CS 450: Numerical Analysis\(^1\)
Boundary Value Problems for Ordinary Differential Equations

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\(^1\) These 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

$$y'(t) = A(t)y(t) + b(t) \quad \Rightarrow \quad Y'(t)u(t) + Y(t)u'(t) = A(t)Y(t)u(t) + b(t),$$

$$Y'(t) = A(t)Y(t) \quad \Rightarrow \quad u'(t) = Y(t)^{-1}b(t).$$

Solution $u(t)$ (and $y(t)$) exists if $Q = B_aY(a) + B_bY(b)$ is invertible:

$$B_aY(a)u(a) + B_bY(b)\left(\int_a^b u'(s)ds\right) = c,$$

$$u(a) = \left(\frac{Q}{B_aY(a) + B_bY(b)}\right)^{-1}\left(c - B_bY(b)\int_a^b u'(s)ds\right).$$
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 fundamental matrix and the 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 $y(t)$,

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

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

$$= \Phi(t)c + Y(t)Q^{-1}\left(B_aY(a)\int_a^t Y^{-1}(s)b(s)ds - B_bY(b)\int_t^b Y^{-1}(s)b(s)ds\right).$$
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
   \[ h(x) = B_a x + B_b y_x(b) - c, \text{ where } y_x(b) \text{ is the IVP solution with } y_x(a) = x. \]

**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 satisfy boundary conditions, finite difference methods 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,**

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

**The resulting system of equations can be solved by standard methods and is linear if** $\hat{f}$ **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:

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

where \((A + B)u = [3 \ 0 \ \cdots \ 0 \ -3]^T\).
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 $f(t, y) = f(t)$,
    
    $$
    r(t, x) = v'(t, x) - f(t) = \sum_{j=1}^{n} x_j \phi'_j(t) - f(t).
    $$

- In particular, we seek to minimize the objective function,
  
  $$
  F(x) = \frac{1}{2} \int_{a}^{b} ||r(t, x)||^2 dt.
  $$

- The first-order optimality conditions of the optimization problem are a system of linear equations $Ax = b$:
  
  $$
  0 = \frac{dF}{dx_i} = \int_{a}^{b} r(t, x)^T \frac{dr}{dx_i} dt = \int_{a}^{b} r(t, x)^T \phi'_i(t) dt = \sum_{j=1}^{n} x_j \int_{a}^{b} \phi'_j(t)^T \phi'_i(t) dt - \int_{a}^{b} f(t)^T \phi'_i(t) dt
  $$
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 \( w_i(t) = \phi_i \).

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

\[
0 = \sum_{j=1}^{n} x_j \left[ \int_a^b \phi_j'(t)^T \phi_i(t) dt - \int_a^b f(t)^T \phi_i(t) dt \right].
\]
Second-Order BVPs: Poisson Equation

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

Consider the Poisson equation \( u''(t) = f(t) \) 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 \( t_n = t_{n+1} = b \).

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

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

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 ODEs such as Poisson in weak form:

If the test functions \( \{ \phi_i \}_{i=1}^n \) satisfy the boundary conditions,

\[
0 = \int_a^b r(t, x) \phi_i(t) dt = \sum_{j=1}^n x_j \int_a^b \phi_j''(t) \phi_i(t) dt - \int_a^b f(t) \phi_i(t) dt
\]

\[
= \sum_{j=1}^n x_j \left( \phi_j'(b) \phi_i(b) - \phi_j'(a) \phi_i(a) - \int_a^b \phi_j'(t) \phi_i'(t) dt \right) - \int_a^b f(t) \phi_i(t) dt
\]

\[
= - \sum_{j=1}^n x_j \int_a^b \phi_j'(t) \phi_i'(t) dt - \int_a^b f(t) \phi_i(t) dt.
\]

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.
A typical second-order scalar ODE BVP eigenvalue problem is to find eigenvalue $\lambda$ and eigenfunction $u$ to satisfy

$$u'' = \lambda f(t, u, u'),$$

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

$$\frac{y_{i+1} - 2y_i + y_{i-1}}{g_i h^2} = \lambda y_i.$$
Using Generalized Matrix Eigenvalue Problems

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).