

CS 450: Numerical Analysis¹

Boundary Value Problems for Ordinary Differential Equations

University of Illinois at Urbana-Champaign

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 $\mathbf{y}(t)$ at boundary.
 - ▶ *Neumann boundary conditions* specify values of derivative $\mathbf{f}(t, \mathbf{y})$ at boundary.
- ▶ Consider a first order ODE $\mathbf{y}'(t) = \mathbf{f}(t, \mathbf{y})$ with *linear boundary conditions* on domain $t \in [a, b]$:

$$\mathbf{B}_a \mathbf{y}(a) + \mathbf{B}_b \mathbf{y}(b) = \mathbf{c}$$

- ▶ *IVPs are a special case of Dirichlet condition with $\mathbf{B}_a = \mathbf{I}$, $\mathbf{B}_b = \mathbf{0}$.*
- ▶ *Conditions are **separated** if they do not couple different boundary points, i.e., for all i , the i th row of either \mathbf{B}_a or \mathbf{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 $\mathbf{y}'(t) = \mathbf{A}(t)\mathbf{y}(t) + \mathbf{b}(t)$ are linear combinations of solutions to linear homogeneous ODE IVPs $\mathbf{y}'(t) = \mathbf{A}(t)\mathbf{y}(t)$:

- ▶ Let the solutions $\mathbf{y}_i(t)$ to the homogeneous ODE, $\mathbf{y}'_i(t) = \mathbf{A}(t)\mathbf{y}_i(t)$, with initial conditions $\mathbf{y}_i(a) = \mathbf{e}_i$ be columns of

$$\mathbf{Y}(t) = [\mathbf{y}_1(t) \quad \cdots \quad \mathbf{y}_n(t)] = \mathbf{I} + \int_a^t \mathbf{A}(s)\mathbf{Y}(s)ds.$$

- ▶ The ODE BVP solutions are then given by $\mathbf{y}(t) = \mathbf{Y}(t)\mathbf{u}(t)$ for some $\mathbf{u}(t)$, with

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

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

- ▶ Solution $\mathbf{u}(t)$ (and $\mathbf{y}(t)$) exists if $\mathbf{Q} = \mathbf{B}_a\mathbf{Y}(a) + \mathbf{B}_b\mathbf{Y}(b)$ is invertible:

$$\mathbf{B}_a\mathbf{Y}(a)\mathbf{u}(a) + \mathbf{B}_b\mathbf{Y}(b)\left(\mathbf{u}(a) + \int_a^b \mathbf{u}'(s)ds\right) = \mathbf{c},$$

$$\mathbf{u}(a) = \left(\underbrace{\mathbf{B}_a\mathbf{Y}(a) + \mathbf{B}_b\mathbf{Y}(b)}_{\mathbf{Q}}\right)^{-1}\left(\mathbf{c} - \mathbf{B}_b\mathbf{Y}(b) \int_a^b \mathbf{u}'(s)ds\right).$$

Green's Function Form of Solution for Linear ODE BVPs

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

$$\mathbf{y}(t) = \Phi(t)\mathbf{c} + \int_a^b \mathbf{G}(t, s)\mathbf{b}(s)ds$$

$\Phi(t) = \mathbf{Y}(t)\mathbf{Q}^{-1}$ is the *fundamental matrix* and the *Green's function* is

$$\mathbf{G}(t, s) = \mathbf{Y}(t)\mathbf{Q}^{-1}\mathbf{I}(s)\mathbf{Y}^{-1}(s), \quad \mathbf{I}(s) = \begin{cases} \mathbf{B}_a\mathbf{Y}(a) & : s < t \\ -\mathbf{B}_b\mathbf{Y}(b) & : s \geq t \end{cases}$$

- ▶ From our expression for $\mathbf{u}(a)$ and the integral equation for $\mathbf{y}(t)$,

$$\begin{aligned} \mathbf{y}(t) &= \mathbf{Y}(t)\mathbf{Q}^{-1}\left(\mathbf{c} - \mathbf{B}_b\mathbf{Y}(b) \int_a^b \mathbf{u}'(s)ds\right) + \mathbf{Y}(t) \int_a^t \mathbf{u}'(s)ds \\ &= \Phi(t)\mathbf{c} + \mathbf{Y}(t)\mathbf{Q}^{-1}\left(-\mathbf{B}_b\mathbf{Y}(b) \int_a^b \mathbf{u}'(s)ds + \mathbf{Q} \int_a^t \mathbf{u}'(s)ds\right) \\ &= \Phi(t)\mathbf{c} + \mathbf{Y}(t)\mathbf{Q}^{-1}\left(\mathbf{B}_a\mathbf{Y}(a) \int_a^t \mathbf{Y}^{-1}(s)\mathbf{b}(s)ds - \mathbf{B}_b\mathbf{Y}(b) \int_t^b \mathbf{Y}^{-1}(s)\mathbf{b}(s)ds\right). \end{aligned}$$

