PhD Course in Simulation

Course Meeting 4 – BVP

Lars Eriksson

Associate Professor
Department of Electrical Engineering
Linkoping University
lars.erikssonk@liu.se

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1. BVP

BVP – Preliminaries

- ODE + boundary values

$$\boldsymbol{y}' = \boldsymbol{f}(t, \boldsymbol{y}), \qquad 0 < t < b$$
$$\boldsymbol{g}(\boldsymbol{y}(0), \boldsymbol{y}(b)) = 0$$

–m components
–m two point boundary values

- Linear BVP

$$\boldsymbol{y}' = A(t)\boldsymbol{y} + \boldsymbol{q}(t), \qquad 0 < t < b$$
$$B_0\boldsymbol{y}(0) + B_b\boldsymbol{y}(b) = \boldsymbol{b}$$

- Nonlinear notation for $\boldsymbol{g}(\boldsymbol{u}, \boldsymbol{v})$

$$B_0 = \frac{\partial \boldsymbol{g}}{\partial \boldsymbol{u}}, \quad B_b = \frac{\partial \boldsymbol{g}}{\partial \boldsymbol{v}}$$

BVP – Existence and Uniqueness

- IVP theory is nice; attempt to extend it to BVP

$$\begin{aligned} &\boldsymbol{y}' = \boldsymbol{f}(t, \boldsymbol{y}), \qquad 0 < t < b \\ &\boldsymbol{g}(\boldsymbol{y}(0), \boldsymbol{y}(b)) = 0 \end{aligned} \tag{1}$$

- Start with IVP with $\boldsymbol{c}$ unknown

$$\begin{aligned} &\boldsymbol{y}' = \boldsymbol{f}(t, \boldsymbol{y}), \qquad 0 < t < b \\ &\boldsymbol{y}(0) = \boldsymbol{c} \end{aligned}$$

  The solution at b is $\boldsymbol{y}(b; \boldsymbol{c})$

- Insert solution in (1), m nonlinear functions

$$\boldsymbol{h}(\boldsymbol{c}) = \boldsymbol{g}(c, \boldsymbol{y}(b; c)) = 0$$

  many, one, or no solution – No guarantees

- IVP for LTV

$$\begin{aligned} \boldsymbol{y}' &= A(t)\boldsymbol{y} + \boldsymbol{q}(t), \qquad 0 < t < b \\ \boldsymbol{y}(0) &= \boldsymbol{c} \end{aligned}$$

- Fundamental solution from ODE theory, $Y(t)$
  Fulfills $Y' = A(t)Y$, with $Y(0) = I$
- Solution to IVP

$$\boldsymbol{y}(t) = Y(t)\left[\boldsymbol{c} + \int_0^t Y^{-1}(s)\boldsymbol{q}(s)ds\right]$$

Linear BVP – Existence and Uniqueness

- Consider BVP

$$\begin{aligned} \boldsymbol{y}' &= A(t)\boldsymbol{y} + \boldsymbol{q}(t), \qquad 0 < t < b \\ B_0\boldsymbol{y}(0) &+ B_b\boldsymbol{y}(b) = \boldsymbol{b} \end{aligned} \tag{1}$$

- Solve as IVP with $\boldsymbol{y}(0) = \boldsymbol{c}$

$$\boldsymbol{y}(t) = Y(t)\left[\boldsymbol{c} + \int_0^t Y^{-1}(s)\boldsymbol{q}(s)ds\right]$$

and insert into (1)

$$\underbrace{B_0 Y(0) + B_b Y(b)}_{Q}\,\boldsymbol{c} = \boldsymbol{b} - B_b\, Y(b)\int_0^b Y^{-1}(s)\boldsymbol{q}(s)ds$$

Linear BVP – Existence and Uniqueness

Theorem:
Let $A(t)$ and $\boldsymbol{q}(t)$ be continuous and define

$$Q = B_0 + B_b Y(b)$$

then:

- BVP has a unique solution iff Q is nonsingular
- if Q is nonsingular then the solution is given by

$$\begin{aligned} \boldsymbol{y}' &= A(t)\boldsymbol{y} + \boldsymbol{q}(t), \qquad 0 < t < b \\ \boldsymbol{y}(0) &= \boldsymbol{c} \end{aligned}$$

  with

$$\boldsymbol{c} = Q^{-1}\left[\boldsymbol{b} - B_b\, Y(b) \int_0^b Y^{-1}(s)\boldsymbol{q}(s)ds\right]$$

2. Fundamental Solution and Greens Function

Scaled Fundamental Solution, $\Phi(t)$

- $Y(t)$ is scaled for an IVP, $Y(0) = I$
- Defining

$$\Phi = Y(t)Q^{-1}$$

gives a function that fulfills the following

$$\Phi' = A(t)\Phi, \qquad 0 < t < b$$
$$B_0\Phi(0) + B_b\Phi(b) = I$$

$$\Rightarrow \Phi(t) \text{ scaled for BVP.}$$

- Inserting it into the theorem gives the solution

$$\boldsymbol{y}(t) = \Phi(t)\boldsymbol{b} + \int_0^b G(t,s)\boldsymbol{q}(s)ds$$

Green's Function $G(t, s)$

- The solution

$$\boldsymbol{y}(t) = \Phi(t)\boldsymbol{b} + \int_0^b G(t,s)\boldsymbol{q}(s)ds$$

- Green's function (solution operator)

$$G = \begin{cases} \Phi(t)B_0\Phi(0)\Phi^{-1}(s), & s \le t \\ -\Phi(t)B_b\Phi(b)\Phi^{-1}(s), & s > t \end{cases}$$

- *Outside this course:*
  Green's function also appears when solving PDEs
  –Poisson Equation, Diffusion equation
  There called: Green's function, source function, fundamental solution, Gaussian, propagator

3. BVP Stability

Stability

- Recall: Stability – "Perturbation" propagation
- BVP: Test function + boundary conditions

$$\boldsymbol{y}' = \begin{pmatrix} \lambda & 0 \\ 0 & -\lambda \end{pmatrix} \boldsymbol{y}, \qquad \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \boldsymbol{y}(0) + \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} \boldsymbol{y}(b) = \begin{pmatrix} 1 \\ 1 \end{pmatrix}$$

With $\mathrm{Re}(\lambda) \leq 0$,
–ODE is unstable but
–BVP is stable!

