CS 450: Numerical Analysis

Boundary Value Problems for Ordinary Differential Equations

University of Illinois at Urbana-Champaign

¹These slides have been drafted by Edgar Solomonik as lecture templates and supplementary material for the book “Scientific Computing: An Introductory Survey” by Michael T. Heath (slides).
Boundary Conditions

- Often we seek to solve a differential equation that satisfies conditions on its values and derivatives on parts of the domain boundary.
  - **Dirichlet boundary conditions** specify values of \( y(t) \) at boundary.
  - **Neumann boundary conditions** specify values of derivative \( f(t, y) \) at boundary.

- Consider a first order ODE \( y'(t) = f(t, y) \) with **linear boundary conditions** on domain \( t \in [a, b] \):
  \[
  B_a y(a) + B_b y(b) = c
  \]

- **IVPs are a special case of Dirichlet condition with** \( B_a = I, B_b = 0 \).

- **Conditions are separated** if they do not couple different boundary points, i.e., for all \( i \), the \( i \)th row of either \( B_a \) or \( B_b \) is zero.

- **Higher-order boundary conditions** can be reduced to linear boundary conditions in the same way as a nonlinear ODE is reduced to a linear ODE.
Existence of Solutions for Linear ODE BVPs

- The solutions of linear ODE BVP $y'(t) = A(t)y(t) + b(t)$ are linear combinations of solutions to linear homogeneous ODE IVPs $y'(t) = A(t)y(t)$:
  - Let the solutions $y_i(t)$ to the homogeneous ODE, $y_i'(t) = A(t)y_i(t)$, with initial conditions $y_i(a) = e_i$ be columns of
    $$Y(t) = [y_1(t) \ldots y_n(t)] = I + \int_a^t A(s)Y(s)ds.$$
  - The ODE BVP solutions are then given by $y(t) = Y(t)u(t)$ for some $u(t)$, with
    $$y'(t) = A(t)y(t) + b(t) \Rightarrow Y'(t)u(t) + Y(t)u'(t) = A(t)Y(t)u(t) + b(t),$$
    $$Y'(t) = A(t)Y(t) \Rightarrow u'(t) = Y(t)^{-1}b(t).$$

- Solution $u(t)$ (and $y(t)$) exists if $Q = B_aY(a) + B_bY(b)$ is invertible:
  $$B_aY(a)u(a) + B_bY(b)\left(\int_a^b u'(s)ds\right) = c,$$
  $$u(a) = \left(\frac{B_aY(a) + B_bY(b)}{Q}\right)^{-1}\left(c - B_bY(b)\int_a^b u'(s)ds\right).$$
Green’s Function Form of Solution for Linear ODE BVPs

- For any given \( b(t) \) and \( c \), the solution to the BVP can be written in the form:

\[
y(t) = \Phi(t)c + \int_a^b G(t,s)b(s)ds
\]

\( \Phi(t) = Y(t)Q^{-1} \) is the \textit{fundamental matrix} and the \textit{Green’s function} is

\[
G(t,s) = Y(t)Q^{-1}I(s)Y^{-1}(s), \quad I(s) = \begin{cases} B_aY(a) & : s < t \\ -B_bY(b) & : s \geq t \end{cases}
\]

- From our expression for \( u(a) \) and the integral equation for \( y(t) \),

\[
y(t) = Y(t)Q^{-1} \left(c - B_bY(b) \int_a^b u'(s)ds\right) + Y(t) \int_a^t u'(s)ds
\]

\[
= \Phi(t)c + Y(t)Q^{-1} \left(-B_bY(b) \int_a^b u'(s)ds + Q \int_a^t u'(s)ds\right)
\]

\[
= \Phi(t)c + Y(t)Q^{-1} \left(B_aY(a) \int_a^t Y^{-1}(s)b(s)ds - B_bY(b) \int_t^b Y^{-1}(s)b(s)\right).
\]
Conditioning of Linear ODE BVPs

- For any given \( b(t) \) and \( c \), the solution to the BVP can be written in the form:

\[
y(t) = \Phi(t)c + \int_a^b G(t, s)b(s)ds
\]

\( \Phi(t) = Y(t)Q^{-1} \) is the fundamental matrix, which like the Green’s function is associated with the homogeneous ODE as well as its linear boundary condition matrices \( B_a \) and \( B_b \), but is independent \( b(t) \) and \( c \).

- The absolute condition number of the BVP is \( \kappa = \max\{||\Phi||_\infty, ||G||_\infty\} \):

  This sensitivity measure enables us to bound the perturbation \( ||\hat{y} - y||_\infty \) with respect to the magnitude of a perturbation to \( b(t) \) or \( c \).
Shooting Method for ODE BVPs

For linear ODEs, we construct solutions from IVP solutions in $Y(t)$, which suggests the *shooting method* for solving BVPs by reduction to IVPs:

*For $k = 1, 2, \ldots$ repeat until convergence:*

1. construct approximate initial value guesses $\hat{y}^{(k)}(a) \approx y(a)$,
2. solve the resulting IVP,
3. check the quality of the solution at the new boundary,
   $$\|B_b \hat{y}^{(k)}(b) - B_a \hat{y}^{(k)}(a) - c\|,$$
4. pick the initial conditions for the next shot, $\hat{y}^{(k+1)}(a)$ by treating $\hat{y}^{(l)}(a)$ for $l = 1, \ldots, k$ as guesses $x(1), \ldots, x(k)$ to root finding procedure for
   $$h(x) = B_a x + B_b y_x(b) - c,$$
   where $y_x(b)$ is the IVP solution with $y_x(a) = x$.

