Lecture Notes to Accompany

Scientific Computing

An Introductory Survey
Second Edition

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Chapter 10

Boundary Value Problems for Ordinary Differential Equations

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Boundary Value Problems

Side conditions prescribing solution or derivative values at specified points required to make solution of ODE unique

In initial value problem, all side conditions specified at single point, say t_0

In boundary value problem (BVP), side conditions specified at more than one point

kth order ODE, or equivalent first-order system, requires k side conditions

For ODE, side conditions typically specified at two points, endpoints of interval [a,b], so we have two-point boundary value problem

Boundary Value Problems, continued

General first-order two-point BVP has form

$$y' = f(t, y),$$
 $a < t < b,$

with boundary conditions

$$g(y(a), y(b)) = o,$$

where $f: \mathbb{R}^{n+1} \to \mathbb{R}^n$ and $g: \mathbb{R}^{2n} \to \mathbb{R}^n$

Boundary conditions are *separated* if any given component of g involves solution values only at a or at b, but not both

Boundary conditions are linear if of form

$$B_a y(a) + B_b y(b) = c,$$

where $oldsymbol{B}_a, oldsymbol{B}_b \in \mathbb{R}^{n imes n}$ and $oldsymbol{c} \in \mathbb{R}^n$

BVP is *linear* if both ODE and boundary conditions are linear

Example: Separated Linear BC

Two-point BVP for second-order scalar ODE

$$u'' = f(t, u, u'), \qquad a < t < b,$$

with boundary conditions

$$u(a) = \alpha, \qquad u(b) = \beta,$$

is equivalent to first-order system of ODEs

$$\begin{bmatrix} y_1' \\ y_2' \end{bmatrix} = \begin{bmatrix} y_2 \\ f(t, y_1, y_2) \end{bmatrix}, \quad a < t < b,$$

with separated linear boundary conditions

$$\begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix} \begin{bmatrix} y_1(a) \\ y_2(a) \end{bmatrix} + \begin{bmatrix} 0 & 0 \\ 1 & 0 \end{bmatrix} \begin{bmatrix} y_1(b) \\ y_2(b) \end{bmatrix} = \begin{bmatrix} \alpha \\ \beta \end{bmatrix}$$

Existence and Uniqueness

Unlike IVP, with BVP we cannot begin at initial point and continue solution step by step to nearby points

Instead, solution determined everywhere simultaneously, so existence and/or uniqueness may not hold

For example,

$$u'' = -u, \qquad 0 < t < b,$$

with boundary conditions

$$u(0) = 0, \qquad u(b) = \beta,$$

with b integer multiple of π , has infinitely many solutions if $\beta = 0$, but no solution if $\beta \neq 0$

Existence and Uniqueness, continued

In general, solvability of BVP

$$y' = f(t, y), \qquad a < t < b,$$

with boundary conditions

$$g(y(a), y(b)) = o,$$

depends on solvability of algebraic equation

$$g(x, y(b; x)) = o,$$

where y(t;x) denotes solution to ODE with initial condition y(a)=x for $x\in\mathbb{R}^n$

Solvability of latter system is difficult to establish if $oldsymbol{g}$ is nonlinear

Existence and Uniqueness, continued

For *linear* BVP, existence and uniqueness are more tractable

Consider linear BVP

$$y' = A(t) y + b(t), \qquad a < t < b,$$

where $\boldsymbol{A}(t)$ and $\boldsymbol{b}(t)$ are continuous, with boundary conditions

$$B_a y(a) + B_b y(b) = c$$

Let Y(t) denote matrix whose ith column, $y_i(t)$, called ith mode, is solution to y' = A(t)y with initial condition $y(a) = e_i$

Then BVP has unique solution if, and only if, matrix

$$Q \equiv B_a Y(a) + B_b Y(b)$$

is nonsingular

Existence and Uniqueness, continued

Assuming Q is nonsingular, define

$$\Phi(t) = Y(t) Q^{-1}$$

and Green's function

$$G(t,s) = \begin{cases} \Phi(t)B_a\Phi(a)\Phi^{-1}(s), & a \le s \le t \\ -\Phi(t)B_b\Phi(b)\Phi^{-1}(s), & t < s \le b \end{cases}$$

