AMSC/CMSC 661 Scientific Computing II

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Solution of Ordinary Differential Equations, Boundary Value Problems

Part 1

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These notes are based on the 2003 textbook
of Stig Larsson and Vidar Thomée.

Ordinary Differential Equations, Boundary Value Problems

Ordinary Differential Equations, Boundary Value Problems = ODE/BVP

The plan:

- The problem and boundary conditions
- A motivating problem
- The Maximum Principle
- The Green's function
- The variational formulation
- Regularity of the solution
- Solution and error estimates using finite differences
- Solution and error estimates using finite elements

The philosophy:

- To solve differential equations, we need to understand a lot about theory and a lot about computation.
- This is much easier to master for ODEs than for PDEs.
- Therefore, we will study the theory (all 9 pages of it!) in great detail for ODEs, so that when we get to PDEs, we will see where the ideas come from and we will be able to take some results on faith.
- We will also study the computation in great detail for ODEs, so that it will give us a firm foundation upon which to build the tools for PDEs.

Reference: Sections 2.1-2.4, 4.1, 5.1.

The problem and boundary conditions (p. 15)

Find the function $u(x)$ that satisfies

$$\mathcal{A}u = -(au')' + bu' + cu = f \text{ in } \Omega = (0,1)$$

$$u(0) = u_0, \;\; u(1) = u_1,$$

where the functions $a(x), b(x), c(x), f(x)$ and the numbers u_0 and u_1 are given.

Note: We have scaled the problem to the interval $x \in [0,1] \equiv \bar{\Omega}$ for convenience, without loss of generality.

Assumptions:

- The coefficients a, b, and c may depend on x.
- The coefficients a, b, and c are smooth functions; i.e., they have as many continuous derivatives as we need.
- $a(x) \geq a_0 > 0$ for $x \in \bar{\Omega}$. (Why?)
- $c(x) \geq 0$ for $x \in \bar{\Omega}$. (The reason is not as obvious.)

Motivation: These assumptions will lead us to methods that can be extended to elliptic PDEs. We will use different tools for hyperbolic and parabolic PDEs.

A motivating problem (Selvadurai, p. 236)

(See also Section 1.3, p. 7)

Here is an example of how ODE-BVPs arise in modeling physical problems.

- Suppose we have a piece of steel that is
  - homogeneous (of uniform content).
  - isotropic (with properties independent of direction of measurement).
- We know that steel conducts heat: it feels cold to the touch, because it conducts heat away from our finger.
- Fourier (1768-1830) derived a good model of this heat conduction, relating the amount of heat entering or escaping from a small piece of the metal to the rate at which the temperature T changes normal to the surface.

- To keep the model simple, we make two wild assumptions:
  - The piece of steel is infinite in y and z (or at least so large that it doesn't matter), but is bounded by $x = 0$ and $x = 1$,
  - and any external source of heat (which is energy) is applied at $(0, y, z)$ for all values of y and z, so the only direction left to study is x.

Let's see what happens.

According to Fourier's model, the amount of heat entering a volume V of steel is

$$\int_V (aT')' dV$$

where a is the constant of proportionality between temperature and heat. (This is known as the thermal conductivity of the steel.
Typical units: joules/(sec m K), where K is degrees in Kelvin.)

If there is a heat source f within that volume, then it generates an amount of heat equal to

$$\int_V f dV.$$

The heat contained in V is

$$\int_V \rho c \frac{\partial T}{\partial t} dV$$

where ρ and c are two constants depending on the material: ρ is the mass-density of the steel
(Typical units: kg/m^3)
and c is its specific heat
(Typical units: joules/(kg K).

To balance things out, we must have

$$\int_V \left((aT')' + f - \rho c \frac{\partial T}{\partial t} \right) dV = 0,$$

and taking limits over small volumes yields

$$(aT')' + f = \rho c \frac{\partial T}{\partial t}.$$

Finally, if we assume steady state, in which T is unchanging in time, we obtain the equation

$$(aT')' + f = 0,$$

and we can solve this for values of T in the interior of the steel once we know what is happening at the boundary.

