Numerical methods for dynamical systems

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Part VII

Numerical methods for BVP-ODE

Part 7. Section 1
Introduction to Two-point Boundary Value Problems

Initial value problem (IVP)

Definition of IVP

$$\dot{\mathbf{y}} = f(t, \mathbf{y}) \quad \text{with} \quad \mathbf{y}(0) = \mathbf{y}_0$$

The IVP is **autonomous** if f does not explicitly depend on t: $\dot{\mathbf{y}} = f(\mathbf{y})$

Remark: we can always transform a non autonomous problem into an autonomous one.

Recipe to make IVP autonomous

It is sufficient to increase the dimension of the problem:

- adding an equation of the form $\dot{y}_{n+1} = 1$ with $y_{n+1}(0) = 0$
- substituting each occurrence of t by y_{n+1}.

Initial value problem (IVP)

Definition of IVP

$$\dot{\mathbf{y}} = f(t, \mathbf{y}) \quad \text{with} \quad \mathbf{y}(0) = \mathbf{y}_0$$

IVP has a unique solution if:

- f is continuous with respect to time t
- f is Lipschitz with respect to $\mathbf{y}$ that is:

$$\forall t, \forall \mathbf{y}_1, \mathbf{y}_2 \in \mathbb{R}^n, \exists L > 0, \quad \| f(t, \mathbf{y}_1) - f(t, \mathbf{y}_2) \| \leq \; L \| \mathbf{y}_1 - \mathbf{y}_2 \|$$

Remark it is still true for piece-wise Lipschitz functions.

Remark the uniqueness is lost if continuity is only considered.

Solution are usually only numerically computed

Many numerical integration methods exist to solve IVP-ODE

Definition of IVP for second order ODE

$$\ddot{\mathbf{y}} = f(t, \mathbf{y}, \dot{\mathbf{y}}) \quad \text{with} \quad \mathbf{A}\mathbf{y}(a) + \mathbf{B}\mathbf{y}(b) = \boldsymbol{\alpha} \quad \text{and} \quad a \leqslant t \leqslant b. \tag{1}$$

with

- $\mathbf{y} \in \mathbb{R}^n$
- **A** and **B** are matrices of dimension $n \times n$.
- $\boldsymbol{\alpha} \in \mathbb{R}^n$

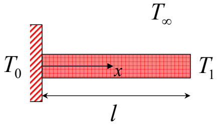
Note: usually boundary conditions are given in a separated form

$$\mathbf{A}\mathbf{y}(a) = c_1 \quad \text{and} \quad \mathbf{B}\mathbf{y}(b) = c_2$$

Different kinds of boundary conditions are considered

- Dirichelet or of first kind: $\mathbf{y}(a) = \boldsymbol{\alpha}$ and $\mathbf{y}(b) = \boldsymbol{\beta}$
- Neumann or of second kind: $\dot{\mathbf{y}}(a) = \boldsymbol{\alpha}$ and $\dot{\mathbf{y}}(b) = \boldsymbol{\beta}$
- Robin or Third or Mixed kind: $\boldsymbol{A}_1\mathbf{y}(a) + \mathbf{A}_2\dot{\mathbf{y}}(a) = \boldsymbol{\alpha}$ and $\mathbf{B}_1\mathbf{y}(b) + \mathbf{B}_2\dot{\mathbf{y}}(b) = \boldsymbol{\beta}$.

Example of BVP-ODE: cooling fin



Mathematical model

$$\frac{d^2T}{dx^2} - \frac{hP}{kA}(T - T_\infty) = 0 \quad \text{with} \quad T(x=0) = T_0 \quad \text{and} \quad T(x=L) = T_1$$

with

- h heat transfer coefficient
- k thermal conductivity
- P perimeter of the fin
- A cross section area of the fin
- T_∞ ambient temperature

BVP-ODE existence and uniqueness of the solution

This study of existence and uniqueness are defined as the study of the roots of a certain equations over IVP-ODE.

In particular, we study

$$\dot{\mathbf{u}} = f(t, \mathbf{u}) \quad \text{and} \quad \mathbf{u}(a) = \mathbf{s} \tag{2a}$$

$$\Phi(s) \equiv (\mathbf{A}\mathbf{s} + \mathbf{B}\mathbf{u}(b; \mathbf{s})) - \alpha = 0 \tag{2b}$$

with $\mathbf{u}(b; \mathbf{s})$ is the solution of IVP-ODE at time b from initial condition $\mathbf{s}$.

