Two-point Boundary Value Problems: Numerical Approaches

Math 615, Spring 2014

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

Outline

classical ODE problems: IVP vs BVP

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

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

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

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

classical ODE problems: IVP vs BVP

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

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

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

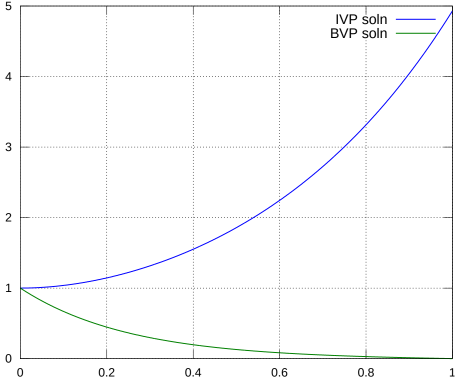
- both problems can be solved by hand
- in fact, the ODE has constant coefficients so we can find *characteristic polynomial* and *general solution* . . . like this: if $y(x) = e^{rx}$ then $r^2 + 2r - 8 = (r + 4)(r - 2) = 0$ so

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

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

viewing solns with MATLAB

```
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')
```



obvious name: “two-point BVP”

- *Example 2* above is called a “two-point BVP”
- a two-point BVP includes an ODE and the value(s) 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)
- we will also consider boundary value problems for PDEs in this course (i.e. problems including no initial values)

a standard manipulation of a 2nd order ODE

Consider the general linear 2nd-order ODE:

$$y'' + p(x)y' + q(x)y = r(x) \tag{1}$$

Also consider the general 2nd-order ODE:

$$y'' = f(x, y, y') \tag{2}$$

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

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

- equation (2) is equivalent to

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

- first order systems are the form in which to apply a numerical ODE solver

why IVP are *better* problems than BVPs

- IVPs have unique solutions
- we say they are "well-posed"; specifically:

Theorem

Consider the system of ODEs

$$\frac{d\mathbf{y}}{dt} = \mathbf{f}(t, \mathbf{y}), \qquad (3)$$

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, this theorem also covers IVPs for 2nd-order scalar ODEs

warning about apparently-easy BVPs

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

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

- 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 $c_1 = 1$
- ... but then the second condition says

$$\text{“} \qquad 0 = y(1) = -1 + c_2 \sin(\pi) \qquad \text{”}$$

  and this has no solution because $\sin(\pi) = 0$
- this is a constant-coefficient problem for which all the “parts” are “well-behaved” ... but it is a BVP

Outline

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:

$$\rho c \frac{\partial u}{\partial t} = \frac{\partial}{\partial x}\left(k(x)\frac{\partial u}{\partial x}\right) + r(x)u + s(x) \qquad (4)$$

- recall that, roughly speaking, ρ is a density, c a specific heat, $k(x)$ a conductivity, $r(x)$ a reaction coefficient, and $s(x)$ is an external source of heat

an equilibrium heat example, cont

- *equilibrium* means no change in time; the equilibrium version of (4) is this:

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

- we can use ordinary derivative notation; the equilibrium equation is an ODE:

$$(k(x)u')' + r(x)u = -s(x) \tag{5}$$

- suppose the rod has length L
- example boundary values are *(i)* insulation at the left end and *(ii)* zero temperature at the right end:

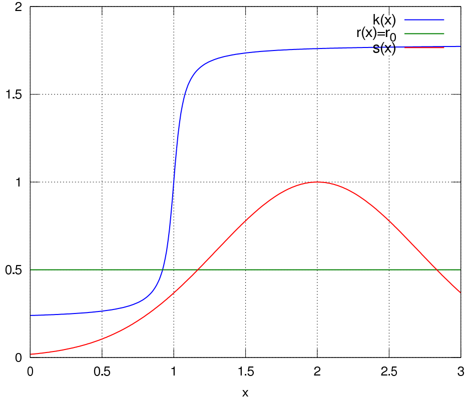
$$u'(0) = 0, \qquad u(L) = 0 \tag{6}$$

an equilibrium heat example, cont

- some concrete choices in my example include $L = 3$ and:

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

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



an equilibrium heat example, cont

- 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)')
```

an equilibrium heat example, cont

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

$$(k(x)u')' + r_0 u = -s(x), \qquad u'(0) = 0, \quad u(3) = 0 \quad (7)$$

- $u(x)$ 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 $r_0 > 0$: constant rate of linear-in-temperature heating
  - source term $s(x)$: an external heat source concentrated around $x = 2$
- *Question*: what is $u(0)$, the temperature at the left end?
- I will call this my "serious problem", and solve it numerically two different ways

plan from here

1. 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”

Outline

1. classical IVPs and BVPs with by-hand solutions
2. a serious problem: 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

finite differences

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

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

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
- make sure you could solve this yourself!

toy example: approximated by finite differences

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

$$\Delta x = 1/J$$

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

- 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 $j = 2, \dots, J$ 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: $Y_1 = 0,\ Y_{J+1} = 0$

toy example: approximated by finite differences, cont

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

$$\begin{aligned} Y_1 &= 0 \\ Y_1 - 2Y_2 + Y_3 &= 12x_2^2\Delta x^2 \\ Y_2 - 2Y_3 + Y_4 &= 12x_3^2\Delta x^2 \\ \vdots \quad &\quad \vdots \\ Y_{J-1} - 2Y_J + Y_{J+1} &= 12x_J^2\Delta x^2 \\ Y_{J+1} &= 0 \end{aligned}$$

toy example: as matrix problem

- this is a matrix problem:

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

- 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
- use MATLAB's `sparse` to store it
- the *locations* of nonzero entries, and the nonzero values, are stored; this saves space
- the backslash command in MATLAB is an "expert system"
  - recognizes sparsity pattern
  - exploits it to speed up matrix/vector operations
- use `spy` and `full` to see sparse matrices

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:

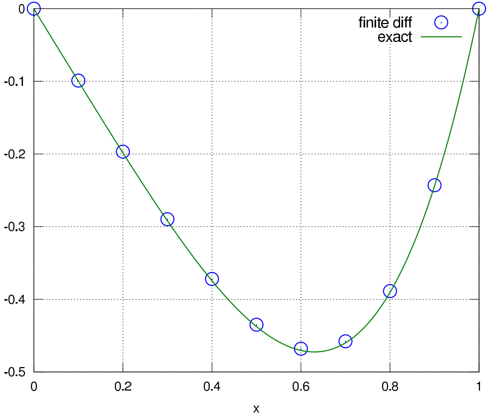
```
Y = A \ b;   % solve A Y = b
```

- 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')
```

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

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



toy example with finite differences: brief analysis

regarding the result on the previous slide:

- recall the *exact* solution is $y(x) = x^4 - x$
- and

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

- applied to $f(x) = y(x)$, for which $y^{(4)}(x) = 24$, we see that the finite difference approximation to the second derivative in the ODE $y'' = 12x^2$ 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 truncation error is known!

toy example with finite differences: brief analysis, cont

- let $e_j = Y_j - y(x_j)$, the *error* we care about
- by subtraction,

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

  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 the picture a few slides back was good …but showed slight errors close to screen resolution

Outline

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* MATLAB's `ode45`
- 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 $w'(0) = A$
- "hitting the target" is getting the desired boundary value $w(1) = 0$
- "aiming" and "hitting the target" is *shooting*

toy example shooting, cont

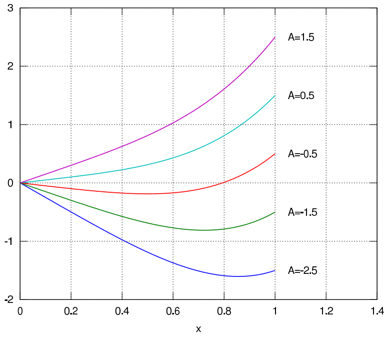
- for illustrating the method on this easy problem, I'll skip using a numerical ODE solver because the ODE IVP

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

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:



toy example shooting, cont, cont

- we have "aimed" (by choosing A) and "shot" five times
- a "shot" is a computation of the solution to an ODE IVP
  - generally this would be a numerical solution
- on previous slide 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

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":

$$w'' = 12x^2, \qquad w(0) = 0, \quad w'(0) = A \tag{8}$$

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

$$F(A) = \Big(w(1), \text{ where } w \text{ solves } (8)\Big)$$

- 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

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 condition A, should be zero: $F(A) = 0$"

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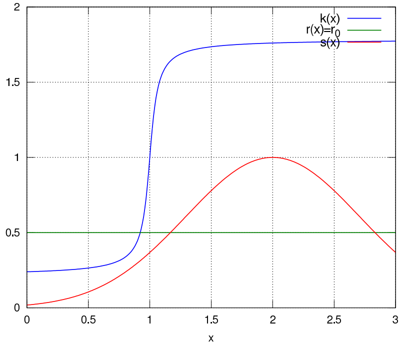
recall the serious example

