L;

plot(x,k(x),x,r0*ones(size(x)),x,s(x))

grid on, xlabel x

legend('k(x)','r(x)=r_0','s(x)')
```



summary of "serious example"

 we now have a non-constant-coefficient boundary value problem to solve:

 $(k(x)u')' + r_0u = -s(x), \qquad u'(0) = 0, \quad u(3) = 0$ (8)

- *u*(*x*) represents the equilibrium distribution of temperature in a rod with these properties:
 - conductivity k(x): the first third [0, 1] is a material with much lower conductivity than the last two-thirds [2, 3]
 - reaction rate r₀ > 0: constant rate of linear-in-temperature heating
 - source term s(x): an external heat source concentrated around x = 2
- worth drawing a picture of the rod and its surroundings: shading for *k*(*x*), candles for *s*(*x*), insulated end, refrigerated end, ...
- a concrete *Question*: what is *u*(0), the temperature at the left end?

Two-point Boundary Value Problems: Numerical Approaches Bueler

classical IVPs and BVPs

serious example

finite difference

shooting

serious example: solved

plan from here

- introduce finite difference approach on really-easy "toy" two-point BVP
- 2 introduce shooting method on same toy problem
- 3 demonstrate both approaches on "serious problem"

classical IVPs and BVPs

serious example

finite difference

shooting

serious example: solved

Outline

Classical IVPs and BVPs with by-hand solutions

2 a more serious example: a BVP for equilibrium heat

3 finite difference solution of two-point BVPs

4 shooting to solve two-point BVPs

5 a more serious example: solutions



Two-point Boundary Value Problems: Numerical Approaches Bueler

classical IVPs and BVPs

serious example

finite difference

shooting

serious example: solved

finite differences

- finite difference methods for two-point BVPs generalize to PDEs ... as demonstrated in the rest of Math 615!
- but here we are just solving ODEs

 recall I showed this using a Taylor's-theorem-with-remainder argument:

$$\frac{f(x-h)-2f(x)+f(x+h)}{h^2}=f''(x)+\frac{f^{(4)}(\nu)}{12}h^2$$

Two-point Boundary Value Problems: Numerical Approaches Bueler

classical IVPs and BVPs

serious example

finite difference

shooting

serious example: solved

toy example problem

consider this easy BVP:

$$y'' = 12x^2, \qquad y(0) = 0, \quad y(1) = 0$$

- it has exact solution $y(x) = x^4 x$
- ... please check my last claim
- ... and be sure you could construct this exact solution by integrating

Two-point Boundary Value Problems: Numerical Approaches Bueler

classical IVPs and BVPs

serious example

finite difference

shooting

serious example: solved

toy example: approximated by finite differences

• cut up the interval [0, 1] into J subintervals:

$$\Delta x = 1/J$$

$$x_j = 0 + (j-1)\Delta x$$
 $(j = 1, ..., J+1)$

- note that my indices run from j = 1 to j = J + 1
- let Y_j be the approximation to $y(x_j)$
- for each of $j = 2, \ldots, J$ we approximate

$$y''=12x^2$$

by

$$\frac{Y_{j-1} - 2Y_j + Y_{j+1}}{\Delta x^2} = 12x_j^2$$

• the boundary conditions are: $Y_1 = 0$, $Y_{J+1} = 0$

Two-point Boundary Value Problems: Numerical Approaches Bueler

classical IVPs and BVPs

serious example

finite difference

shooting

serious example: solved

toy example: approximated by finite differences, cont

 so now we have a linear system of J + 1 equations in J + 1 unknowns:

 $Y_{1} = 0$ $Y_{1} - 2Y_{2} + Y_{3} = 12\Delta x^{2}x_{2}^{2}$ $Y_{2} - 2Y_{3} + Y_{4} = 12\Delta x^{2}x_{3}^{2}$ $\vdots \qquad \vdots$ $Y_{J-1} - 2Y_{J} + Y_{J+1} = 12\Delta x^{2}x_{J}^{2}$ $Y_{J+1} = 0$

Two-point Boundary Value Problems: Numerical Approaches Bueler

classical IVPs and BVPs

serious example

finite difference

shooting

serious example: solved

toy example: as matrix problem

• this is a matrix problem:

$$\begin{bmatrix} 1 & 0 & 0 & 0 & \dots & 0 \\ 1 & -2 & 1 & 0 & \dots & 0 \\ 0 & 1 & -2 & 1 & & 0 \\ \vdots & & & \ddots & & \\ & & & 1 & -2 & 1 \\ 0 & \dots & & 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} Y_1 \\ Y_2 \\ Y_3 \\ \vdots \\ Y_J \\ Y_{J+1} \end{bmatrix} = \begin{bmatrix} 0 \\ 12\Delta x^2 x_2^2 \\ 12\Delta x^2 x_3^2 \\ \vdots \\ 12\Delta x^2 x_J^2 \\ 0 \end{bmatrix}$$

Two-point Boundary Value Problems: Numerical Approaches Bueler

classical IVPs and BVPs

serious example

finite difference

shooting

serious example: solved

exercises

• i.e.

 $A\mathbf{Y} = \mathbf{b}$

toy example: as matrix problem in OCTAVE

- the matrix A is tridiagonal
- which is usually true of finite difference methods for two-point boundary value problems for second order ODEs
- A has lots of zero entries, so in MATLAB/OCTAVE we store it as a "sparse" matrix
- this means that the *locations* of nonzero entries, and the matrix entries at those locations, are stored; this saves space
- also there are "expert systems" in MATLAB/OCTAVE which recognize sparsity and then try to exploit it to speed up matrix/vector operations
- practical MATLAB/OCTAVE advice: learn how to use spy and full to see these sparse matrix structures

Two-point Boundary Value Problems: Numerical Approaches Bueler

classical IVPs and BVPs

serious example

finite difference

shooting

serious example: solved

toy example: as matrix problem in OCTAVE, cont

setting up the matrix problem looks like:

```
J = 10; dx = 1/J; x = (0:dx:1)';
b = zeros(J+1,1);
b(2:J) = 12 * dx^2 * x(2:J).^2;
A = sparse(J+1,J+1);
A(1,1) = 1.0; A(J+1,J+1) = 1.0;
for j=2:J
    A(j,[j-1, j, j+1]) = [1, -2, 1];
end
```

• solving the matrix problem looks like:

 $Y = A \setminus b$; % solve A Y = b

plot on next page from

```
% also get exact soln on fine grid:
xf = 0:1/1000:1; yexact = xf.^4 - xf;
plot(x,Y,'o','markersize',12,xf,yexact)
grid on, xlabel x, legend('finite diff','exact')
```

Two-point Boundary Value Problems: Numerical Approaches Bueler

classical IVPs and BVPs

serious example

finite difference

shooting

serious example: solved

toy example: as matrix problem in OCTAVE, cont, cont

 gives result which is better than we have any reason to expect:



Two-point Boundary Value Problems: Numerical Approaches Bueler

classical IVPs and BVPs

serious example

finite difference

shooting

serious example: solved

toy example with finite differences: brief analysis

regarding how the result on the previous slide can be so suspiciously nice:

- recall that the *exact* solution is $y(x) = x^4 x$
- recall we had

$$\frac{f(x-h)-2f(x)+f(x+h)}{h^2}=f''(x)+\frac{f^{(4)}(\nu)}{12}h^2$$

applied to f(x) = y(x), for which y⁽⁴⁾(x) = 24 is constant, we see that the finite difference approximation to the second derivative in the ODE y'' = 12x² has error at most

$$\frac{y^{(4)}(\nu)}{12}\Delta x^2 = \frac{24}{12}(0.1)^2 = 0.02$$

because $\Delta x = 0.1$

• this is a rare case where the *local truncation error* is a known constant ... and fairly small

Two-point Boundary Value Problems: Numerical Approaches Bueler

classical IVPs and BVPs

serious example

finite difference

shooting

serious example: solved

toy example with finite differences: brief analysis, cont

- let $e_j = Y_j y(x_j)$
- by subtraction,

$$rac{e_{j-1}-2e_j+e_{j+1}}{\Delta x^2}=0.02$$

and $e_0 = e_{J+1} = 0$

so (after bit of not-too-hard thought)

$$e_j = 0.01 x_j (x_j - 1)$$

SO

$$\max_{j} |Y_{j} - y(x_{j})| = \max_{j} |e_{j}| = 0.0025$$

• which explains why picture a few slides back was good ... but showed slight errors close to screen resolution

Two-point Boundary Value Problems: Numerical Approaches Bueler

classical IVPs and BVPs

serious example

finite difference

shooting

serious example: solved

Outline

Classical IVPs and BVPs with by-hand solutions

- 2 a more serious example: a BVP for equilibrium heat
- Inite difference solution of two-point BVPs
- 4 shooting to solve two-point BVPs
- 5 a more serious example: solutions



Two-point Boundary Value Problems: Numerical Approaches Bueler

classical IVPs and BVPs

serious example

finite difference

shooting

serious example: solved

toy example problem again: shooting

• recall this "toy" ODE BVP:

$$y'' = 12x^2, \qquad y(0) = 0, \quad y(1) = 0$$

(which has exact solution $y(x) = x^4 - x$)

- this time we think: *if only it were an ODE IVP then we could apply a numerical ODE solver like* ode45 *or* lsode
- indeed, this ODE IVP

$$w'' = 12x^2, \qquad w(0) = 0, \quad w'(0) = A$$

can be solved by a numerical ODE solver, for any A

