Boundary-value problems for ODEs

General case: $\vec{y}\,'=\vec{f}\,(\vec{y},x)$

(As a reminder, can reduce higher-order equations to a 1st order set.)

Needs to be solved for $a\leq x\leq b$ given some conditions at *a* and *b*:

$$\vec{p}\,(\vec{y}(a),\vec{y}(b))=0$$

Even more generally, conditions at some points between *a* and *b* may be specified (multipoint problems).

Most important in physics: second order equation

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

in particular, the linear case $y''+g(x)y'+k(x)y=s(x)$

with boundary conditions $y(a)=C_1;\ y(b)=C_2$ (Dirichlet or first type)

$y'(a)=C_1;\ y'(b)=C_2$ (Neumann or second type)

$r_1 y(a)+s_1 y'(a)=C_1;\ r_2 y(b)+s_2 y'(b)=C_2$ (Robin or third type)

or a mixture of different types.

Often arise as steady-state equations.

Advection-diffusion: flux $j = v(x)c(x) - D(x)\frac{\partial c(x)}{\partial x}$ *c* is the particle concentration

Continuity equation $\frac{\partial c}{\partial t} + \frac{\partial j}{\partial x} = 0 \Rightarrow$

$$\frac{\partial c}{\partial t} = -\frac{\partial (v(x)c(x))}{\partial x} + \frac{\partial}{\partial x}\left[D(x)\frac{\partial c(x)}{\partial x}\right]$$

$$\frac{\partial c}{\partial t} = 0 \quad \Rightarrow \quad \frac{d}{dx}\left[D(x)\frac{dc(x)}{dx}\right] - \frac{d(v(x)c(x))}{dx} = 0$$

Confined between 2 walls, at *a* and *b*. Absorbing wall – c = 0 (Dirichlet).

Impenetrable wall – j = 0 (Robin; Neumann when v=0), in which case

$$v(x)c(x) - D(x)\frac{dc(x)}{dx} = 0 \quad \Rightarrow \quad c(x) = c_0 \exp\left(\int \frac{v(x)}{D(x)}dx\right)$$

This is the Boltzmann distribution, since $v/D = F/k_B T$ (Einstein relation).

Poisson equation for the electrostatic potential

$$\nabla^2 \phi = -\rho/\epsilon_0$$

If the charge distribution is spherically symmetric, $\rho = \rho(r)$,

$$\frac{d^2\phi}{dr^2} + \frac{2}{r}\frac{d\phi}{dr} = -\rho(r)/\epsilon_0$$

Substitute $\phi = y/r$. $\quad \frac{d\phi}{dr} = \frac{1}{r}\frac{dy}{dr} - \frac{y}{r^2}; \quad \frac{d^2\phi}{dr^2} = \frac{1}{r}\frac{d^2y}{dr^2} - \frac{2}{r^2}\frac{dy}{dr} + \frac{2y}{r^3}$

$$\frac{1}{r}\frac{d^2y}{dr^2} = -\rho(r)/\epsilon_0$$

If there is a point charge q at the centre, $y(0)=q/(4\pi\varepsilon_0)$.

Related: eigenvalue (or Sturm-Liouville) problem

$$-\frac{d}{dx}\left[p(x)\frac{dy}{dx}\right]+q(x)y=\lambda w(x)y$$

$$r_1 y(a)+s_1 y'(a)=0;\ r_2 y(b)+s_2 y'(b)=0$$

Solutions only exist for specific $\lambda = \lambda_i$, in which case they are defined up to an arbitrary factor.

Often arise from time-dependent equations after separation of variables.