Intuitively: if $\mathbf{s}^*$ is the root of $\Phi(\mathbf{s})$ we expect that $\mathbf{u}(t; \mathbf{s}^*) = \mathbf{y}(t)$ that is the solution of BVP-ODE.

Theorem

Let $f(t, \mathbf{u})$ be continuous on $a \leqslant t \leqslant b$ and $|\mathbf{u}| < \infty$ and satisfy Lipschitz condition on $\mathbf{u}$. Then the BVP-ODE (1) has as many solution as there are distinct root $\mathbf{s} = \mathbf{s}^\nu$ of (2b). These solutions are $\mathbf{y}(t) = \mathbf{u}(t, \mathbf{s}^\nu)$ the solution of (2a) with initial condition $\mathbf{s}^\nu$.

Theorem of existence and uniqueness of BVP-ODE

Let $f(t, \mathbf{u})$ satisfy on $a \leqslant t \leqslant b$, $|\mathbf{u}| < \infty$

i. $f(t, \mathbf{u})$ is continuous;
ii. $\frac{\partial f_i(t,\mathbf{u})}{\partial u_j}$ is continuous for $i, j = 1, 2, \ldots, n$;
iii. $\left\| \frac{\partial f(t,\mathbf{u})}{\partial \mathbf{u}} \right\|_\infty \leqslant k(t)$.

Furthermore, let the matrices $\mathbf{A}$ and $\mathbf{B}$ and the scalar function $k(t)$ satisfy

1. $(\mathbf{A} + \mathbf{B})$ non-singular;
2. $\int_a^b k(x)dx \leqslant \ln\left(1 + \frac{\lambda}{m}\right)$ for some $0 < \lambda < 1$ with

$$m = \left\| (\mathbf{A} + \mathbf{B})^{-1} \mathbf{B} \right\|_\infty .$$

Then the BVP-ODE (1) has a unique solution for each α.

Remark

It is not so easy

Examples of BVP-ODE

Initial problem

$$\ddot{y} + y = 0$$

with conditions:

- $y(0) = 0$ and $y(\frac{\pi}{2}) = 1$ then there is a unique solution $\sin(t)$
- $y(0) = 0$ and $y(\pi) = 0$ then there is an infinite number of solutions $c_1 \sin(t)$
- $y(0) = 0$ and $y(\pi) = 1$ there is no solution

Conclusion

BVP-ODE do not behave so nicely than IVP-ODE!

Part 7. Section 2
Numerical solution: shooting methods

Simple shooting method to solve BVP-ODE 1D

Introductory example

$$\ddot{y} = f(t, y, \dot{y}) \quad \text{with} \quad y(a) = \alpha \quad \text{and} \quad y(b) = \beta$$

Transforming differential equation into first order

$$\begin{aligned} \dot{y}_1 &= y_2 \\ \dot{y}_2 &= f(t, y_1, y_2) \end{aligned}$$

and we set the initial conditions:

$$y_1(a) = \alpha \quad \text{and} \quad y_2(a) = s$$

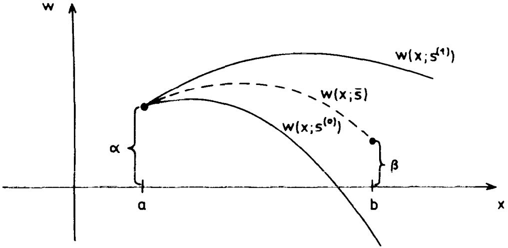
So we have to find s which is a root of $y_1(b; s) - \beta = 0$

Hence we can use any root finding algorithm to do so such as bisection or Newton-like methods

BVP-ODE: Bisection-based root finding 1D

- Inputs:
  - s_1 such that $y_1(b; s_1) - \beta < 0$
  - s_2 such that $y_1(b; s_2) - \beta > 0$
- Process: compute center s_c of interval $[s_1, s_2]$, assuming $s_1 < s_2$, solve IVP-ODE with s_c
  - if $y_1(b; s_c) - \beta < 0$ then redo with interval $[s_c, s_2]$
  - otherwise redo with interval $[s_1, s_c]$

  until he width of interval is small enough



Remark

As in general $F(s) = y_1(b; s) - \beta$ is continuously differentiable as $y_1(b; s_1)$ is, Newton's method can be used.