With such physical problems in mind, we return to the study of theory of ODE-BVPs.

The Maximum Principle (p. 15)

Consider a special case of our problem

$$\mathcal{A}u = -(au')' + bu' + cu = f \text{ in } \Omega = (0, 1)$$

$$u(0) = u_0, \;\; u(1) = u_1,$$

by letting $a = 1$, $b = c = 0$:

$$-u'' = f \text{ in } \Omega = (0,1).$$

Now integrate:

$$-u'(y) + u'(0) = \int_0^y (-u'')ds = \int_0^y f(s)ds$$

so

$$\int_0^x -u'(y) + u'(0)dy = \int_0^x \int_0^y (-u'')dsdy = \int_0^x \int_0^y f(s)dsdy$$

and

$$-u(x) + u(0) + xu'(0) = \int_0^x \int_0^y f(s)dsdy$$

gives a formula for $u(x)$.

To find $u'(0)$, plug in $x = 1$:

$$-u_1 + u_0 + u'(0) = \int_0^1 \int_0^y f(s)dsdy$$

A further special case

$$u(x) - u(0) - u'(0)x = -\int_0^x \int_0^y f(s)dsdy$$

If $f(x) = 0$, then this formula says

$$u(x) = u(0) + u'(0)x,$$

and using the boundary conditions, we obtain

$$u'(0) = u_1 - u_0,$$

so

$$u(x) = u_0(1-x) + u_1 x.$$

Thus, the solution values lie between the numbers u_0 and u_1, so the max and the min of the solution occur at the boundary. This is called the maximum principle (minimum principle), and it is an important tool in developing bounds on the solution.

The Maximum Principle

$$\mathcal{A}u = -(au')' + bu' + cu = f \text{ in } \Omega = (0,1)$$

Theorem 2.1a (p. 16): Assume

- $u \in \mathcal{C}^2(\bar{\Omega})$;
- $\mathcal{A}u \leq 0$ in Ω.

Then

- If $c = 0$, then
$$\max_{x \in \bar{\Omega}} u(x) = \max(u_0, u_1).$$
- If $c(x) \geq 0$ for $x \in \Omega$, then
$$\max_{x \in \bar{\Omega}} u(x) \leq \max(u_0, u_1, 0).$$

Proof:

- Assume that $c = 0$ and $\mathcal{A}u<0$ in Ω. Suppose that u has a maximum at $\bar{x} \in \Omega$. Then (by rules we learned in calculus) $u'(\bar{x}) = 0$ and $u''(\bar{x}) \leq 0$, so
$$\begin{aligned} \mathcal{A}u(\bar{x}) &= -(au')'(\bar{x}) \\ &= -a'(\bar{x})u'(\bar{x}) - a(\bar{x})u''(\bar{x}) \\ &= 0 - a(\bar{x})u''(\bar{x}) \geq 0, \end{aligned}$$
a contradiction. So our result holds if $\mathcal{A}u<0$.

  Let's relax this to $\mathcal{A}u\leq 0$, and again assume that u has a maximum at $\bar{x} \in \Omega$. Let
$$\phi(x) = e^{\lambda x},$$
  Note that
$$\begin{aligned} \mathcal{A}\phi &= -(a\phi')' + b\phi' \\ &= -a'\lambda\phi - a\lambda^2\phi + b\lambda\phi \\ &= [-a\lambda^2 + \lambda(b - a')]\phi \end{aligned}$$
  Now choose λ so large that $\mathcal{A}\phi < 0$ on Ω.

  Suppose that u has a maximum at $\bar{x} \in \Omega$ that is strictly bigger than u_0 and u_1. Then, for ϵ sufficiently small, this is also true for $v = u + \epsilon\phi$, but $\mathcal{A}v < 0$ on $\bar{\Omega}$, and this contradicts what we just proved above. Therefore, our result holds when $\mathcal{A}u\leq 0$.

