CS 450: Numerical Anlaysis[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 $\boldsymbol{y}(t)$ at boundary.*
  - *Neumann boundary conditions specify values of derivative $\boldsymbol{f}(t, \boldsymbol{y})$ at boundary.*
- Consider a first order ODE $\boldsymbol{y}'(t) = \boldsymbol{f}(t, \boldsymbol{y})$ with *linear boundary conditions* on domain $t \in [a, b]$:

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

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

$$\boldsymbol{Y}(t) = \begin{bmatrix} \boldsymbol{y}_1(t) & \cdots & \boldsymbol{y}_n(t) \end{bmatrix} = \boldsymbol{I} + \int_a^t \boldsymbol{A}(s)\boldsymbol{Y}(s)ds.$$

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

$$\begin{aligned} \boldsymbol{y}'(t) = \boldsymbol{A}(t)\boldsymbol{y}(t) + \boldsymbol{b}(t) \quad &\Rightarrow \quad \boldsymbol{Y}'(t)\boldsymbol{u}(t) + \boldsymbol{Y}(t)\boldsymbol{u}'(t) = \boldsymbol{A}(t)\boldsymbol{Y}(t)\boldsymbol{u}(t) + \boldsymbol{b}(t), \\ \boldsymbol{Y}'(t) = \boldsymbol{A}(t)\boldsymbol{Y}(t) \quad &\Rightarrow \quad \boldsymbol{u}'(t) = \boldsymbol{Y}(t)^{-1}\boldsymbol{b}(t). \end{aligned}$$

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

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

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

Green's Function Form of Solution for Linear ODE BVPs

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

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

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

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

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

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

Conditioning of Linear ODE BVPs

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

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

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

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

  This sensitivity measure enables us to bound the perturbation $||\hat{\boldsymbol{y}} - \boldsymbol{y}||_\infty$ *with respect to the magnitude of a perturbation to* $\boldsymbol{b}(t)$ *or* $\boldsymbol{c}$*.*

Shooting Method for ODE BVPs

- For linear ODEs, we construct solutions from IVP solutions in $\boldsymbol{Y}(t)$, 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 $\hat{\boldsymbol{y}}^{(k)}(a) \approx \boldsymbol{y}(a)$,*
  2. *solve the resulting IVP,*
  3. *check the quality of the solution at the new boundary,*
  $$||\boldsymbol{B}_b\hat{\boldsymbol{y}}^{(k)}(b) - \boldsymbol{B}_a\hat{\boldsymbol{y}}^{(k)}(a) - \boldsymbol{c}||,$$
  4. *pick the initial conditions for the next shot, $\hat{\boldsymbol{y}}^{(k+1)}(a)$ by treating $\hat{\boldsymbol{y}}^{(l)}(a)$ for $l = 1, \ldots, k$ as guesses $\boldsymbol{x}^{(1)}, \ldots, \boldsymbol{x}^{(k)}$ to root finding procedure for*
  $$\boldsymbol{h}(\boldsymbol{x}) = \boldsymbol{B}_a\boldsymbol{x} + \boldsymbol{B}_b\boldsymbol{y}_{\boldsymbol{x}}(b) - \boldsymbol{c}, \text{ where } \boldsymbol{y}_{\boldsymbol{x}}(b) \text{ is the IVP solution with } \boldsymbol{y}_{\boldsymbol{x}}(a) = \boldsymbol{x}.$$
- *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 $\hat{\boldsymbol{y}}_k \approx \boldsymbol{y}(t_k)$ by finite-difference formulae, for example,*

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

  - *The resulting system of equations can be solved by standard methods and is linear if $\boldsymbol{f}$ 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 $t_1, \ldots, t_n$, $t_{i+1} - t_i = h$.

  - *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:*

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

where $(\boldsymbol{A}+\boldsymbol{B})\boldsymbol{u} = \begin{bmatrix} 3 & 0 & \cdots 0 & -3 \end{bmatrix}^T$.

Collocation Methods

Demo: Sparse matrices

- *Collocation methods* approximate $\boldsymbol{y}$ by representing it in a basis

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

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

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

  - *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 $\boldsymbol{f}(t, y) = \boldsymbol{f}(t)$,*

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

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

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

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

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

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*

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

  - *Again, we obtain a system of equations of the form $\boldsymbol{A}\boldsymbol{x} = \boldsymbol{b}$, where*

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

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

  Linear system with the stiffness matrix $\boldsymbol{A}$ and load vector $\boldsymbol{b}$ is

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

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* $u''(t) = f(t)$ with boundary conditions $u(a) = u(b) = 0$ and define a localized basis of hat functions:

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

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

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

  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,*

$$\int_a^b f(t)\phi_i(t)dt = \int_a^b u''(t)\phi_i(t)dt = u'(b)\underbrace{\phi_i(b)}_{0} - u'(a)\underbrace{\phi_i(a)}_{0} - \int_a^b u'(t)\phi_i'(t)dt$$
$$= -\int_a^b u'(t)\phi_i'(t)dt.$$

  - *Note that the final equation contains no second derivatives, and subsequently we can form the linear system $\boldsymbol{Ax} = \boldsymbol{b}$ 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 to find eigenvalue λ and eigenfunction u to satisfy

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

  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 $\boldsymbol{A}\boldsymbol{y} = \lambda \boldsymbol{y}$ 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*

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

    where both $\boldsymbol{A}$ and $\boldsymbol{B}$ are tridiagonal.

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