In that case, we uses the recurrence

$$s_{i+1} = s_i + \frac{F(s_i)}{F'(s_i)}$$

to generate initial conditions to the IVP-ODE

$$\begin{aligned} \dot{y}_1 &= y_2 \\ \dot{y}_2 &= f(t, y_1, y_2) \end{aligned} \quad \text{with} \quad y_1(a) = \alpha \quad \text{and} \quad y_2(a) = s_i$$

Note that, the derivative F' of F is

$$F'(s) = \frac{\partial y_1(t; s)}{\partial s}$$

Variational equations

Theorem

Let $f(t, \mathbf{y})$ be Lipschitz in $\mathbf{y}$ on $R = a \leqslant t \leqslant b$ and $|\mathbf{y}| < \infty$. And let the Jacobian of f w.r.t. $\mathbf{y}$ have continuous element on R that is the n-th order matrix

$$\mathbf{J}(t, \mathbf{y}) \equiv \frac{\partial f(t, \mathbf{y})}{\partial \mathbf{y}} = \left(\frac{\partial f_i(t, \mathbf{y})}{\partial \mathbf{y}_i} \right)$$

is continuous on R. Then for any $\boldsymbol{\alpha}$ the solution $\mathbf{y}(t; \boldsymbol{\alpha})$ is continuously differentiable. Moreover, the derivative of $\frac{\partial \mathbf{y}(t;\boldsymbol{\alpha})}{\partial \alpha_i} \equiv \boldsymbol{\xi}(t)$ is the solution on $[a, b]$ of the linear system

$$\dot{\boldsymbol{\xi}}(t) = \mathbf{J}(t, \mathbf{y})\boldsymbol{\xi}(t) \quad \text{with} \quad \boldsymbol{\xi}(a) = \mathbf{e}_k = (0, 0, \ldots, 1, \ldots, 0)$$

Remark: for applying Newton-based method for BVP-ODE 1D

- an augmented IVP-ODE with variational equation may be considered
- a finite difference approach may also be used

We want to solve

$$F(s) = y_1(b; s) - \beta = 0$$

To avoid complex computation using variational equations, a finite difference may be used

$$\Delta F(s_i) = \frac{F(s_i + \Delta s_i) - (F(s_i)}{\Delta s_i}$$

then the following recurrence may be used

$$s_{i+1} = s_i + \frac{F(s_i)}{\Delta F(s_i)}$$

Remark computing $\Delta F(s_i)$ involves solving IVP-ODE.

BVP-ODE more general case

Full nonlinear BVP-ODE

$$\dot{\mathbf{y}} = f(t, \mathbf{y})$$
$$a \leqslant t \leqslant b$$
$$g(\mathbf{y}(a), \mathbf{y}(b)) = \mathbf{0} \quad (m\text{non-linear equations})$$

Using translation to IVP-ODE we need to solve

$$F(\mathbf{s}) \equiv g(\mathbf{s}, y(b; \mathbf{s})) = 0$$

Remark Newton's method has to be used to solve non-linear systems of equations!

Comment

Shooting methods are very "simple" methods to solve BVP but they cannot address all the classes of BVP-ODE.

Multiple shooting methods

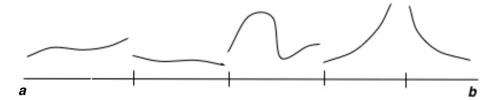
Note some numerical stability problems can be appeared with simple shooting method especially when b is large.

Idea of multiple shooting method

Consider more tight interval on which doing the shooting. So it is applied on a mesh

$$a = t_0 < t_2 < \cdots < t_N = b$$

So solve IVP-ODE on each sub-interval $[t_i, t_{i+1}]$ and add continuity constraints on the pieces of solution



Multiple shooting methods – cont'

With this methods we have to solve

$$\begin{aligned} \dot{\mathbf{y}}_i &= f(t, \mathbf{y}_i) \quad \text{with} \quad t_{i-1} < t < t_i \\ \mathbf{y}(t_{i-1}) &= \mathbf{c}_{i-1} \end{aligned}$$

Then the solution of BVP-ODE $\mathbf{y}(t)$ will be defined by piece such that

$$\mathbf{y}(t) = \mathbf{y}_i(t) \quad \text{for} \quad t_{i-1} < t < t_i, i = 1, 2, \dots, N$$

where

$$\begin{aligned} \mathbf{y}(t_{i-1}) &= \mathbf{c}_{i-1} \\ g(\mathbf{c}_0, \mathbf{y}_N(b; \mathbf{c}_{N-1})) &= \mathbf{0} \end{aligned}$$

In consequence with have to solve a system of dimension $Nm \times Nm$.