- Now we assume that $c \geq 0$ in Ω (instead of $c = 0$). If $u \leq 0$ in Ω, then our result holds. Otherwise, let

$$u(\bar{x}) = \max_{x \in \bar{\Omega}} u(x) > 0,$$

  with $\bar{x} \neq 0, 1$. Let the interval (α, β) containing $\bar{x}$ be the largest one for which u is positive. Then $\mathcal{A}u - cu \leq 0$ in this interval, too.

  Therefore, Part 1 of our theorem, applied to the operator $\mathcal{A}u - cu \leq 0$ on the interval (α, β) shows that $u(\bar{x}) = \max(u(\alpha), u(\beta))$, but that would mean that $u(\alpha)$ or $u(\beta)$ is positive, so the interval could not be the largest, a contradiction unless $u(\bar{x}) = \max(u(0), u(1))$, as desired. []

The Minimum Principle

$$\mathcal{A}u = -(au')' + bu' + cu = f \text{ in } \Omega = (0, 1)$$

Theorem 2.1b (p. 16): Assume

- $u \in \mathcal{C}^2(\bar{\Omega})$;
- $\mathcal{A}u \geq 0$ in Ω.

Then

- If $c = 0$, then

$$\min_{x \in \bar{\Omega}} u(x) = \min(u_0, u_1).$$

- If $c(x) \geq 0$ for $x \in \Omega$, then

$$\min_{x \in \bar{\Omega}} u(x) \geq \min(u_0, u_1, 0).$$

A stronger variant of the Maximum Principle

Corollary 2.1a: Assume

- $u \in \mathcal{C}^2(\bar{\Omega})$;
- $\mathcal{A}u \leq 0$ in Ω.

Then

- If $c = 0$ and

$$\max_{x \in \bar{\Omega}} u(x) = u(\bar{x})$$

  with $\bar{x} \in \Omega$, then u is constant in $\bar{\Omega}$.

- If $c(x) \geq 0$ for $x \in \Omega$, and

$$\max_{x \in \bar{\Omega}} u(x) = u(\bar{x}) \geq 0$$

with $\bar{x} \in \Omega$, then u is constant in $\bar{\Omega}$.

Proof: Omitted.

Uses of the Maximum Principle

- Bounding the solution in terms of the data.
- Proving uniqueness of solutions.
- Proving stability of solutions.
- Monotonicity properties.

Bounding the solution in terms of the data

Notation: The sup-norm (p. 231) is defined by

$$\|u\|_{\mathcal{C}} = \max_{x \in \bar{\Omega}} |u(x)|$$

Theorem 2.2 (p. 17): If $u \in \mathcal{C}^2$, then

$$\|u\|_{\mathcal{C}} \leq \max(|u_0|, |u_1|) + C\|\mathcal{A}u\|_{\mathcal{C}}$$

where the constant C depends on a, b, and c.

Note: People in this field have the rather sloppy habit of calling all constants C, even if there are two different constants in the same theorem. Your textbook follows this custom.

Proof: p. 17.

Usefulness: Even if $f(x)$ is not always ≥ 0 in Ω, we have an upper and lower bound on the solution.

Proving uniqueness

Corollary 2.2a: Our problem has a unique solution.

Proof: Suppose we have two solutions u and v, and let $w = u - v$. Then

$$\begin{aligned} \mathcal{A}w &= 0, \\ w(0) &= 0, \\ w(1) &= 0. \end{aligned}$$

Therefore, Theorem 2.2 tells us that $w(x) = 0$ for $x \in \Omega$, so $u = v$. []

Proving stability

Corollary 2.2b: Our problem is stable: small changes in the data make small changes in the solution.