String vibrations

$$\rho\frac{\partial^2 u}{\partial t^2}=T\frac{\partial^2 u}{\partial x^2}$$

ρ is the linear mass density, T is the tension

$$u(x,t)=e^{i\omega t}y(x) \qquad -\frac{d^2 y}{dx^2}=\frac{\rho\omega^2}{T}y \qquad \lambda=\frac{\rho\omega^2}{T}$$

$$y(0)=y(L)=0$$

Time-independent Schrödinger equation

1D: $$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2}+U(x)\psi=E\psi$$

If infinitely high walls, 0 at the walls; otherwise, 0 at infinity.

3D: for a spherically symmetric potential *U*(*r*),

$$\psi(r,\theta,\phi)=\frac{1}{r}R(r)Y_{lm}(\theta,\phi)$$

$$R''(r)+\frac{2m}{\hbar^2}\left[E-\frac{\hbar^2 l(l+1)}{2mr^2}-U(r)\right]R(r)=0$$

Again, no first derivative.

At 0, R(r) never grows faster than $1/\sqrt{r}$, so R(0)=0. Also, for bound states, R(∞)=0.

Sometimes higher-order equations do arise. Beam deflection equation.:

$$\frac{d^4y}{dx^2}=\frac{w(x)}{EI}$$

w(x) – load; E – Young's modulus, I – moment of inertia

$$y''+g(x)y'+k(x)y=s(x)$$

For simplicity, consider Dirichlet problem $y(a)=C_1;\ y(b)=C_2$

Know how to solve the initial value problem, i.e., if both y(a) and y'(a) are known. $y'=z;\ z'=-g(x)z-k(x)y+s(x)$ Solve, e.g., using RK4.

But, of course, we do not know y'(a). Let us guess: take $y'(a)=A^{(0)}$. Solve the initial value problem, get $y(b) = B^{(0)}$. In general, $B^{(0)}\neq C_2$. Take another guess $y'(a)=A^{(1)}$. Get $y(b)=B^{(1)}$. Etc. We see that y(b) is some function of y'(a): **y(b) = F[y'(a)]**. We can calculate the value of this function for any argument. The correct value of y'(a) is the solution of the equation

$$F[y'(a)]=C_2$$

Solve it using the secant method. We have $F[A^{(0)}]=B^{(0)};\ F[A^{(1)}]=B^{(1)}$.

The next approximation to the root is $A^{(2)}=\dfrac{A^{(0)}(B^{(1)}-C_2)+A^{(1)}(C_2-B^{(0)})}{B^{(1)}-B^{(0)}}$

In principle, should continue until iterations converge, but ...

$$y''+g(x)y'+k(x)y=s(x) \qquad y(a)=C_1;\; y(b)=C_2$$

But our problem is linear! Suppose $y^{(0)}$ is the solution with $y(a)=C_1$ and $y'(a)=A^{(0)}$; $y^{(1)}$ is the solution with $y(a)=C_1$ and $y'(a)=A^{(1)}$. Then $y=(1-\theta)y^{(0)}+\theta y^{(1)}$ is the solution with $y(a)=C_1$ and $y'(a)=(1-\theta)A^{(0)}+\theta A^{(1)}$. Our next iteration has $y(a)=C_1$ and $y'(a)=A^{(1)}=$

$$\frac{A^{(0)}(B^{(1)}-C_2)+A^{(1)}(C_2-B^{(0)})}{B^{(1)}-B^{(0)}}, \text{ so } \theta=\frac{C_2-B^{(0)}}{B^{(1)}-B^{(0)}}.$$

Due to uniqueness,

$$y^{(2)}=\frac{y^{(0)}(B^{(1)}-C_2)+y^{(1)}(C_2-B^{(0)})}{B^{(1)}-B^{(0)}}.$$

But then

$$y^{(2)}(b)=\frac{y^{(0)}(b)(B^{(1)}-C_2)+y^{(1)}(b)(C_2-B^{(0)})}{B^{(1)}-B^{(0)}}$$

$$=\frac{B^{(0)}(B^{(1)}-C_2)+B^{(1)}(C_2-B^{(0)})}{B^{(1)}-B^{(0)}}=C_2$$

So the value at b is exactly C_2, and we have converged perfectly in 1 step!