Then solution to BVP given by

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

This result also gives absolute condition number for BVP,

$$\kappa = \max\{\|\Phi\|_{\infty}, \|G\|_{\infty}\}$$

Conditioning and Stability

Conditioning or stability of BVP depends on interplay between growth of solution modes and boundary conditions

For IVP, instability is associated with modes that grow exponentially as time increases

For BVP, solution is determined everywhere simultaneously, so there is no notion of "direction" of integration in interval [a,b]

Growth of modes increasing with time is limited by boundary conditions at b, and "growth" of decaying modes is limited by boundary conditions at a

For BVP to be well-conditioned, growing and decaying modes must be controlled appropriately by boundary conditions imposed

Numerical Methods for BVPs

For IVP, initial data supply all information necessary to begin numerical solution method at initial point and step forward from there

For BVP, we have insufficient information to begin step-by-step numerical method, so numerical methods for solving BVPs are more complicated than those for solving IVPs

We consider four types of numerical methods for two-point BVPs:

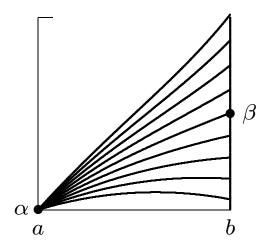
- Shooting
- Finite difference
- Collocation
- Galerkin

Shooting Method

In statement of two-point BVP, we are given value of u(a)

If we also knew value of u'(a), then we would have IVP that we could solve by methods previously discussed

Lacking that information, we try sequence of increasingly accurate guesses until we find value for u'(a) such that when we solve resulting IVP, approximate solution value at t=b matches desired boundary value, $u(b)=\beta$



Shooting Method, continued

For given γ , value at b of solution u(b) to IVP

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

with initial conditions

$$u(a) = \alpha, \qquad u'(a) = \gamma,$$

can be considered as function of γ , say $g(\gamma)$

Then BVP becomes problem of solving equation $g(\gamma) = \beta$

One-dimensional zero finder can be used to solve this scalar equation

Example: Shooting Method

Consider two-point BVP for second-order ODE

$$u'' = 6t,$$
 0 < t < 1,

with BC

$$u(0) = 0,$$
 $u(1) = 1$

For each guess for u'(0), we integrate ODE using classical fourth-order Runge-Kutta method to determine how close we come to hitting desired solution value at t=1

We transform second-order ODE into system of two first-order ODEs

$$\begin{bmatrix} y_1' \\ y_2' \end{bmatrix} = \begin{bmatrix} y_2 \\ 6t \end{bmatrix}$$

We try initial slope of $y_2(0) = 1$

Using step size h = 0.5, we first step from $t_0 = 0$ to $t_1 = 0.5$

Classical fourth-order Runge-Kutta method gives approximate solution value at t_1

$$y^{(1)} = y^{(0)} + \frac{h}{6}(k_1 + 2k_2 + 2k_3 + k_4)$$

$$= \begin{bmatrix} 0 \\ 1 \end{bmatrix} + \frac{0.5}{6} \left(\begin{bmatrix} 1 \\ 0 \end{bmatrix} + 2 \begin{bmatrix} 1.0 \\ 1.5 \end{bmatrix} + 2 \begin{bmatrix} 1.375 \\ 1.500 \end{bmatrix} + \begin{bmatrix} 1.75 \\ 3.00 \end{bmatrix} \right) = \begin{bmatrix} 0.625 \\ 1.750 \end{bmatrix}$$

Next we step from $t_1 = 0.5$ to $t_2 = 1$, getting

$$y^{(2)} = \begin{bmatrix} 0.625 \\ 1.750 \end{bmatrix} + \frac{0.5}{6} \left(\begin{bmatrix} 1.75 \\ 3.00 \end{bmatrix} + 2 \begin{bmatrix} 2.5 \\ 4.5 \end{bmatrix} \right)$$
$$+ 2 \begin{bmatrix} 2.875 \\ 4.500 \end{bmatrix} + \begin{bmatrix} 4 \\ 6 \end{bmatrix} = \begin{bmatrix} 2 \\ 4 \end{bmatrix},$$