Multiple shooting methods – cont'

In summary we have to solve

$$H(\mathbf{c}) = \mathbf{0}$$

So Newton's method has to be used

$$A\delta^{\eta} = -H(c^{\eta}) \quad \text{with} \quad A = \frac{\partial H}{\partial c}|_{c^{\eta}}$$
$$c^{\eta+1} = c^{\eta} + \delta^{\eta}$$

and A has particular structure

$$\mathbf{A} = \begin{bmatrix} -\mathbf{Y}_1(t_1) & \mathbf{I} & & & \\ & -\mathbf{Y}_2(t_2) & \mathbf{I} & & \\ & & \ddots & \ddots & \\ & & & -\mathbf{Y}_{N-1}(t_{N-1}) & \mathbf{I} \\ \mathbf{B}_a & & & & \mathbf{B}_b\mathbf{Y}_N(b) \end{bmatrix}$$

Summary

This multiple shooting approach is more robust than simple shooting approach but it is more computer expensive.

Part 7. Section 3
Finite difference approach

Problem statement

We consider the boundary problem

$$\ddot{y} = f(t, y, \dot{y})$$
$$y(a) = \alpha \qquad\qquad y(b) = \beta$$

If u, v, and w are continuous and $v(t) > 0$ on $[a, b]$ then this problem has a unique solution.

Idea of the methods

Discretized the ODE

We will consider an equidistant partition of $[a, b]$ into $m + 1$ pieces $[t_k, t_{k+1}]$ for $k = 0, 1, \dots, m$ is performed

$$t_k = a + kh, \quad k = 0, 1, \dots, m + 1, \quad \text{and} \quad h = \frac{b - a}{m + 1}$$

$$\ddot{y} = f(t, y, \dot{y}) \equiv u(t) + v(t)y(t) + w(t)\dot{y}(t)$$

Applying finite difference on that equation we have

$$\begin{aligned} y_0 &= \alpha \\ \frac{y_{k+1} - 2y_k + y_{k-1}}{h^2} &= u_k + v_k y_k + w_k \frac{y_{k+1} - y_{k-1}}{2h}, \quad k = 0, 1, \ldots, m \\ y_{m+1} &= \beta \end{aligned}$$

where $u_k = u(t_k)$

The linear system is *tridiagonal* as can be seen by rewriting the system

$$\begin{aligned} y_0 &= \alpha \\ \left(-1 - \frac{w_k}{2}h\right) y_{k-1} + (2 + h^2 v_k) y_k + \left(-1 + \frac{w_k}{2}h\right) y_{k+1} &= -h^2 u_k, \quad k = 0, 1, \ldots, m \\ y_{m+1} &= \beta \end{aligned}$$

In matrix form we have

$$
\begin{pmatrix}
2+h^2v_1 & -1+\frac{w_1}{2}h & 0 & \cdots & 0 \\
-1-\frac{w_2}{2}h & 2+h^2v_2 & -1+\frac{w_2}{2}h & & \vdots \\
\vdots & \ddots & \ddots & \ddots & \vdots \\
\vdots & & -1-\frac{w_{m-1}}{2}h & 2+h^2v_{m-1} & -1+\frac{w_{m-1}}{2}h \\
0 & \cdots & 0 & -1-\frac{w_m}{2}h & 2+h^2v_m
\end{pmatrix}
\times
\begin{pmatrix} y_1 \\ y_2 \\ \vdots \\ y_{m-1} \\ y_m \end{pmatrix}
=
\begin{pmatrix}
-h^2u_1-\alpha(-1-\frac{w_1}{2}h) \\
-h^2u_2 \\
\vdots \\
-h^2u_{m-1} \\
-h^2u_m-\beta(-1+\frac{w_m}{2}h)
\end{pmatrix}
$$