Generalizations

1. Applies straightforwardly to more general Robin boundary conditions. Vary y'(a), as before, but keeping $r_1 y(a)+s_1 y'(a)=\text{const}$.

2. When the equation is nonlinear, same approach, but one iteration is not enough.

3. For a set of N linear equations,

$$y_{(n)}''+g_{(n)}(x)\,y_{(n)}'+k_{(n)}(x)\,y_{(n)}=s_{(n)}(x) \qquad y_{(n)}(a)=C_{(n)1};\ y_{(n)}(b)=C_{(n)2}$$

need to determine N initial derivatives using N conditions at b.

$$\vec{F}[\vec{y}\,'(a)]=\vec{C}_2$$

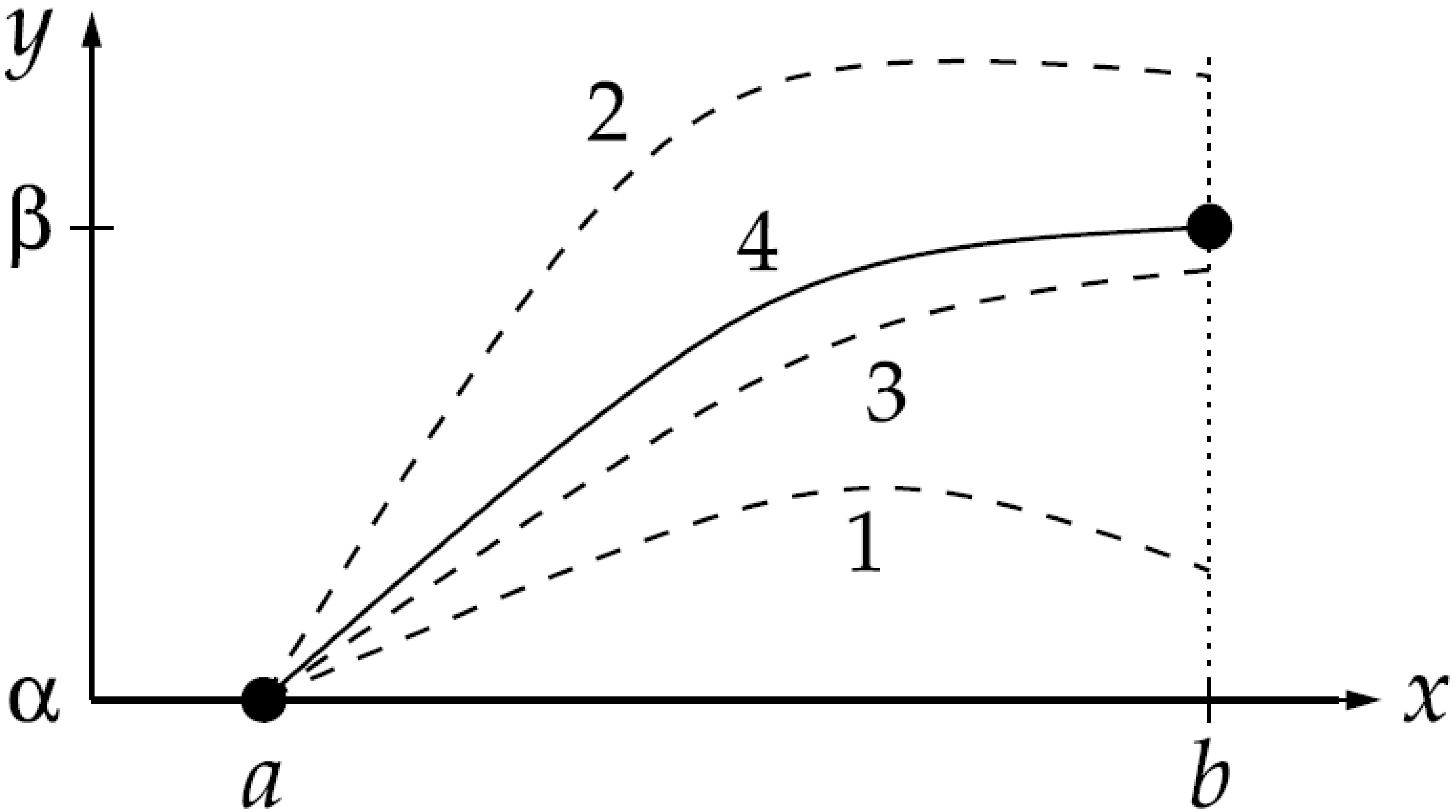
No straightforward generalization of the secant method, have to use Newton. Calculate Jacobian matrix (need N+1 attempts instead of 2), but still converges in 1iteration.