so we have hit $y_1(1) = 2$ instead of desired value $y_1(1) = 1$

We try again, this time with initial slope $y_2(0) = -1$, obtaining

$$y^{(1)} = \begin{bmatrix} 0 \\ -1 \end{bmatrix} + \frac{0.5}{6} \left(\begin{bmatrix} -1 \\ 0 \end{bmatrix} + 2 \begin{bmatrix} -1.0 \\ 1.5 \end{bmatrix} \right)$$
$$+ 2 \begin{bmatrix} -0.625 \\ 1.500 \end{bmatrix} + \begin{bmatrix} -0.25 \\ 3.00 \end{bmatrix} = \begin{bmatrix} -0.375 \\ -0.250 \end{bmatrix},$$

$$y^{(2)} = \begin{bmatrix} -0.375 \\ -0.250 \end{bmatrix} + \frac{0.5}{6} \left(\begin{bmatrix} -0.25 \\ 3.00 \end{bmatrix} + 2 \begin{bmatrix} 0.5 \\ 4.5 \end{bmatrix} + 2 \begin{bmatrix} 0.875 \\ 4.500 \end{bmatrix} + \begin{bmatrix} 2 \\ 6 \end{bmatrix} \right) = \begin{bmatrix} 0 \\ 2 \end{bmatrix},$$

so we have hit $y_1(1) = 0$ instead of desired value $y_1(1) = 1$

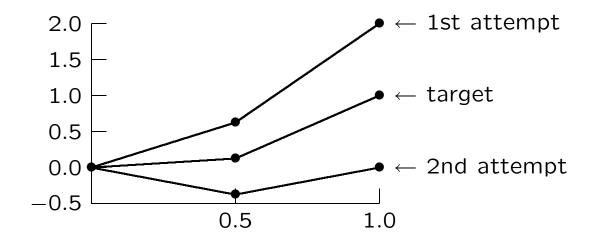
We now have initial slope bracketed between -1 and 1

We omit further iterations necessary to identify correct initial slope, which turns out to be $y_2(0) = 0$:

$$y^{(1)} = \begin{bmatrix} 0 \\ 0 \end{bmatrix} + \frac{0.5}{6} \left(\begin{bmatrix} 0 \\ 0 \end{bmatrix} + 2 \begin{bmatrix} 0.0 \\ 1.5 \end{bmatrix} \right)$$
$$+ 2 \begin{bmatrix} 0.375 \\ 1.500 \end{bmatrix} + \begin{bmatrix} 0.75 \\ 3.00 \end{bmatrix} \right) = \begin{bmatrix} 0.125 \\ 0.750 \end{bmatrix},$$

$$y^{(2)} = \begin{bmatrix} 0.125 \\ 0.750 \end{bmatrix} + \frac{0.5}{6} \left(\begin{bmatrix} 0.75 \\ 3.00 \end{bmatrix} + 2 \begin{bmatrix} 1.5 \\ 4.5 \end{bmatrix} + 2 \begin{bmatrix} 1.875 \\ 4.500 \end{bmatrix} + \begin{bmatrix} 3 \\ 6 \end{bmatrix} \right) = \begin{bmatrix} 1 \\ 3 \end{bmatrix},$$

so we have indeed hit target solution value, $y_1(1) = 1$



Multiple Shooting

Simple shooting method inherits stability (or instability) of associated IVP, which may be unstable even when BVP is stable

Such ill-conditioning may make it difficult to achieve convergence of iterative method for solving nonlinear equation

Potential remedy is $multiple\ shooting$, in which interval [a,b] is divided into subintervals, and shooting is carried out on each

Requiring continuity at internal mesh points provides BC for individual subproblems

Multiple shooting results in larger *system* of nonlinear equations to solve

Finite Difference Method

Finite difference method converts BVP into system of algebraic equations by replacing all derivatives by finite difference approximations

For example, to solve two-point BVP

$$u'' = f(t, u, u'), \qquad a < t < b,$$

with BC

$$u(a) = \alpha, \qquad u(b) = \beta,$$

we introduce mesh points $t_i = a + ih$, i = 0, 1, ..., n + 1, where h = (b - a)/(n + 1)

We already have $y_0 = u(a) = \alpha$ and $y_{n+1} = u(b) = \beta$, and we seek approximate solution value $y_i \approx u(t_i)$ at each mesh point t_i , $i = 1, \ldots, n$