Solution of tridiagonal linear system can be efficiently solved if it has the diagonal dominant property that is

$$\mid 2+h^2v_k \mid > \mid 1+\frac{h}{2}w_k \mid + \mid 1-\frac{h}{2}w_k \mid$$

This inequality is satisfied if $v_k > 0$ and the discretization is such that $\mid \frac{h}{2}w_k \mid < 1$

Finite difference produces

$$\begin{aligned} y_0 &= \alpha \\ \frac{y_{k+1} - 2y_k + y_{k-1}}{h^2} &= f(t_k, y_k, \frac{y_{k+1} - y_{k-1}}{2h}) \quad k = 0, 1, \dots, m \\ y_{m+1} &= \beta \end{aligned}$$

and one gets

$$\begin{aligned} 2y_1 - y_2 + h^2 f(t_1, y_1, \frac{y_2 - \alpha}{2h}) - \alpha &= 0 \\ -y_{k-1} + 2y_k - y_{k+1} + h^2 f(t_k, y_k, \frac{y_{k+1} - y_{k-1}}{2h}) &= 0 \quad k = 2, \dots, m-1 \\ -y_{m-1} + 2y_m + h^2 f(t_m, y_m, \frac{\beta - y_{m-1}}{2h}) - \beta &= 0 \end{aligned}$$

this system has a unique solution if $h < \frac{2}{M}$ where M is such that $\mid f_z(t, y, z) \mid < M$ for all $(t, y, z) \in \{[1, b],] - \infty, \infty[^2$

We can solve this system with Newton-like methods such that

$$J(\mathbf{y}^{[i]})u = -F(\mathbf{y}^{[i]})$$
$$\mathbf{y}^{[i+1]} = \mathbf{y}^{[i]} + u$$

with the tridiagonal Jacobian matrix defined by

$$J(\mathbf{y})_{k\ell} = \begin{cases} -1 + \frac{h}{2} f_z(t_k, y_k, \frac{y_{k+1} - y_{k-1}}{2h}), k = \ell - 1, \ell = 2, \ldots, m \\ 2 + h^2 f_y(t_k, y_k, \frac{y_{k+1} - y_{k-1}}{2h}), k = \ell, \ell = 1, \ldots, m \\ -1 + \frac{h}{2} f_z(t_k, y_k, \frac{y_{k+1} - y_{k-1}}{2h}), k = \ell, \ell = 1, \ldots, m - 1 \end{cases}$$

Remark we need a good initial guess to apply Newton method

Part 7. Section 4

A few words on initial guess

Many methods to solve BVP-ODE require an initial guess to start the computation (Newton like approach) but for nonlinear problems it is difficult.

One common approach is to used *Homotopy continuation* methods. The idea is to transform continuously a simpler (e.g., linear) problem to solve to our nonlinear problem to solve.

First we need to introduce a parameter α so ODE is transformed into

$$\dot{y} = f(t, y, \alpha)$$

This parameterization is such that $\alpha = 1$ is our original problem and $\alpha 0$ is our simpler problem.

-set $\alpha_0 = 0$ and initial mesh $x_0^0 < x_1^0 \cdots x_{N_0}^0$;
-invoke the BV solver to determine the discrete solution on this mesh, $(y_0^0, y_1^0 \cdots y_{N_0}^0)$;
-set $j = 0$;
-Repeat until ($\alpha_j = 1$ or all attempts fail);
    -choose the next value, α_{j+1};
    -choose the initial mesh for the next problem,$x_0^{j+1}, x_1^{j+1} \cdots x_{N_{j+1}}^{j+1}$;
        (Usually this mesh will be equal to or a refinement of $x_0^j, x_1^j \cdots x_{N_j}^j$)
    -choose an initial guess for the solution at $x_0^{j+1}, x_1^{j+1} \cdots x_{N_{j+1}}^{j+1}$;
        This will involve referring to $y_0^j, y_1^j \cdots y_{N_j}^j$.
    -invoke BV solver on problem determined by α_{j+1} with initial mesh and corresponding initial guess $y_0^{j+1}, y_1^{j+1} \cdots y_{N_{j+1}}^{j+1}$;
    -if (BV solver was successfull) then
        -set $j = j + 1$;
    -else
        -consider reducing α_{j+1} for the next attempted step;
-end Repeat