Same for other types equations, e.g., first order.

4. Periodic boundary conditions [y(a)=y(b); y'(a)=y'(b)]. 2 matching conditions.

5. For N nonlinear equations, still use Newton, but need more iterations.

This method is called the shooting method.



Širca, Horvat, Computational Methods for Physicists, Springer, 2012.

"Shoot", correct your angle based on the result, "shoot" again, repeat until convergence.

For the Newton method, instead of doing multiple shooting to calculate the derivatives numerically, may be a better idea to write down and solve the differential equation for the derivative.

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

Suppose $y_s(x)$ is a solution. Consider $y_s(x)+\delta y(x)$.

$$(y_s(x)+\delta y(x))' = f(y_s(x)+\delta y(x), x)$$

$$y'_s(x)+\delta y'(x) = f(y_s(x), x)+(\partial f/\partial y)\big|_{y_s}\delta y(x)$$

$$\delta y'(x) = (\partial f/\partial y)\big|_{y_s}\delta y(x)$$

Solve the equations for y and δy concurrently.

Note that nonlinear equations, even with all the boundary conditions, are not guaranteed to have a unique solution. As always, may converge to different solutions depending on the starting point.

Uniqueness of solutions of non-linear problems is much harder to fathom than in linear problems: a seemingly simple problem $y'' = -\delta e^y$ with conditions $y(0) = y(1) = 0$ (Gelfand–Bratu equation of diffusion-reaction kinetics in a layer) has two solutions for $0 < \delta < \delta_c \approx 3.51$ while the solution does not exist for $\delta > \delta_c$. For the spherical diffusion-reaction problem $y'' + (2/x)y' = \phi^2 y + \exp[\gamma\beta(1-y)/(1+\beta(1-y))]$ with conditions $y'(0) = 0$, $y(1) = 1$ at least 15 solutions are known to exist. How do we numerically compute all of them?

S. Širca, M. Horvat, *Computational Methods for Physicists*, Graduate Texts in Physics, 401
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The eigenvalue problem

$$-\frac{d}{dx}\left[p(x)\frac{dy}{dx}\right]+q(x)y=\lambda w(x)y$$

$$r_1 y(a)+s_1 y'(a)=0;\ r_2 y(b)+s_2 y'(b)=0$$

Here y'(a) can be chosen arbitrarily – since both the equation and the boundary conditions are homogeneous, increasing it simply increases the solution by the same factor. Instead, λ is varied.

If *a* and/or *b* are ∞, replace with a large finite number. Use the theoretical asymptotic solution, if possible, especially if decays slowly (e.g., Poisson equation).

Error is of the same order as the method used to solve the initial-value problem. But, of course, zero on both boundaries and maximum somewhere in the middle.

Sometimes, shooting across the whole interval is problematic, e.g., when a or b is $\pm\infty$ or a singular point.

Example: solving the Schrödinger eq. for a potential well. Generally, for λ not equal to one of the eigenvalues, a sum of a growing and a decaying exponentials. Even if you are slightly off the right λ, (or simply due to the round-off error) the growing exponential will dominate.