Stability

- Stability constant

$$\kappa = \max(||\Phi||_\infty, ||G||_\infty)$$

- Bounds on $\boldsymbol{y}$

$$||\boldsymbol{y}|| = \max_{0 \le t \le b} |\boldsymbol{y}(t)| \le \kappa \left(|\boldsymbol{b}| + \int_0^b |\boldsymbol{q}(s)| ds \right)$$

- Perturbations: $\boldsymbol{\beta} = \hat{\boldsymbol{b}} - \boldsymbol{b}$, $\boldsymbol{\delta} = \hat{\boldsymbol{q}}(t) - \boldsymbol{q}(t)$, $\boldsymbol{x}(t) = \hat{\boldsymbol{y}}(t) - \boldsymbol{y}(t)$

$$||\boldsymbol{x}|| \le \kappa \left(|\boldsymbol{\beta}| + \int_0^b |\boldsymbol{\delta}(s)| ds \right)$$

Stability – Green's function nicely bounded

Stability – Dichotomy

- Consider separated boundary conditions

$$B_0\Phi(0) = P = \begin{pmatrix} I_k & 0 \\ 0 & 0 \end{pmatrix}, \quad B_b\Phi(b) = I - P$$

Green's function now becomes

$$G = \begin{cases} \Phi(t)P\Phi^{-1}(s), & s \le t \\ -\Phi(t)(I-P)\Phi^{-1}(s), & s > t \end{cases}$$

- Dichotomy (Exponential)

$$\begin{aligned} ||\Phi(t)P\Phi^{-1}(s)|| &\le K\left(e^{\alpha\,(s-t)}\right), && s \le t \\ ||\Phi(t)(I-P)\Phi^{-1}(s)|| &\le K\left(e^{\beta\,(t-s)}\right), && s > t \end{aligned}$$

Dichotomy – Stability

4. Nonlinear BVP

Nonlinear BVP

- General theory only covers the local behavior around one solution $\boldsymbol{y}(t)$
- Consider variation equation, with $\boldsymbol{y}(t)$ solution to $\boldsymbol{y}' = \boldsymbol{f}(t, \boldsymbol{y})$

$$\boldsymbol{z}' = A(t, \boldsymbol{y}(t))\boldsymbol{z}, \qquad A(t, \boldsymbol{y}) = \frac{\partial f(t, \boldsymbol{y})}{\partial \boldsymbol{y}}$$

- Isolated solution, uniqueness around a trajectory
  Condition, Q nonsingular.

5. Solving BVP Numerically – Shooting

Shooting

- BVP to IVP

$$\begin{cases} \boldsymbol{y}' = \boldsymbol{f}(t, \boldsymbol{y}), & 0 < t < b \\ \boldsymbol{g}(\boldsymbol{y}(0), \boldsymbol{y}(b)) = 0 \end{cases} \quad \Rightarrow \quad \begin{cases} \boldsymbol{y}' = \boldsymbol{f}(t, \boldsymbol{y}), & 0 < t < b \\ \boldsymbol{y}(0) = \boldsymbol{c} \end{cases}$$

- Equation solving for $\boldsymbol{h}(\boldsymbol{c}) = \boldsymbol{g}(c, \boldsymbol{y}(b; c)) = 0$
  - Solve IVP for $\boldsymbol{c}^\nu$
  - Solve the linearized problem with $A(t_n) = \frac{\partial \boldsymbol{f}}{\partial \boldsymbol{y}}(t_n, \boldsymbol{y}^\nu_{n_\nu})$
  - Newton's method to update $\boldsymbol{c}^{\nu+1} = \boldsymbol{c}^\nu - \left(\frac{\partial \boldsymbol{h}}{\partial \boldsymbol{c}}\right)^{-1} \boldsymbol{h}(\boldsymbol{c})$
    Where $\frac{\partial \boldsymbol{h}}{\partial \boldsymbol{c}} = Q$
    Q obtained from the variational ODE.

Multiple Shooting

Reduces sensitivity when the ODE is unstable.

6. Solving BVP Numerically – Finite Difference Methods

Finite Difference Methods

- Build mesh, N steps.
- Apply discretization method (symmetric)
- Reformulate problem to equation solving in each step

$$\frac{\boldsymbol{y}_n - \boldsymbol{y}_{n-1}}{h_n} = \boldsymbol{f}(t_{n-\frac{1}{2}}, \frac{\boldsymbol{y}_n + \boldsymbol{y}_{n-1}}{2}), \quad n = 1, \ldots, N$$

and at the boundary

$$\boldsymbol{g}(y_0, \boldsymbol{y}_N) = 0$$

giving $m\,(N+1)$ equations

Use variational formulation around trajectory and apply (quasi-)Newton methods.
–Solution of sparse linear systems.