Conditioning of Linear ODE BVPs

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

$$\mathbf{y}(t) = \mathbf{\Phi}(t)\mathbf{c} + \int_a^b \mathbf{G}(t, s)\mathbf{b}(s)ds$$

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

- ▶ The absolute condition number of the BVP is $\kappa = \max\{\|\mathbf{\Phi}\|_\infty, \|\mathbf{G}\|_\infty\}$:
This sensitivity measure enables us to bound the perturbation $\|\hat{\mathbf{y}} - \mathbf{y}\|_\infty$ with respect to the magnitude of a perturbation to $\mathbf{b}(t)$ or \mathbf{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 $k = 1, 2, \dots$ 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 $l = 1, \dots, k$ as guesses $x^{(1)}, \dots, x^{(k)}$ 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 (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, \dots, t_n , so that $\hat{\mathbf{y}}_k \approx \mathbf{y}(t_k)$ by finite-difference formulae, for example,

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

- ▶ *The resulting system of equations can be solved by standard methods and is linear if \mathbf{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.*

Finite Difference Methods

- ▶ Lets 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, \dots, 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 $i \in \{2, \dots, n - 1\}$,

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

- ▶ These correspond to a linear system based on matrices:

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

where $(\mathbf{A} + \mathbf{B})\mathbf{u} = [3 \quad 0 \quad \dots \quad 0 \quad -3]^T$.

Collocation Methods

- ▶ *Collocation methods* approximate \mathbf{y} by representing it in a basis

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

- ▶ Seek to satisfy for collocation points t_1, \dots, t_n with $t_1 = a$ and $t_n = b$,

$$\forall_{i \in \{2, \dots, n-1\}} \quad \mathbf{v}'(t_i, \mathbf{x}) = \mathbf{f}(t_i, \mathbf{v}(t_i, \mathbf{x})).$$

- ▶ 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 ϕ_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 $\mathbf{f}(t, y) = \mathbf{f}(t)$,

$$\mathbf{r}(t, \mathbf{x}) = \mathbf{v}'(t, \mathbf{x}) - \mathbf{f}(t) = \sum_{j=1}^n x_j \phi_j'(t) - \mathbf{f}(t).$$

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

$$F(\mathbf{x}) = \frac{1}{2} \int_a^b \|\mathbf{r}(t, \mathbf{x})\|_2^2 dt.$$

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

$$\begin{aligned} \mathbf{0} &= \frac{dF}{dx_i} = \int_a^b \mathbf{r}(t, \mathbf{x})^T \frac{d\mathbf{r}}{dx_i} dt = \int_a^b \mathbf{r}(t, \mathbf{x})^T \phi_i'(t) dt \\ &= \sum_{j=1}^n x_j \underbrace{\int_a^b \phi_j'(t)^T \phi_i'(t) dt}_{a_{ij}} - \underbrace{\int_a^b \mathbf{f}(t)^T \phi_i'(t) dt}_{b_i} \end{aligned}$$

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*

$$\int_a^b \mathbf{r}(t, \mathbf{x})^T \mathbf{w}_i(t) dt = 0, \forall i \in \{1, \dots, n\}.$$

- ▶ *Again, we obtain a system of equations of the form $\mathbf{Ax} = \mathbf{b}$, where*

$$a_{ij} = \int_a^b \phi'_j(t)^T \mathbf{w}_i(t), \quad b_i = \int_a^b \mathbf{f}(t)^T \mathbf{w}_i(t).$$

- ▶ *The collocation method is a weighted residual method where $\mathbf{w}_i(t) = \delta(t - t_i)$.*
- ▶ The Galerkin method is a weighted residual method where $\mathbf{w}_i = \phi_i$.

*Linear system with the **stiffness matrix** \mathbf{A} and **load vector** \mathbf{b} is*

$$\mathbf{0} = \sum_{j=1}^n x_j \underbrace{\int_a^b \phi'_j(t)^T \phi_i(t) dt}_{a_{ij}} - \underbrace{\int_a^b \mathbf{f}(t)^T \phi_i(t) dt}_{b_i}.$$

Second-Order BVPs: Poisson Equation

In practice, BVPs are at least second order and its 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:

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

for $i \in \{1, \dots, n\}$, 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,

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

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} .

Weak Form and the Finite Element Method

- ▶ 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 ϕ_i satisfies the boundary conditions, the ODE satisfies the weak form,

$$\begin{aligned}\int_a^b f(t)\phi_i(t)dt &= \int_a^b u''(t)\phi_i(t)dt = u'(b)\underbrace{\phi_i(b)}_0 - u'(a)\underbrace{\phi_i(a)}_0 - \int_a^b u'(t)\phi_i'(t)dt \\ &= - \int_a^b u'(t)\phi_i'(t)dt.\end{aligned}$$

- ▶ Note that the final equation contains no second derivatives, and subsequently we can form the linear system $\mathbf{Ax} = \mathbf{b}$ 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, \dots, 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 $\mathbf{A}\mathbf{y} = \lambda\mathbf{y}$ 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, \dots, 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*

$$A\mathbf{y} = \lambda B\mathbf{y},$$

where both A and B are tridiagonal.

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