Solution: start at the boundaries, solve to a point in the middle, match there.

For eigenvalue problems, keep in mind that we only need to match up to a factor.

Conversely, if there is a singularity in the middle of the interval, start at the singularity and integrate towards the ends.

May need to divide into many subintervals and match at all internal boundaries. Multiple (or parallel) shooting. May be a good idea even without singularities.

We have seen that quite a few second-order equations are linear and do not contain the first derivative. There is a special method for solving such equations called Numerov's method.

$$y''+k(x)y=s(x)$$

Use the notation $y_n=y(x_n)$, $k_n=k(x_n)$, $s_n=s(x_n)$.

$$y_{n+1}=y(x_n+h)=y_n+y'_n h+\frac{1}{2}y''_n h^2+\frac{1}{6}y_n^{(3)}h^3+\frac{1}{24}y_n^{(4)}h^4+\frac{1}{120}y_n^{(5)}h^5+O(h^6)$$

$$y_{n-1}=y(x_n-h)=y_n-y'_n h+\frac{1}{2}y''_n h^2-\frac{1}{6}y_n^{(3)}h^3+\frac{1}{24}y_n^{(4)}h^4-\frac{1}{120}y_n^{(5)}h^5+O(h^6)$$

$$y_{n+1}+y_{n-1}=2y_n+y''_n h^2+\frac{1}{12}y_n^{(4)}h^4+O(h^6)$$

$$y''_n=s_n-k_n y_n \qquad y^{(4)}=(y'')''=(s-ky)''$$

$$y_n^{(4)}=\frac{(s-ky)_{n+1}-2(s-ky)_n+(s-ky)_{n-1}}{h^2}+O(h^2)=$$

$$\frac{s_{n+1}-2s_n+s_{n-1}-k_{n+1}y_{n+1}+2k_n y_n-k_{n-1}y_{n-1}}{h^2}+O(h^2)$$

$$y_{n+1}+y_{n-1}=2y_n+y''_n h^2+\frac{1}{12}y_n^{(4)}h^4+O(h^6) \qquad y''_n=s_n-k_n y_n$$

$$y_n^{(4)}=\frac{s_{n+1}-2s_n+s_{n-1}-k_{n+1}y_{n+1}+2k_n y_n-k_{n-1}y_{n-1}}{h^2}+O(h^2)$$

$$y_{n+1}(1+k_{n+1}h^2/12)=y_n(2-k_n h^2+k_n h^2/6)-y_{n-1}(1+k_{n-1}h^2/12)$$
$$+s_n h^2+(s_{n+1}-2s_n+s_{n-1})h^2/12+O(h^6)$$

$$\boxed{y_{n+1}=\frac{y_n(2-5k_n h^2/6)-y_{n-1}(1+k_{n-1}h^2/12)+(s_{n+1}+10s_n+s_{n-1})h^2/12}{1+k_{n+1}h^2/12}+O(h^6)}$$

A multistep method – need to know 2 previous values. As for Verlet, the global accuracy is 2 orders lower, so it is a 4th order method, like RK4, but only 1 function calculation per step instead of 4.

For the shooting method the fact that we need to know 2 values is not a problem: y_0 is fixed by the boundary condition and then, instead of choosing the derivative arbitrarily and iterating, we choose y_1 arbitrarily.