Finite Difference Method, continued

We replace derivatives by finite difference quotients, such as

$$u'(t_i) \approx \frac{y_{i+1} - y_{i-1}}{2h}$$

and

$$u''(t_i) \approx \frac{y_{i+1} - 2y_i + y_{i-1}}{h^2},$$

yielding system of equations

$$\frac{y_{i+1} - 2y_i + y_{i-1}}{h^2} = f\left(t_i, y_i, \frac{y_{i+1} - y_{i-1}}{2h}\right),$$

to be solved for unknowns y_i , i = 1, ..., n

System of equations may be linear or nonlinear, depending on whether f is linear or nonlinear

Finite Difference Method, continued

In this example, system to be solved is tridiagonal, which saves on both work and storage compared to general system of equations

This is generally true of finite difference methods: they yield sparse systems because each equation involves few variables

Example: Finite Difference Method

Consider two-point BVP

$$u'' = 6t,$$
 0 < t < 1,

with BC

$$u(0) = 0,$$
 $u(1) = 1$

To keep computation to minimum, we compute approximate solution at one mesh point in interval [0, 1], t = 0.5

Including boundary points, we have three mesh points, $t_0 = 0$, $t_1 = 0.5$, and $t_2 = 1$

From BC, we know that $y_0 = u(t_0) = 0$ and $y_2 = u(t_2) = 1$, and we seek approximate solution $y_1 \approx u(t_1)$

Approximating second derivative by standard finite difference quotient at t_1 gives equation

$$\frac{y_2 - 2y_1 + y_0}{h^2} = f\left(t_1, y_1, \frac{y_2 - y_0}{2h}\right)$$

Substituting boundary data, mesh size, and right hand side for this example,

$$\frac{1 - 2y_1 + 0}{(0.5)^2} = 6t_1,$$

or

$$4 - 8y_1 = 6(0.5) = 3$$

so that

$$y(0.5) \approx y_1 = 1/8 = 0.125$$

which agrees with approximate solution at t = 0.5 that we previously computed by shooting method

In a practical problem, much smaller step size and many more mesh points would be required to achieve acceptable accuracy

We would therefore obtain *system* of equations to solve for approximate solution values at mesh points, rather than single equation as in this example

Collocation Method

Collocation method approximates solution to BVP by finite linear combination of basis functions

For two-point BVP

$$u'' = f(t, u, u'), \qquad a < t < b,$$

with BC

$$u(a) = \alpha, \qquad u(b) = \beta,$$

we seek approximate solution of form

$$u(t) \approx v(t, \boldsymbol{x}) = \sum_{i=1}^{n} x_i \phi_i(t),$$

where ϕ_i are basis functions defined on [a,b] and ${\boldsymbol x}$ is n-vector of parameters to be determined

Collocation Method

Popular choices of basis functions include polynomials, B-splines, and trigonometric functions

Basis functions with global support, such as polynomials or trigonometric functions, yield spectral or pseudospectral method

Basis functions with highly localized support, such as B-splines, yield *finite element method*

Collocation Method, continued

To determine vector of parameters x, define set of n collocation points, $a=t_1<\cdots< t_n=b$, at which approximate solution v(t,x) is forced to satisfy ODE and boundary conditions

Common choices of collocation points include equally-spaced mesh or Chebyshev points

Suitably smooth basis functions can be differentiated analytically, so that approximate solution and its derivatives can be substituted into ODE and BC to obtain system of algebraic equations for unknown parameters \boldsymbol{x}

Example: Collocation Method

Consider again two-point BVP

$$u'' = 6t,$$
 0 < t < 1,

with BC

$$u(0) = 0,$$
 $u(1) = 1$

To keep computation to minimum, we use one interior collocation point, t = 0.5

Including boundary points, we have three collocation points, $t_0 = 0$, $t_1 = 0.5$, and $t_2 = 1$, so we will be able to determine three parameters

As basis functions we use first three monomials, so approximate solution has form

$$v(t, x) = x_1 + x_2 t + x_3 t^2$$

Derivatives of approximate solution function with respect to t are given by

$$v'(t, x) = x_2 + 2x_3t,$$
 $v''(t, x) = 2x_3$

Requiring ODE to be satisfied at interior collocation point $t_2=0.5$ gives equation