- solving this ODE IVP involves "aiming" by guessing an initial slope w'(0) = A
- ... and "hitting the target" is getting the desired boundary value w(1) = 0 correct, so that y(x) = w(x) in that case

Two-point Boundary Value Problems: Numerical Approaches Bueler

classical IVPs and BVPs

serious example

finite difference

shooting

serious example: solved

toy example shooting, cont

 for illustrating the method, I'll skip the use of a numerical ODE solver because the ODE IVP

$$w'' = 12x^2, \qquad w(0) = 0, \quad w'(0) = A$$

has a solution we can get by-hand:

$$w(x) = x^4 + Ax$$

• plotting for A = -2.5, -1.5, -0.5, 0.5, 1.5 gives this figure:



Two-point Boundary Value Problems: Numerical Approaches Bueler

classical IVPs and BVPs

serious example

finite difference

shooting

serious example: solved

toy example shooting, cont, cont

- we have "aimed" (by choosing A) and "shot" five times
- "shot" = (computed the solution to an ODE IVP); generally this would be solving the ODE IVP numerically
- we missed every time
- but we have bracketed the correct right-hand boundary condition y(1) = 0 with the two values A = -1.5 and A = -0.5
- a numerical *equation* solver can refine the search to converge to the correct *A* value . . . which we know would by A = -1 in this case
- ... the last idea is best illustrated by example

Two-point Boundary Value Problems: Numerical Approaches Bueler

classical IVPs and BVPs

serious example

finite difference

shooting

serious example: solved

shooting: solving the boundary condition equation

recall our ODE BVP

 $y'' = 12x^2, \qquad y(0) = 0, \quad y(1) = 0$

is replaced by this ODE IVP when "shooting":

$$w'' = 12x^2, \qquad w(0) = 0, \quad w'(0) = A$$

• the x = 1 endpoint value of w(x) is a function of A:

$$F(A) = (w(1), \text{ where } w \text{ solves } (9))$$

• and so we solve this equation because we want y(1) = 0:

$$F(A) = 0$$

- in this easy problem, $w(x) = x^4 + Ax$
- so we solve F(A) = 1 + A = 0 and get A = -1
- generally we solve *F*(*A*) = 0 numerically, e.g. by the *bisection* or *secant* methods

Two-point Boundary Value Problems: Numerical Approaches Bueler

classical IVPs and BVPs

serious example

finite difference

shooting

(9)

serious example: solved

shooting: general strategy for two-point ODE BVPs

- identify one end of the interval x = b as the target
- at the other end *x* = *a*, identify some additional initial conditions which would give a well-posed ODE IVP
- for various guesses of those additional initial conditions,
 "shoot" by solving the corresponding ODE IVP from x = a to x = b
- ask whether you "hit the target" by asking whether the boundary conditions at *x* = *b* are satisfied
- automate the adjustment process by using an equation solver (e.g. bisection or secant method) on the equation that says "the discrepancy between the solution of the ODE IVP at *x* = *b* and the desired boundary conditions at *x* = *b*, as a function of the additional initial conditions, should be zero: *F*(*A*) = 0"

Two-point Boundary Value Problems: Numerical Approaches Bueler

classical IVPs and BVPs

serious example