Another approach.

$$y''+g(x)y'+k(x)y=s(x) \qquad y(a)=C_1;\; y(b)=C_2$$

Introduce a mesh $\{x_n\}$, where $x_0=a$, $x_M=b$, $x_n=a+hn$.

$$y_n=y(x_n);\; g_n=g(x_n);\; k_n=k(x_n);\; s_n=s(x_n)$$

Approximate the derivatives by finite differences directly in the ODE.

$$y''_n=\frac{y_{n+1}-2y_n+y_{n-1}}{h^2}+O(h^2);\; y'_n=\frac{y_{n+1}-y_{n-1}}{2h}+O(h^2)$$

$$\frac{y_{n+1}-2y_n+y_{n-1}}{h^2}+g_n\frac{y_{n+1}-y_{n-1}}{2h}+k_n y_n-s_n+O(h^2)=0,\quad n=1,\ldots,M-1$$

Boundary conditions:

$$y_0=C_1$$
$$y_M=C_2$$

A system of M+1 linear equations, M+1 unknowns. A unique solution, unless degenerate. Tridiagonal. The error is of the same order as the discretization error, i.e., $O(h^2)$. Can use higher-order discretizations, but generally won't be tridiagonal. Numerov is an exception!

Neumann boundary condition on the left boundary

$$y''+g(x)y'+k(x)y=s(x) \qquad y'(a)=C_1;\ y(b)=C_2$$

$$\frac{y_{n+1}-2y_n+y_{n-1}}{h^2}+g_n\frac{y_{n+1}-y_{n-1}}{2h}+k_n y_n-s_n+O(h^2)=0,\quad n=1,\dots,M-1$$

$$y_M=C_2$$

On the left boundary: $y'(a)=y'_0=\dfrac{y_1-y_{-1}}{2h}+O(h^2)$

Involves a non-existent site -1. Alternatively, forward difference

$y'_0=\dfrac{y_1-y_0}{h}+O(h),$ but lower order.

Solution: introduce “ghost” site -1. Two more equations: the discretization of the ODE at site 0,

$\dfrac{y_1-2y_0+y_{-1}}{h^2}+g_0\dfrac{y_1-y_{-1}}{2h}+k_0y_0-s_0=0,$ and the BC, $\dfrac{y_1-y_{-1}}{2h}=C_1.$

$$\frac{2(y_1-y_0)}{h^2}+k_0y_0-2C_1/h+g_0C_1-s_0=0$$

Still M+1 eqs. and as many unknowns; tridiagonal

Another possibility: a second-order 1st derivative discretization not involving site -1.

$$y_1 = y_0 + y'_0 h + \frac{1}{2} y''_0 h^2 + O(h^3) \qquad y_2 = y_0 + 2y'_0 h + 2y''_0 h^2 + O(h^3)$$

$$c_0 y_0 + c_1 y_1 + c_2 y_2 = (c_0 + c_1 + c_2) y_0 + (c_1 + 2c_2) h y'_0 + (c_1/2 + 2c_2) h^2 y''_0 + O(h^3)$$

$$= h y'_0 + O(h^3)$$

$$c_0 + c_1 + c_2 = 0;\ c_1 + 2c_2 = 1;\ c_1/2 + 2c_2 = 0 \ \Rightarrow\ c_0 = -3/2;\ c_1 = 2;\ c_2 = -1/2$$

$$y'_0 = \frac{4y_1 - 3y_0 - y_2}{2h} = C_1 \ \Rightarrow\ \text{get } y_0\text{, insert in}$$

$$\frac{y_2 - 2y_1 + y_0}{h^2} + g_1 \frac{y_2 - y_0}{2h} + k_1 y_1 - s_1 = 0$$

For systems of linear ODEs, the matrix is block-tridiagonal. Still possible to solve faster than a general set of linear equations.

N = 3, M = 5 (3 equations, 6 grid points).