Proof: Suppose that

$$\mathcal{A}u = f_1, \;\; u(0) = u_0, \;\; u(1) = u_1,$$

$$\mathcal{A}v = f_2, \;\; v(0) = v_0, \;\; v(1) = v_1.$$

Then, letting $w = u - v$, we see that

$$\begin{aligned} \mathcal{A}w &= f_1 - f_2, \\ w(0) &= u_0 - v_0, \\ w(1) &= u_1 - v_1, \end{aligned}$$

Now apply the stability estimate Theorem 2.2 to w:

$$\|w\|_{\mathcal{C}} \leq \max(|w_0|, |w_1|) + C\|\mathcal{A}w\|_{\mathcal{C}} = \max(|u_0 - v_0|, |u_1 - v_1|) + C\|f_1 - f_2\|_{\mathcal{C}},$$

and stability is established. []

Monotonicity

Corollary 2.2c: Suppose

$$\mathcal{A}u = f, \;\; u(0) = u_0, \;\; u(1) = u_1,$$

$$\mathcal{A}v = g, \;\; v(0) = v_0, \;\; v(1) = v_1.$$

If $f(x) \leq g(x)$ for all $x \in \Omega$, and if $u_0 \leq v_0$ and $u_1 \leq v_1$, then $u(x) \leq v(x)$ for all $x \in \Omega$.

Proof: Again let $w = u - v$ Then $\mathcal{A}w \leq 0$ in Ω, so the Maximum Principle says that $u(x) - v(x) = w(x) \leq \max(u_0 - v_0, u_1 - v_1, 0) \leq 0$ for $x \in \Omega$. []

The Green's function (p. 18)

$$\mathcal{A}u = -(au')' + bu' + cu = f \text{ in } \Omega = (0,1)$$

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

For convenience, again we work with a special case: $b = 0$. ($b \neq 0$ in Problem 2.5)

Our goals: To prove that a solution exists, and to express the solution in terms of the solution to two simpler problems:

Problem 1: $\mathcal{A}U_0 = 0$, $U_0(0) = 1$, $U_0(1) = 0$.
Problem 2: $\mathcal{A}U_1 = 0$, $U_1(0) = 0$, $U_1(1) = 1$.
(We take the existence of the solution to these two problems on faith, from theory developed in ODE courses.)

Note that the Minimum Principle implies that $U_0, U_1 \geq 0$ on Ω.

Now define

$$K(x) = aU_0U_1' - aU_0'U_1.$$

Then

$$\begin{aligned} K'(x) &= U_0(aU_1')' + U_0'aU_1' - (aU_0')'U_1 - aU_0'U_1' \\ &= U_0cU_1 - cU_0U_1 \\ &= 0. \end{aligned}$$

Therefore, K is constant, and our data at $x = 0$ gives

$$K(0) = a(0)U_1'(0) = K \geq 0.$$

But $K > 0$ since, if not, $U_1(0) = U_1'(0)$ and U_1 would be identically zero.

Now define

$$u(x) = \int_0^1 G(x,y)f(y)dy$$

where the Green's function is defined by

$$G(x,y) = \begin{cases} \frac{1}{\kappa}U_0(x)U_1(y) & \text{for } 0 \leq y \leq x \leq 1, \\ \frac{1}{\kappa}U_1(x)U_0(y) & \text{for } 0 \leq x \leq y \leq 1, \end{cases}$$

and $\kappa = a(x)(U_0(x)U_1'(x) - U_0'(x)U_1(x))$ =constant> 0.

We now verify that u solves our problem.

First notice that $u(0) = 0$ and $u(1) = 0$, so the boundary conditions hold.

We now verify that u solves $\mathcal{A}u = f$.

Next notice that for $0 < x < 1$,

$$u(x) = \int_0^x G(x,y)f(y)dy + \int_x^1 G(x,y)f(y)dy$$

and a formula from calculus tells us that if

$$z(x) = \int_0^x F(y)dy$$

then $z'(x) = F(x)$.

Unquiz 1: Use these facts to verify that $\mathcal{A}u(x) = f(x)$ for $x \in \Omega$.