**Multiple shooting** employs the shooting method over subdomains:

- The shooting problems on subdomains are interdependent, as they must satisfy continuity conditions on boundaries between them, leading to a system of nonlinear equations.
- Improves on conditioning of shooting method, which can suffer from ill-conditioning of large IVPs.
Finite Difference Methods

- Rather than solve a sequence of IVPs that satisfy the ODEs until they (approximately) satisfy boundary conditions, we can refine an approximation that satisfies the boundary conditions, until it satisfies the ODE:

  - **Finite difference methods** work by obtaining a solution on points $t_1, \ldots, t_n$, so that $\hat{y}_k \approx y(t_k)$ by finite-difference formulae, for example,

    
    $$f(t, y) = y'(t) \approx \frac{y(t + h) - y(t - h)}{2h} \Rightarrow f(t_k, \hat{y}_k) = \frac{\hat{y}_{k+1} - \hat{y}_{k-1}}{t_{k+1} - t_{k-1}}.$$

  - The resulting system of equations can be solved by standard methods and is linear if $f$ is linear.

- Convergence to solution is obtained with decreasing step size $h$ so long as the method is consistent and stable:

  - Consistency implies that the truncation error goes to zero.
  - Stability ensures input perturbations have bounded effect on solution.
Let's derive the finite difference method for the ODE BVP defined by

$$u'' + 7(1 + t^2)u = 0$$

with boundary conditions $u(-1) = 3$ and $u(1) = -3$, using a centered difference approximation for $u''$ on $t_1, \ldots, t_n$, $t_{i+1} - t_i = h$.

We have equations $u(-1) = u(t_1) = u_1 = 3$, $u(1) = u(t_n) = u_n = 3$ and $n - 2$ finite difference equations, one for each $i \in \{2, \ldots, n-1\}$,

$$\frac{u_{i+1} - 2u_i + u_{i-1}}{h^2} + 7(1 + t_i^2)u_i = 0.$$

These correspond to a linear system based on matrices:

$$A = \begin{bmatrix} 1/h^2 & -2/h^2 & 1/h^2 \\
1/h^2 & \ddots & \ddots & \ddots \\
\ddots & \ddots & \ddots & 1/h^2 \\
1/h^2 & -2/h^2 & 1/h^2 & 1 \\
\end{bmatrix} \quad \text{and} \quad B = \begin{bmatrix} 0 & 0 \\
0 & 7(1 + t_2^2) \\
\ddots & \ddots \\
7(1 + t_{n-1}^2) & 0 & 0 \\
\end{bmatrix},$$

where $(A + B)u = [3 \ 0 \ \cdots \ 0 \ -3]^T$. 

Demo: Finite differences
Collocation Methods

- **Collocation methods** approximate \( y \) by representing it in a basis

\[
y(t) \approx v(t, x) = \sum_{i=1}^{n} x_i \phi_i(t).
\]

- Seek to satisfy for collocation points \( t_1, \ldots, t_n \) with \( t_1 = a \) and \( t_n = b \),

\[
\forall i \in \{2, \ldots, n-1\} \quad v'(t_i, x) = f(t_i, v(t_i, x)).
\]

- Two more equations typically obtained from boundary conditions at \( t_1, t_n \).

- Choices of basis functions give different families of methods:
  - **Spectral methods** use polynomials or trigonometric functions for \( \phi_i \), which are nonzero over most of \([a, b]\), and have the advantage of corresponding to eigenfunctions of differential operators.
  - **Finite element** methods leverage basis functions with local support (e.g. B-splines) and yield sparsity in the resulting problem since many pairs of basis functions have disjoint support.
Solving BVPs by Optimization

▶ To improve robustness, define and minimize a residual error over the whole domain rather than at collocation points.

▶ For simplified scenario \( f(t, y) = f(t) \),

\[
\mathbf{r}(t, \mathbf{x}) = \mathbf{v}'(t, \mathbf{x}) - f(t) = \sum_{j=1}^{n} x_j \phi'_j(t) - f(t).
\]

▶ In particular, we seek to minimize the objective function,

\[
F(\mathbf{x}) = \frac{1}{2} \int_{a}^{b} ||\mathbf{r}(t, \mathbf{x})||^2 dt.
\]