X	X	X	X	X	X	O	O	O	O	O	O	O	O	O	O	O	O
X	X	X	X	X	X	O	O	O	O	O	O	O	O	O	O	O	O
X	X	X	X	X	X	O	O	O	O	O	O	O	O	O	O	O	O
X	X	X	X	X	X	X	X	X	O	O	O	O	O	O	O	O	O
X	X	X	X	X	X	X	X	X	O	O	O	O	O	O	O	O	O
X	X	X	X	X	X	X	X	X	O	O	O	O	O	O	O	O	O
O	O	O	X	X	X	X	X	X	X	X	X	O	O	O	O	O	O
O	O	O	X	X	X	X	X	X	X	X	X	O	O	O	O	O	O
O	O	O	X	X	X	X	X	X	X	X	X	O	O	O	O	O	O
O	O	O	O	O	O	X	X	X	X	X	X	X	X	X	O	O	O
O	O	O	O	O	O	X	X	X	X	X	X	X	X	X	O	O	O
O	O	O	O	O	O	X	X	X	X	X	X	X	X	X	O	O	O
O	O	O	O	O	O	O	O	O	X	X	X	X	X	X	X	X	X
O	O	O	O	O	O	O	O	O	X	X	X	X	X	X	X	X	X
O	O	O	O	O	O	O	O	O	X	X	X	X	X	X	X	X	X
O	O	O	O	O	O	O	O	O	O	O	O	X	X	X	X	X	X
O	O	O	O	O	O	O	O	O	O	O	O	X	X	X	X	X	X
O	O	O	O	O	O	O	O	O	O	O	O	X	X	X	X	X	X

Advection-diffusion equation

$$\frac{d}{dx}\left[D(x)\frac{d\,c(x)}{dx}\right]-\frac{d\,(v(x)\,c(x))}{dx}=0$$

$$D=\text{const},\ v=\text{const}\ \Rightarrow\ Dc''-vc'=0 \qquad c=C_0+C_1\exp\left(\frac{v}{D}x\right)$$

$$D\frac{c_{n+1}-2c_n+c_{n-1}}{h^2}-v\frac{c_{n+1}-c_{n-1}}{2h}=0$$

Diagonal matrix element – $2D/h^2$. Off-diagonal – $2D/h^2 \pm v/2h$.

Define Péclet number $\mathrm{Pe}=\frac{vh}{2D}$. If Pe>~1, off-diagonal elements will dominate and the matrix may become singular. Generally, for

$-y''+p(x)\,y'+q(x)\,y=r(x)$ may happen if $h>2/\max|p(x)|$.

Similar to the issue of stability of initial-value problems.

Use backward difference for the 1st derivative:

$$D\frac{c_{n+1}-2c_n+c_{n-1}}{h^2}-v\frac{c_n-c_{n-1}}{h}=0$$

Eigenvalue problem

$$-\frac{d}{dx}\left[p(x)\frac{dy}{dx}\right]+q(x)y=\lambda w(x)y$$

$$r_1 y(a)+s_1 y'(a)=0;\; r_2 y(b)+s_2 y'(b)=0$$

$$-\frac{p_{n+1/2}(y_{n+1}-y_n)-p_{n-1/2}(y_n-y_{n-1})}{h^2}+q_n y_n=\lambda w_n y_n$$

Eigenvalue problem for this linear tridiagonal system. There are special methods.

Will get M-1 eigenvalues; of course, the original problem has infinitely many.

The error is $O(k^4h^2)$, where k is the number of the eigenvalue. Relative error is $O(k^2h^2)$. Grows rapidly with k.

Advantage: get all eigenvalues at once. Disadvantage: error increases with k, because the same mesh size is used for all eigenvalues. But for the case when there is no 1st derivative, there is a correction that makes the error independent of k!

Richardson extrapolation

$$y''+g(x)y'+k(x)y=s(x)$$

$$r_1 y(a)+s_1 y'(a)=C_1;\; r_2 y(b)+s_2 y'(b)=C_2$$

$$\frac{y_{n+1}-2y_n+y_{n-1}}{h^2}+g_n\frac{y_{n+1}-y_{n-1}}{2h}+k_n y_n-s_n=0$$

The error contains only even-order terms, because the errors of the discretizations contain only even-order terms:

$$y_n^h-\tilde{y}(x_n)=A_1 h^2+A_2 h^4+A_3 h^6+\ldots$$

Repeat on the mesh with step h/2:

$$y_n^{h/2}-\tilde{y}(x_n)=A_1(h/2)^2+A_2(h/2)^4+A_3(h/2)^6+\ldots$$

$$y_n^{(h,h/2)}=\frac{4}{3}y_n^{h/2}-\frac{1}{3}y_n^h$$

$$y_n^{(h,h/2)}-\tilde{y}(x_n)=-A_2 h^4/4+O(h^6)$$

Can be continued.