finite difference

shooting

serious example: solved

Outline

Classical IVPs and BVPs with by-hand solutions

- 2 a more serious example: a BVP for equilibrium heat
- Inite difference solution of two-point BVPs
- 4 shooting to solve two-point BVPs
- **5** a more serious example: solutions



Two-point Boundary Value Problems: Numerical Approaches Bueler

classical IVPs and BVPs

serious example

finite difference

shooting

serious example: solved

recall the serious example

• recall the "serious" non-constant-coefficient BVP:

$$(k(x)u')' + r_0u = -s(x), \qquad u'(0) = 0, \quad u(3) = 0,$$
 (10)

- *u*(*x*) is the equilibrium temperature in a rod
- the conductivity k(x) has a big jump at x = 1 and the heat source s(x) is concentrated at x = 2:



Two-point Boundary Value Problems: Numerical Approaches Bueler

classical IVPs and BVPs

serious example

finite difference

shooting

serious example: solved

finite differences: need staggered grid

- finite difference approach first
- as before: *J* subintervals, $\Delta x = 1/J$, and

$$x_j = (j - 1)\Delta x$$
 for $j = 1, ..., J + 1$

- let U_j be our finite diff. approx. to $u(x_j)$
- let $k_j = k(x_j)$ and $s_j = s(x_j)$; we know these exactly
- note: if q(x) = -k(x)u'(x)—think Fourier!—then we are solving

$$-q'+r_0u=-s(x)$$

· the finite difference version looks like

$$-\frac{q_{j+1/2}-q_{j-1/2}}{\Delta x}+r_0U_j=-s(x_j)$$

• or

$$\frac{k(x_{j+1/2})\frac{U_{j+1}-U_{j}}{\Delta x}-k(x_{j-1/2})\frac{U_{j}-U_{j-1}}{\Delta x}}{\Delta x}+r_{0}U_{j}=-s(x_{j})$$

Two-point Boundary Value Problems: Numerical Approaches Bueler

classical IVPs and BVPs

serious example

finite difference

shooting

serious example: solved

finite differences: need staggered grid, cont

• ... or (just notation)

$$\frac{k_{j+\frac{1}{2}}(U_{j+1}-U_j)-k_{j-\frac{1}{2}}(U_j-U_{j-1})}{\Delta x^2}+r_0U_j=-s_j$$

or (clear denominators)

$$k_{j+\frac{1}{2}}(U_{j+1}-U_j)-k_{j-\frac{1}{2}}(U_j-U_{j-1})+r_0\Delta x^2 U_j=-s_j\Delta x^2$$

or

$$k_{j-\frac{1}{2}}U_{j-1} - \left(k_{j-\frac{1}{2}} + k_{j+\frac{1}{2}} - r_0\Delta x^2\right)U_j + k_{j+\frac{1}{2}}U_{j+1} = -s_j\Delta x^2$$

- like the "toy" example earlier, this last form is a tridiagonal matrix equation AU = b
- note we actually evaluate the conductivity k(x), and the flux q, on the staggered grid
- the deeper reason *why* we use the staggered grid will be revealed later in class ...

Two-point Boundary Value Problems: Numerical Approaches Bueler

classical IVPs and BVPs

serious example

finite difference

shooting

serious example: solved

finite differences: remember the boundary conditions

- recall we have boundary condition u'(0) = 0
- approximate this by

$$\frac{U_2 - U_1}{\Delta x} = 0$$

or

 $-U_1 + U_2 = 0$

- we will see there is a more-accurate way later ...
- also we have u(L) = 0 so

$$U_{J+1}=0$$

Two-point Boundary Value Problems: Numerical Approaches Bueler

classical IVPs and BVPs

serious example

finite difference

shooting

serious example: solved

finite differences for the "serious problem"

- now for an actual code: see varheatFD.m online
- the ODE setup:

```
L = 3;

k = @(x) 0.5 * atan((x-1.0) * 20.0) + 1.0;

s = @(x) exp(-(x-2.0).^2);

r0 = 0.5;

dx = L / J;

x = (0:dx:L)'; % regular grid

xstag = ((dx/2):dx:L-(dx/2))'; % staggered grid

kstag = k(xstag); % k(x) on staggered grid
```

• the matrix problem setup:

```
% right side is J+1 length column vector
b = [0;
        - dx^2 * s(x(2:J));
      0];
% matrix is tridiagonal
A = sparse(J+1,J+1);
A(1,[1 2]) = [-1.0 1.0];
for j=1:J-1
      A(j+1,j) = kstag(j);
      A(j+1,j+1) = - kstag(j) - kstag(j+1) + r0 * dx^2;
      A(j+1,J+1) = 1.0;
```

Two-point Boundary Value Problems: Numerical Approaches Bueler

classical IVPs and BVPs

serious example

finite difference

shooting

serious example: solved

finite differences for the "serious problem", cont

 it is good to use "spy (A)" at this point to see the matrix structure; this is the J = 10 case



Two-point Boundary Value Problems: Numerical Approaches Bueler

classical IVPs and BVPs

serious example

finite difference

shooting

serious example: solved

finite differences for the "serious problem", cont, cont

the matrix solve:

 $U = A \setminus b$; % soln is J+1 column vector

the plot details:

```
figure(1)
plot(x,k(x),'r',x,s(x),'b',...
        x,U','g*','markersize',3)
grid on, xlabel x
legend('k(x)','s(x)','solution U_j')
```

Two-point Boundary Value Problems: Numerical Approaches Bueler

classical IVPs and BVPs

serious example

finite difference

shooting

serious example: solved

finite difference solution to "serious problem"

• the picture when J = 60:



Two-point Boundary Value Problems: Numerical Approaches Bueler

classical IVPs and BVPs

serious example

finite difference

shooting

serious example: solved

finite difference solution to "serious problem", cont

- recall our concrete goal was to estimate u(0)
- clearly we should try different *J* values to estimate:

J	estimate of $u(0)$
10	-13.86507
20	-7.20263
60	-5.66666
200	-5.27443
1000	-5.15199
4000	-5.12965

Two-point Boundary Value Problems: Numerical Approaches Bueler

classical IVPs and BVPs

serious example

finite difference

shooting

serious example: solved

- this suggests that $u(0) \approx -5.13$
- How do we know how wrong we are?

shooting for the "serious problem"

shooting is implemented these codes online:

- varheatSHOOT.m: OCTAVE version using lsode
- varheatSHOOTmat.m: MATLAB version using ode45
- the setup (OCTAVE version):

```
L = 3;

k = 0(x) = 0.5 + atan((x-1.0) + 20.0) + 1.0;

s = 0(x) = xp(-(x-2.0).^2);

r0 = 0.5;

% ODE Y' = G(Y,x) is described by this right-hand side:

G = 0(Y,x) = -Y(2) + k(x); % Y(1) = u

r0 + Y(1) + s(x)]; % Y(2) = q

% bracket unknown u(0)

a = -10.0; % produces u(3) which is too high

b = 0.0; % ... u(3) which is too low
```

Two-point Boundary Value Problems: Numerical Approaches Bueler

classical IVPs and BVPs

serious example

finite difference

shooting

serious example: solved

shooting for the "serious problem", cont

• the *bisection* implementation (OCTAVE version), which starts from initial bracket [a, b] = [-10.0, 0.0]:

```
serious example
N = 100:
                                                             finite difference
for n = 1:N
                                                             shooting
  fprintf('.')
  c = (a+b)/2;
   evaluate F(c) = (estimate of u(3) using u(0)=c)
                                                             exercises
  Y = 1sode(G, [c; 0.0], [0.0 3.0]);
  F = Y(2, 1):
  if abs(F) < 1e-12
    break % we are done
  elseif F \ge 0.0
    a = c;
  else
   b = c;
  end
end
```

Two-point Boundary

Value Problems: Numerical Approaches Bueler

classical IVPs and BVPs

shooting for the "serious problem", cont

• the finish:

```
% redo to get final version on a grid for plot
x = 0:0.05:3.0;
Y = lsode(G,[c; 0.0],x);
u = Y(:,1)';
q = Y(:,2)';
figure(2)
plot(x,k(x),'r',x,s(x),'b',x,u,'g*',x,q,'k')
grid on, xlabel x
legend('k(x)','s(x)','u(x)','g(x)')
```

Two-point Boundary Value Problems: Numerical Approaches Bueler

classical IVPs and BVPs

serious example

finite difference

shooting

serious example: solved

shooting solution to "serious problem"

• the picture:



Two-point Boundary Value Problems: Numerical Approaches Bueler



- default use of lsode gives estimate u(0) = -5.14443
 - How do we know how wrong we are?

minimal conclusion

- finite difference and shooting methods give comparable solutions to this "serious problem"
- closer inspection of the programs above will help understand the methods
- better understanding will also follow from doing the exercises 1 through 5 on the last three slides
- ... which forms Assignment # 3

wo-point Boundary
Value Problems:
Numerical
Approaches
Bueler

classical IVPs and BVPs

serious example

finite difference

shooting

serious example: solved

Outline

Classical IVPs and BVPs with by-hand solutions

- 2 a more serious example: a BVP for equilibrium heat
- Inite difference solution of two-point BVPs
- 4 shooting to solve two-point BVPs
- 5 a more serious example: solutions



Two-point Boundary Value Problems: Numerical Approaches Bueler

classical IVPs and BVPs

serious example

finite difference

shooting

serious example: solved

exercises

1 Solve by-hand this ODE BVP to find y(x):

$$y'' + 2y' + 2y = 0,$$
 $y(0) = 1,$ $y(1) = 0.$

2 Recall Example 3, an impossible-to-solve ODE BVP. Nonetheless there are some values of A in the following problem which allow a solution: find y(x) if

$$y'' + \pi^2 y = 0,$$
 $y(0) = 1,$ $y(1) = A.$

What values of *A* are allowed? For an allowed value of *A*, how many solutions are there?

3 Equation (6) has non-constant coefficients, and essentially it cannot be solved exactly by hand. To develop some sense of the effect of the source term s(x), solve by-hand this ODE BVP

$$(k_0 u')' = -s(x), \qquad u'(0) = 0, \quad u(L) = 0,$$

merely assuming the source is quadratic ($s(x) = ax^2 + bx + c$) and the conductivity is constant ($k_0 > 0$). Compute by-hand u(0). How does the solution u(x) depend on s(x)? (*For example*, how does *u* depend on the sign, values, slope, or concavity of s(x)?) Two-point Boundary Value Problems: Numerical Approaches Bueler

classical IVPs and BVPs

serious example

finite difference

shooting

serious example: solved

exercises, cont

4 Apply the finite difference method to solve this ODE BVP:

$$y'' + \sin(5x)y = x^3 - x,$$
 $y(0) = 0,$ $y(1) = 0.$

In particular, use J = 10, $\Delta x = 1/J$, and $x_j = j\Delta x$ for j = 0, ..., J. Construct the system

 $A\mathbf{y} = \mathbf{b}$

where *A* is a $(J + 1) \times (J + 1)$ matrix, $\mathbf{y} = \{Y_j\}$ approximates the unknowns $\{y(x_j)\}$, and **b** contains the right-side function " $x^3 - x$ " in the ODE. Arrange things so that the first equation in the system represents the boundary condition "y(0) = 0" and the last equation the condition "y(1) = 0". The remaining equations in the system will each hold finite difference approximations of the ODE. Show me your matrix *A* in a non-wasteful way. Solve the system to find \mathbf{y} , and plot it appropriately. Also write a few sentences addressing how to know qualitatively and quantitatively the degree to which your answer is a good approximation.

Two-point Boundary Value Problems: Numerical Approaches Bueler

classical IVPs and BVPs

serious example

finite difference

shooting

serious example: solved

exercises, cont, cont

(The goal of this problem is to understand shooting, though you will not quite put all parts together ...)
 Consider the nonlinear ODE BVP

$$u'' + u^3 = 0,$$
 $u(0) = 1,$ $u(1) = 0.$

This problem is well-suited to the shooting method. Specifically, write a MOP program that uses an ODE solver to solve the following ODE *IVP*

$$u'' + u^3 = 0,$$
 $u(0) = 1,$ $u'(0) = A$

for each of the eleven values A = -5, -4, ..., 4, 5. Plot all eleven solutions, and identify on the plot¹ the *A* value for each curve. Which two *A* values make the computed value u(1) bracket the desired value (boundary condition) "u(1) = 0"?

(With this information in hand you could make a program like varheatSHOOT.m, which uses bisection to converge to an A value so that $u(1) \approx 0$ to many-digit-accuracy.)

Two-point Boundary Value Problems: Numerical Approaches Bueler

classical IVPs and BVPs

serious example

finite difference

shooting

serious example: solved

¹Possibly using the text command in MATLAB/OCTAVE.