- recall the “serious” non-constant-coefficient BVP:

$$(k(x)u')' + r_0 u = -s(x), \qquad u'(0) = 0, \quad u(3) = 0, \quad (9)$$

- $u(x)$ 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 near $x = 2$:



finite differences: need staggered grid

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

$$x_j = (j-1)\Delta x \qquad \text{for } j = 1, \dots, J+1$$

- 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 $q(x) = -k(x)u'(x)$, i.e. Fourier's law for heat flow, then we are solving

$$-q' + r_0 u = -s(x)$$

- the finite difference version looks like

$$-\frac{q_{j+1/2} - q_{j-1/2}}{\Delta x} + r_0 U_j = -s(x_j)$$

- or

$$\frac{k(x_{j+1/2})\frac{U_{j+1}-U_j}{\Delta x} - k(x_{j-1/2})\frac{U_j - U_{j-1}}{\Delta x}}{\Delta x} + r_0 U_j = -s(x_j)$$

finite differences: need staggered grid, cont

- or

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

- 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 $A\mathbf{U} = \mathbf{b}$
- note we evaluate the conductivity $k(x)$, and the flux q, on the staggered grid (i.e. $x_{j+\frac{1}{2}}$ and $x_{j-\frac{1}{2}}$)
- the deeper reason *why* we use the staggered grid will be revealed later in class . . .

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

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

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
```

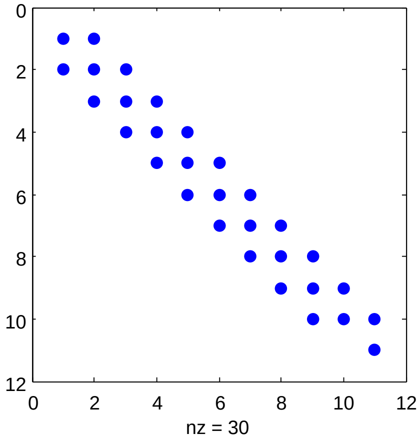
- the matrix problem setup:

```
% 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+2) = kstag(j+1);
end
A(J+1,J+1) = 1.0;
```

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



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

- the matrix solve:

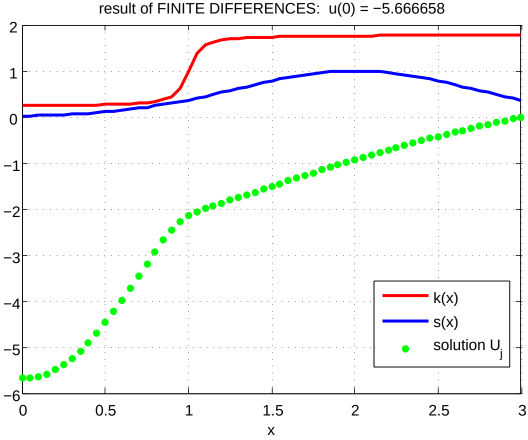
```
U = A \ b;        % soln is J+1 column vector
```

- 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')
```

finite difference solution to “serious problem”

- the picture when $J = 60$:



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

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

shooting for the "serious problem"

- shooting is implemented in this code online:
  - `varheatSHOOT.m`
- the 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;

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

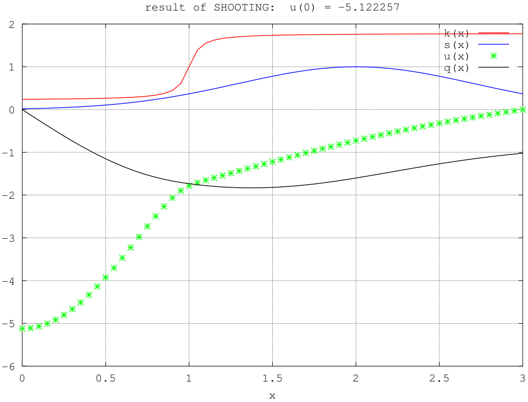
shooting for the "serious problem", cont

- the *bisection* implementation, which starts from initial bracket $[a, b] = [-10.0, 0.0]$:

```
N = 100;
for n = 1:N
  c = (a+b)/2;
  [xout,Y] = ode45(G,[0.0 3.0],[c; 0.0]);
  F = Y(end,1);
  if abs(F) < 1e-12
    break  % we are done
  elseif F >= 0.0
    a = c;
  else
    b = c;
  end
end
```

shooting solution to “serious problem”

- the picture:



- default use of `ode45` gives estimate $u(0) = -5.122257$
- *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 on Assignment # 5