If the equation is nonlinear: $y''=f(y',y,x)$

$$\frac{y_{n+1}-2y_n+y_{n-1}}{h^2}=f\left(\frac{y_{n+1}-y_{n-1}}{2h},y_n,x_n\right)$$

We get a system of nonlinear equations. Iterate. Relaxation method.

1. Multiply the above equation by $h^2/2$ and rewrite as

$$\frac{1}{2}(y_{n+1}+y_{n-1})-(1+\omega-\omega)y_n=\frac{h^2}{2}f\left(\frac{y_{n+1}-y_{n-1}}{2h},y_n,x_n\right)$$

$$(1+\omega)y_n=\frac{1}{2}(y_{n+1}+y_{n-1})+\omega y_n-\frac{h^2}{2}f\left(\frac{y_{n+1}-y_{n-1}}{2h},y_n,x_n\right)$$

$$y_n=\frac{1}{1+\omega}\left[\frac{1}{2}(y_{n+1}+y_{n-1})+\omega y_n-\frac{h^2}{2}f\left(\frac{y_{n+1}-y_{n-1}}{2h},y_n,x_n\right)\right]$$

Iterate:

$$y_n^{(k+1)}=\frac{1}{1+\omega}\left[\frac{1}{2}(y_{n+1}^{(k)}+y_{n-1}^{(k)})+\omega y_n^{(k)}-\frac{h^2}{2}f\left(\frac{y_{n+1}^{(k)}-y_{n-1}^{(k)}}{2h},y_n^{(k)},x_n\right)\right]$$

Generally, not a good idea, but here works if ω is large enough.

$$\frac{y_{n+1}-2y_n+y_{n-1}}{h^2}=f\left(\frac{y_{n+1}-y_{n-1}}{2h},y_n,x_n\right)$$

2. Newton's method. Rewrite as $\vec{F}(\vec{y})=0$, where

$$F_n(\vec{y})=y_n-\frac{1}{2}(y_{n+1}+y_{n-1})+\frac{h^2}{2}f\left(\frac{y_{n+1}-y_{n-1}}{2h},y_n,x_n\right)$$

Newton's iteration:

$$\vec{y}^{(k+1)}=\vec{y}^{(k)}-[\boldsymbol{J}(\vec{y}^{(k)})]^{-1}\vec{F}(\vec{y}^{(k)})$$

Matrix J is tridiagonal, with nonzero matrix elements

$$J_{nn}=\frac{\partial F_n}{\partial y_n}=1+\frac{h^2}{2}\frac{\partial f}{\partial y} \qquad J_{n,n+1}=\frac{\partial F_n}{\partial y_{n+1}}=-1/2+\frac{h}{4}\frac{\partial f}{\partial y'}$$

$$J_{n,n-1}=\frac{\partial F_n}{\partial y_{n-1}}=-1/2-\frac{h}{4}\frac{\partial f}{\partial y'}$$

Converges faster, but is less reliable. Do a few steps of explicit iteration first.

Shooting vs. finite differences/relaxation

Advantages of shooting.

Any initial-value method can be used (easily achieve high accuracy if necessary). Adaptive step is easy (can treat cases where the solution behaves differently in different regions). No need to solve a system of linear equations. Nonlinear ODEs are solved directly. Often more reliable.

Advantages of finite differences.

Boundary conditions are satisfied automatically. Often faster. The issue of, e.g., exponentially growing solutions drowning out exponentially decaying solutions does not arise.