▶ The first-order optimality conditions of the optimization problem are a system of linear equations \( A\mathbf{x} = \mathbf{b} \):

\[
0 = \frac{dF}{dx_i} = \int_{a}^{b} \mathbf{r}(t, \mathbf{x})^T \frac{d\mathbf{r}}{dx_i} dt = \int_{a}^{b} \mathbf{r}(t, \mathbf{x})^T \phi'_i(t) dt
\]

\[
= \sum_{j=1}^{n} x_j \int_{a}^{b} \phi'_j(t)^T \phi'_i(t) dt - \int_{a}^{b} f(t)^T \phi'_i(t) dt
\]
Weighted Residual

- **Weighted residual methods** work by ensuring the residual is orthogonal with respect to a given set of weight functions:
  - Rather than setting components of the gradient to zero, we instead have
    \[
    \int_a^b r(t, x)^T w_i(t) dt = 0, \forall i \in \{1, \ldots, n\}.
    \]
  - Again, we obtain a system of equations of the form \(Ax = b\), where
    \[
    a_{ij} = \int_a^b \phi'_j(t)^T w_i(t), \quad b_i = \int_a^b f(t)^T w_i(t).
    \]
  - The collocation method is a weighted residual method where \(w_i(t) = \delta(t - t_i)\).
  - The Galerkin method is a weighted residual method where \(w_i = \phi_i\).

Linear system with the **stiffness matrix** \(A\) and load vector \(b\) is

\[
0 = \sum_{j=1}^n x_j \underbrace{\int_a^b \phi'_j(t)^T \phi_i(t) dt}_{a_{ij}} - \underbrace{\int_a^b f(t)^T \phi_i(t) dt}_{b_i}.
\]
Second-Order BVPs: Poisson Equation

In practice, BVPs are at least second order and it's advantageous to work in the natural set of variables.

- Consider the *Poisson equation* \( u'' = f(t) \) with boundary conditions \( u(a) = u(b) = 0 \) and define a localized basis of hat functions:

\[
\phi_i(t) = \begin{cases} 
(t - t_{i-1})/h : t \in [t_{i-1}, t_i] \\
(t_{i+1} - t)/h : t \in [t_i, t_{i+1}] \\
0 & \text{otherwise}
\end{cases}
\]

for \( i \in \{1, \ldots, n\} \), handling boundaries via \( t_0 = t_1 = a \) and \( t_{n+1} = t_n = b \).

- Defining residual equation by analogy to the first order case, we obtain,

\[
r = v'' - f, \quad \text{so that} \quad r(t, x) = \sum_{j=1}^{n} x_j \phi_j''(t) - f(t).
\]

However, with our choice of basis, \( \phi_j''(t) \) is undefined, since \( \phi_j'(t) \) is discontinuous at \( t_{j-1}, t_j, t_{j+1} \).
The finite-element method permits a lesser degree of differentiability of basis functions by casting the ODE in weak form:

For any solution $u$, if test function $\phi_i$ satisfies the boundary conditions, the ODE satisfies the weak form,

\[
\int_a^b f(t)\phi_i(t)\,dt = \int_a^b u''(t)\phi_i(t)\,dt = u'(b)\phi_i(b) - u'(a)\phi_i(a) - \int_a^b u'(t)\phi_i'(t)\,dt
\]

\[
= -\int_a^b u'(t)\phi_i'(t)\,dt.
\]

Note that the final equation contains no second derivatives, and subsequently we can form the linear system $Ax = b$ with

\[
a_{ij} = -\int_a^b \phi_j'(t)\phi_i'(t)\,dt, \quad b_i = \int_a^b f(t)\phi_i(t)\,dt.
\]

The finite element method thus searches the larger (once-differentiable) function space to find a solution $u$ that is in a (twice-differentiable) subspace.
Eigenvalue Problems with ODEs

- A typical second-order scalar ODE BVP eigenvalue problem is

\[ u'' = \lambda f(t, u, u'), \quad \text{with boundary conditions } u(a) = 0, u(b) = 0. \]

These can be solved, e.g. for \( f(t, u, u') = g(t)u \) by finite differences:

- Approximating the solution at a set of points \( t_1, \ldots, t_n \) using finite differences,

\[ \frac{y_{i+1} - 2y_i + y_{i-1}}{h^2} = \lambda g_i y_i. \]

- This yields a tridiagonal matrix eigenvalue problem \( Ay = \lambda y \) where

\[ \frac{y_{i+1} - 2y_i + y_{i-1}}{g_i h^2} = \lambda y_i. \]
Generalized matrix eigenvalue problems arise from more sophisticated ODEs,

\[ u'' = \lambda(g(t)u + h(t)u'), \quad \text{with boundary conditions } u(a) = 0, u(b) = 0. \]

Again approximate each of the derivatives at a set of points \( t_1, \ldots, t_n \) using finite differences,

\[ \frac{y_{i+1} - 2y_i + y_{i-1}}{h^2} = \lambda \left( g_i + \frac{y_{i+1} - y_{i-1}}{2h} \right) y_i. \]

These corresponds to a generalized matrix eigenvalue problem

\[ Ay = \lambda By, \]

where both \( A \) and \( B \) are tridiagonal.

Specialized methods exist for solving generalized matrix eigenvalue problems (also referred to as matrix pencil eigenvalue problems).