$$v''(t_2, x) = f(t_2, v(t_2, x), v'(t_2, x)),$$

or

$$2x_3 = 6t_2 = 6(0.5) = 3$$

Left boundary condition at $t_1=0$ gives equation

$$x_1 + x_2t_1 + x_3t_1^2 = x_1 = 0,$$

and right boundary condition at $t_3=1$ gives equation

$$x_1 + x_2t_3 + x_3t_3^2 = x_1 + x_2 + x_3 = 1$$

Solving this system of three equations in three unknowns gives

$$x_1 = 0,$$
 $x_2 = -0.5,$ $x_3 = 1.5,$

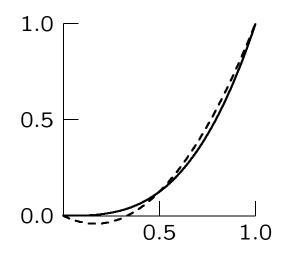
so approximate solution function is quadratic polynomial

$$u(t) \approx v(t, x) = -0.5t + 1.5t^2$$

At interior collocation point, $t_2 = 0.5$, we have approximate solution value

$$u(0.5) \approx v(0.5, x) = 0.125,$$

which agrees with solution value at t=0.5 obtained previously by other two methods



Galerkin Method

Rather than forcing residual to be zero at finite number of points, as in collocation, we could instead minimize residual over entire interval of integration

For example, for scalar *Poisson* equation in one dimension,

$$u'' = f(t), \qquad a < t < b,$$

with homogeneous boundary conditions

$$u(a) = 0, \qquad u(b) = 0,$$

subsitute approximate solution

$$u(t) \approx v(t, \boldsymbol{x}) = \sum_{i=1}^{n} x_i \phi_i(t)$$

into ODE and define residual

$$r(t, \mathbf{x}) = v''(t, \mathbf{x}) - f(t) = \sum_{i=1}^{n} x_i \phi_i''(t) - f(t)$$

Galerkin Method, continued

Using least squares method, we can minimize

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

by setting each component of its gradient to zero, which yields symmetric system of linear algebraic equations Ax = b, where

$$a_{ij} = \int_a^b \phi_j''(t)\phi_i''(t) dt \quad \text{and} \quad b_i = \int_a^b f(t)\phi_i''(t) dt,$$

whose solution gives vector of parameters $oldsymbol{x}$

More generally, weighted residual method forces residual to be orthogonal to each of set of weight functions or test functions w_i , i.e.,

$$\int_{a}^{b} r(t, x) w_{i}(t) dt = 0, \quad i = 1, \dots, n,$$

which yields linear system Ax = b, where now

$$a_{ij} = \int_a^b \phi_j''(t)w_i(t) dt \quad \text{and} \quad b_i = \int_a^b f(t)w_i(t) dt,$$

whose solution gives vector of parameters $oldsymbol{x}$

Galerkin Method, continued

Matrix resulting from weighted residual method is generally not symmetric, and its entries involve second derivatives of basis functions

Both drawbacks overcome by *Galerkin* method, in which weight functions are chosen to be same as basis functions, i.e., $w_i = \phi_i$, $i = 1, \ldots, n$

Orthogonality condition then becomes

$$\int_a^b r(t, \boldsymbol{x}) \phi_i(t) dt = 0, \quad i = 1, \dots, n,$$

or

$$\int_a^b v''(t, \boldsymbol{x}) \phi_i(t) dt = \int_a^b f(t) \phi_i(t) dt, \quad i = 1, \dots, n$$

Galerkin Method, continued

Degree of differentiability can be reduced using integration by parts, which gives

$$\int_{a}^{b} v''(t, \mathbf{x}) \phi_{i}(t) dt = v'(t) \phi_{i}(t) \Big|_{a}^{b} - \int_{a}^{b} v'(t) \phi'_{i}(t) dt
= v'(b) \phi_{i}(b) - v'(a) \phi_{i}(a)
- \int_{a}^{b} v'(t) \phi'_{i}(t) dt$$