We have proved the following theorem:

Theorem 2.3 (Green's Function Theorem) The solution to the problem $\mathcal{A}u(x) = f(x)$ for $x \in (0,1)$, $u(0) = 0$, $u(1) = 0$ is

$$u(x) = \int_0^1 G(x,y) f(y) dy \,.$$

The variational formulation (p. 20)

A powerful tool for solving our ODE-BVP is the observation that the solution solves a problem called the variational formulation.

A digression: Spaces, Spaces, Spaces

Notation to learn:

- The derivative operator $D^\alpha v$ (p. 5),
- The trace operator γv (p. 235),

and the definition of three spaces of functions:

p. 231: $C^k(\Omega)$ = the set of functions with k continuous derivatives on Ω,

$$\begin{aligned} p.233: \quad L_2(\Omega) = &\quad \{v : \|v\|_{L_2} \equiv \left(\int_\Omega |v(x)|^2 dx\right)^{1/2} < \infty\} \\ p.234: \quad H^k(\Omega) = &\quad \{v \in L_2(\Omega) : D^\alpha v \in L_2(\Omega) \text{ if } |\alpha| \le k\} \\ p.238: \quad H_0^1(\Omega) = &\quad \{v \in H^1(\Omega) : \gamma v = 0\} \end{aligned}$$

The spaces H^k are called the Sobolev spaces.

Also, recall from calculus the formula for integration by parts:

$$\int_0^1 uv' dx = uv|_0^1 - \int_0^1 vu' dx.$$

A weak formulation of the ODE-BVP

$$\mathcal{A}u = -(au')' + bu' + cu = f \text{ in } \Omega = (0,1)$$

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

A change in assumptions:

- a, b, c are smooth functions,
- $a(x) \geq a_0 > 0 \ x \in \Omega$,
- $c(x) - b'(x)/2 \geq 0$ for $x \in \Omega$.

Now choose an arbitrary function $\phi \in H_0^1$, and notice that

$$\int_0^1 (-(au')' + bu' + cu)\phi dx = \int_0^1 f\phi dx.$$

Now use integration by parts on the first term:

$$\int_0^1 (au')\phi' + bu'\phi + cu\phi dx = \int_0^1 f\phi dx.$$

Notation:

$$\begin{aligned} a(v,w) &= \int_0^1 (av'w' + bv'w + cvw)dx, \\ (f,w) &= \int_0^1 fw dx \end{aligned}$$

(a is a bilinear form)

So we have shown that if u solves our ODE-BVP, then u satisfies the weak or variational form of the problem: for all $\phi \in H_0^1$,

$$a(u,\phi) = (f,\phi).$$

The converse is not quite true; we say that u is a weak solution of our problem if $u \in H_0^1$ satisfies the variational form of the problem, but it must be in C^2 to solve the strong (original) form of the problem.

In weakness there is strength

The weak formulation has two important uses:

- It provides a set of numerical methods, called Galerkin methods. These come from enforcing $a(u,\phi) = (f,\phi)$ over a subspace of H_0^1. We'll follow up on this when we discuss finite element methods.
- It provides an alternative existence proof for the solution.

More notation: Norms associated with our spaces

The L_2 norm:

$$p.6 : \|v\| = \|v\|_{L_2} = \left(\int_\Omega v^2(x)dx\right)^{1/2}$$

A seminorm:

$$p.7 : |v|_k = \left(\sum_{|\alpha|=k} \|D^\alpha v\|^2 \right)^{1/2}$$

The Sobolev norms:

$$p.7 : \|v\|_k = \left(\sum_{|\alpha|\leq k} \|D^\alpha v\|^2 \right)^{1/2}$$

And one inequality: the Cauchy-Schwarz inequality (p. 226): for all w, v in an inner product space (including Sobolev spaces),

$$|(w,v)| \leq \|w\| \|v\|$$

Bounds leading to an existence proof

$$\begin{aligned} |v(x)|^2 &= \left| \int_0^x v'(y)dy \right|^2 \\ &\leq \int_0^x 1^2 dy \int_0^x (v')^2 dy \\ &\leq x \int_0^1 (v')^2 dy \\ &\leq \|v'\|^2. \end{aligned}$$

so

$$\|v\| \leq \|v'\|.$$

Therefore, for all $v \in H_0^1$,

$$(*) \;\; \|v\|_1 = (\|v\|^2 + \|v'\|^2)^{1/2} \leq \sqrt{2}\|v'\|.$$

Properties of the bilinear form $a(u,v)$

Let $v \in H_0^1$ be arbitrary.

