- Boundary value problems.
- Shooting method.
- Equilibrium boundary value method/ Finite difference method.
- Eigenvalue problems.

Boundary value problems

- Boundary-value problems – involve differential equations with specified boundary conditions: example: one-dimension second order ODE (where p and q are some constants)

$$\frac{d^2y}{dx^2} + p\frac{dy}{dx} + q = f(x)$$

with $y(x_1) = y_1$ and $y(x_2) = y_2$.

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  with $y(x_1) = y_1$ and $y(x_2) = y_2$.
- The boundary-value problem is more difficult to solve than the similar initial-value problem with the same differential equation.

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- A combination of $y(x)$ and $y'(x)$ is specified – mixed boundary conditions

Various ways of solving boundary value problems

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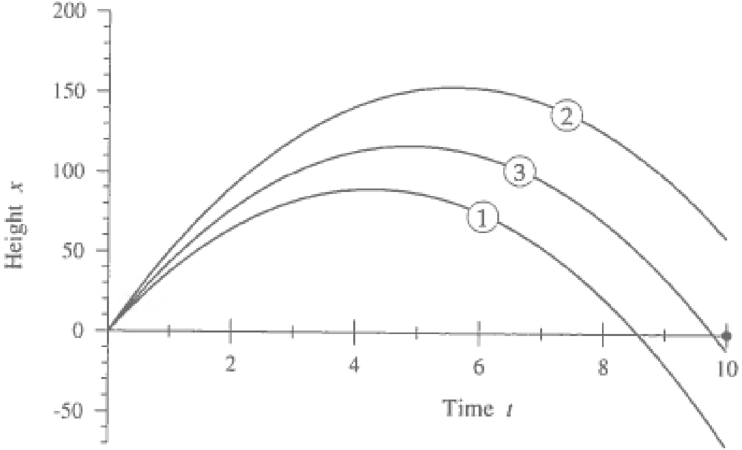
The shooting method



Rather than initial position and velocity, initial and final positions are specified. Start with guess velocity and adjust it to get a solution that satisfies the boundary condition.

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- Only boundary condition on one side is used as one of the initial conditions. The additional initial condition is assumed.
- Then an iterative approach is used to vary the assumed initial condition till the boundary condition on the other side is satisfied.

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- Quite often the fourth-order Runge-Kutta is combined with the secant method.

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- Using secant method for root finding:

$$z_{k+1} = z_k - \frac{c_k - y_2}{c_k - c_{k-1}}(z_k - z_{k-1})$$

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- Substituting the FDAs into the ODE to obtain an algebraic finite difference equation.
- Solving the resulting system of algebraic FDEs (for linear ODEs – a system of linear equations)

- Consider a second order, linear, variable coefficient, boundary value problem with Drichlet boundary conditions:

$$y''(x) + P(x)y'(x) + Q(x)y(x) = F(x)$$

with $y(x_1) = y_1$ and $y(x_N) = y_N$

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- The second order centered difference approximation for y' and y'':

$$y'(x_i) = y'_i = \frac{y_{i+1} - y_{i-1}}{2\Delta x} + \mathcal{O}(\Delta x^2)$$
$$y''(x_i) = y''_i = \frac{y_{i+1} - 2y_i + y_{i-1}}{\Delta x^2} + \mathcal{O}(\Delta x^2)$$

- Substituting this into the differential equation and keeping terms upto order $\mathcal{O}(\Delta x^2)$:

$$\frac{y_{i+1} - 2y_i + y_{i-1}}{\Delta x^2} + P_i\left(\frac{y_{i+1} - y_{i-1}}{2\Delta x} + \right) + Q_i y_i = F_i$$

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- Multiplying by Δx^2 and rearranging:

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- Applying this to all the points on the grid yields a tridiagonal system of equations.
- Number of equations $= N - 2$ – can solve this easily with a linear equation solver. Need to be careful about imposing boundary condition.

Comment on higher order BVP

- Example 4th oder problem:

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

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  and 4 boundary conditions.
- For first/second derivative: $i-1, i, i+1$
  For third/fourth derivative: $i-2, i-1, i, i+1, i+2$
- Leads to a pentadiagonal system.

Neumann boundary condition

- Consider a second order, linear, variable coefficient, boundary value problem with Neumann boundary conditions:

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- The shooting method remains unchanged – except shooting for a value of $y'(x_N)$ rather than $y(x_N)$.
- The equilibrium method needs some modification:

$$\left(1-\frac{\Delta x}{2}P_i\right)y_{i-1}+(-2+\Delta x^2 Q_i)y_i+\left(1+\frac{\Delta x}{2}P_i\right)y_{i+1} = \Delta x^2 F_i$$

  remains the same at all the interior points.

Neumann boundary condition

- We also apply this equation to the boundary point:

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- Again a tridiagonal system of equations.

Boundary condition at infinity

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- Asymptotic solution at large values of x

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- Problem with the method near the boundaries.. central differencing cannot be applied near the boundaries. So, some forward/backward differencing is used there.

Non linear boundary value problems

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- With the finite differencing, this is much more complicated as the corresponding Finite differencing Equation is non-linear. This leads to a non-linear system of FDE's. Have to use Newton's iteration method to solve these.

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Systems of 2nd order boundary value problems

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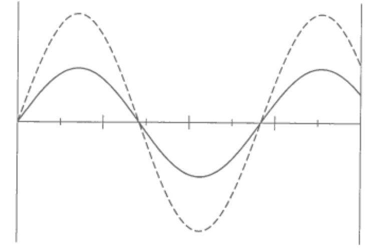
- By either approach, the solution is quite difficult.

Eigenvalue problems



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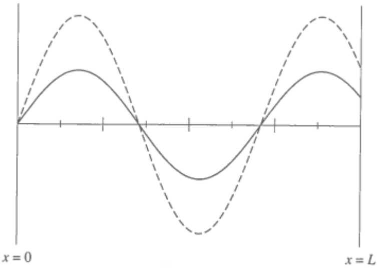

- A special BVP for linear, homogeneous equation. E.g., time-independent Schrödinger equation $-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + V(x)\psi = E\psi$.
- Consider a particle-in-a-box with potential zero within $[0, L]$ and infinite outside this. BC: $\psi = 0$ at $x = 0,\ L$. Cannot adjust $\psi'(0)$ to make ψ vanish at $x = L$ for a general E. Must adjust E (eigenvalue) to ensure $\psi(L) = 0$. Thus, adjust E and not $\psi'(0)$ to satisfy the BC.