Assuming basis functions ϕ_i satisfy homogeneous boundary conditions, so $\phi_i(0) = \phi_i(1) = 0$, orthogonality condition then becomes

$$-\int_{a}^{b} v'(t)\phi'_{i}(t) dt = \int_{a}^{b} f(t)\phi_{i}(t) dt, \quad i = 1, \dots, n,$$

which yields system of linear equations Ax = b, with

$$a_{ij} = -\int_a^b \phi'_j(t)\phi'_i(t) dt$$
 and $b_i = \int_a^b f(t)\phi_i(t) dt$,

whose solution gives vector of parameters $oldsymbol{x}$

 $m{A}$ is symmetric and involves only first derivatives of basis functions

Example: Galerkin Method

Consider again two-point BVP

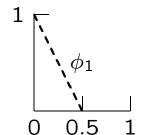
$$u'' = 6t,$$
 0 < t < 1,

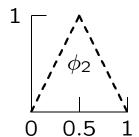
with BC

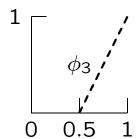
$$u(0) = 0,$$
 $u(1) = 1$

We will approximate solution by piecewise linear polynomial, for which B-splines of degree 1 ("hat" functions) form suitable set of basis functions

To keep computation to minimum, we again use same three mesh points, but now they become knots in piecewise linear polynomial approximation







Thus, we seek approximate solution of form

$$u(t) \approx v(t, x) = x_1 \phi_1(t) + x_2 \phi_2(t) + x_3 \phi_3(t)$$

From BC, we must have $x_1 = 0$ and $x_3 = 1$

To determine remaining parameter x_2 , we impose Galerkin orthogonality condition on interior basis function ϕ_2 and obtain equation

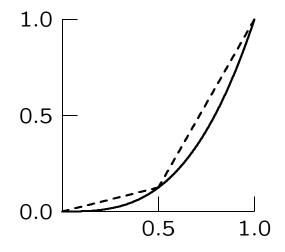
$$-\sum_{j=1}^{3} \left(\int_{0}^{1} \phi'_{j}(t) \phi'_{2}(t) dt \right) x_{j} = \int_{0}^{1} 6t \phi_{2}(t) dt,$$

or, upon evaluating these simple integrals analytically,

$$2x_1 - 4x_2 + 2x_3 = 3/2$$

Substituting known values for x_1 and x_3 then gives $x_2=1/8$ for remaining unknown parameter, so piecewise linear approximate solution is

$$u(t) \approx v(t, x) = 0.125\phi_2(t) + \phi_3(t)$$



We note that v(0.5,x) = 0.125, which again is exact for this particular problem

More realistic problem would have many more interior mesh points and basis functions, and correspondingly many parameters to be determined

Resulting system of equations would be much larger but still sparse, and therefore relatively easy to solve, provided local basis functions, such as "hat" functions, are used

Resulting approximate solution function is less smooth than true solution, but becomes more accurate as more mesh points are used

Eigenvalue Problems

Standard eigenvalue problem for second-order ODE has form

$$u'' = \lambda f(t, u, u'), \qquad a < t < b,$$

with BC

$$u(a) = \alpha, \qquad u(b) = \beta,$$

where we seek not only solution u but also parameter λ as well

Scalar λ (possibly complex) is eigenvalue and solution u corresponding eigenfunction for this two-point BVP

Discretization of eigenvalue problem for ODE results in algebraic eigenvalue problem whose solution approximates that of original problem

Example: Eigenvalue Problem

Consider linear two-point BVP

$$u'' = \lambda g(t)u, \qquad a < t < b,$$

with BC

$$u(a) = 0, \qquad u(b) = 0$$

Introduce discrete mesh points t_i in interval [a,b], with mesh spacing h and use standard finite difference approximation for second derivative to obtain algebraic system

$$\frac{y_{i+1} - 2y_i + y_{i-1}}{h^2} = \lambda g_i y_i, \quad i = 1, \dots, n,$$

where $y_i = u(t_i)$ and $g_i = g(t_i)$, and from BC $y_0 = u(a) = 0$ and $y_{n+1} = u(b) = 0$

Assuming $g_i \neq 0$, divide equation i by g_i for i = 1, ..., n, to obtain linear system

$$Ay = \lambda y$$

where $n \times n$ matrix \boldsymbol{A} has tridiagonal form

$$A = \frac{1}{h^2} \begin{bmatrix} -2/g_1 & 1/g_1 & 0 & \cdots & 0 \\ 1/g_2 & -2/g_2 & 1/g_2 & \ddots & \vdots \\ 0 & \ddots & \ddots & \ddots & 0 \\ \vdots & \ddots & 1/g_{n-1} & -2/g_{n-1} & 1/g_{n-1} \\ 0 & \cdots & 0 & 1/g_n & -2/g_n \end{bmatrix}$$

This standard algebraic eigenvalue problem can be solved by methods discussed previously