Integration by parts, with 'u' $= b$ and 'v' $= v^2/2$:

$$\int_0^1 bv'v dx = \frac{1}{2}bv^2|_0^1 - \int_0^1 \frac{1}{2}b'v^2 dx$$

so

$$\begin{aligned} \int_0^1 bv'v + cv^2 dx &= \frac{1}{2}bv^2|_0^1 + \int_0^1 cv^2 - \frac{1}{2}b'v^2 dx \\ &\geq 0 \end{aligned}$$

since we assumed above just what was needed here: $c(x) - b'(x)/2 \geq 0$.

Combining this with $(*)$, we see that

$$a(v,v) \geq \min_{\bar{\Omega}} a(x) \|v'\|^2 \geq \alpha \|v\|_1^2$$

where $\alpha = a_0/2 > 0$. This property is called coercivity of the bilinear form.

The bilinear form is also bounded:

$$\begin{aligned} |a(v,w)| &= |\int_0^1 (av'w' + bv'w + cvw)dx| \\ &\leq C \int_0^1 |v'w'| + |v'w| + |vw| dx \\ &\leq C\|v\|_1 \|w\|_1 \end{aligned}$$

for all $v, w \in H_0^1$.

Finally, the solution to the weak problem can be bounded in terms of the data:

$$\alpha \|u\|_1^2 \leq a(u,u) = (f,u) \leq \|f\| \|u\| \leq \|f\| \|u\|_1$$

so

$$\|u\|_1 \leq C\|f\|$$

where $C = 1/\alpha = 2/a_0$.

Uniqueness proof

Theorem 2.4 (p. 22): Under our assumptions $a(x) \geq a_0 > 0$ and $c(x) - b'(x)/2 \geq 0$ for $x \in \Omega$, if $f \in L_2$, then there exists a unique solution of $a(u,v) = (f,v)$ for all $v \in H_0^1$, with $\|u\|_1 \leq C\|f\|$.

Proof: Our tool is the Lax-Milgram Lemma (p. 230), which says that the solution exists and is unique if the bilinear form is bounded and coercive and if $L(v) = (f,v)$ is bounded.

We have already verified that $a(u,v)$ is bounded and coercive, so let's check L:

$$|L(v)| = |(f,v)| \leq \|f\| \|v\| \leq \|f\| \|v\|_1$$

for all $v \in H_0^1$, so the result follows. []

Another important tool: minimization of energy

If $b = 0$, then $a(u,v) = a(v,u)$, so a is both symmetric and positive definite. In this case, we can find the solution by minimizing

$$F(u) \equiv \frac{1}{2} a(u,u) - (f,u)$$

for $u \in H_0^1$.

This principle, Dirichlet's principle, is an important computational tool.

Physical interpretation: Suppose we are modeling an elastic string attached at its two endpoints. Then

- $F(u)$ is the potential energy of the string, where u is the deflection.
- $a(u, u)$ is the internal elastic energy.
- (f, u) is the load potential
- In physics, this is sometimes called the principle of minimizing potential energy or minimizing virtual work.

From weak to strong

Under our assumptions, a solution to the weak problem is actually a solution to the strong problem when a is smooth and $f \in L_2$.

Regularity of the solution

Theorem 2.6 (p.23) Assume

- a smooth,
- $f \in L_2$.

Then

$$\|u\|_2 \leq C\|f\|.$$

This is a regularity result; it shows that u, u', and u'' can be bounded in terms of the data f, a rather remarkable fact.